

Validation documentation  
*TCM - Granulated herbal extracts (PhytoComm)*

HiperScan GmbH

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## Contents

|                                                 |           |
|-------------------------------------------------|-----------|
| <b>Introduction</b>                             | <b>9</b>  |
| Context of this document                        | 9         |
| Validity scope of this document                 | 10        |
| Validation concept                              | 10        |
| Model creation procedure and validation runs    | 11        |
| Particularities of individual substance classes | 13        |
| Significance of testing with <i>Apo-Ident</i>   | 14        |
| Conclusion                                      | 15        |
| <b>Explanation of terminology</b>               | <b>16</b> |
| <b>Summary</b>                                  | <b>21</b> |
| Validation samples                              | 21        |
| Validation results                              | 21        |
| <b>Validation reports</b>                       | <b>23</b> |
| Ai Ye                                           | 23        |
| Ba Ji Tian                                      | 27        |
| Bai Guo                                         | 31        |
| Bai He                                          | 35        |
| Bai Hua She She Cao                             | 39        |
| Bai Jiang Cao                                   | 43        |
| Bai Mao Gen                                     | 47        |
| Bai Qian                                        | 51        |
| Bai Shao Yao                                    | 55        |
| Bai Tou Weng                                    | 59        |
| Bai Xian Pi                                     | 63        |
| Bai Zhi                                         | 67        |
| Bai Zhu                                         | 71        |
| Bai Zi Ren                                      | 75        |
| Ban Lan Gen                                     | 79        |
| Ban Xia (Jiang)                                 | 83        |
| Ban Zhi Lian                                    | 87        |
| Bo He                                           | 91        |
| Bu Gu Zhi                                       | 95        |
| Cang Er Zi                                      | 99        |
| Cang Zhu                                        | 103       |
| Ce Bai Ye                                       | 107       |
| Chai Hu                                         | 111       |
| Chan Tui                                        | 115       |
| Che Qian Zi                                     | 119       |
| Chen Pi                                         | 123       |
| Chi Shao (Yao)                                  | 127       |
| Chuan Lian Zi                                   | 131       |
| Chuan Mu Tong                                   | 135       |
| Chuan Niu Xi                                    | 139       |
| Chuan Xin Lian                                  | 143       |
| Chuan Xiong                                     | 147       |
| Chuang Mu Xiang                                 | 151       |
| Ci Wu Jia                                       | 155       |
| Cong Bai                                        | 159       |
| Da Qing Ye                                      | 163       |
| Da Zao                                          | 167       |
| Dan Dou Chi                                     | 171       |
| Dan Shen                                        | 175       |
| Dang Gui                                        | 179       |

|                 |     |
|-----------------|-----|
| Dang Gui Wei    | 183 |
| Dang Shen       | 187 |
| Di Fu Zi        | 191 |
| Di Gu Pi        | 195 |
| Di Long         | 199 |
| Dong Gua Zi     | 203 |
| Du Huo          | 207 |
| Du Zhong        | 211 |
| E Zhu           | 215 |
| Fang Feng       | 219 |
| Fo Shou         | 223 |
| Fu Ling         | 227 |
| Fu Pen Zi       | 231 |
| Fu Shen         | 235 |
| Fu Xiao Mai     | 239 |
| Fu Zi           | 243 |
| Gan Cao         | 247 |
| Gan Jiang       | 251 |
| Ge Gen          | 255 |
| Gou Qi Zi       | 259 |
| Gou Teng        | 263 |
| Gu Sui Bu       | 267 |
| Gua Lou         | 271 |
| Gua Lou Ren     | 275 |
| Guang Huo Xiang | 279 |
| Gui Ban Jiao    | 283 |
| Gui Zhi         | 287 |
| He Huan Pi      | 291 |
| He Shou Wu      | 295 |
| He Ye           | 299 |
| Hei Zhi Ma      | 303 |
| Hong Hua        | 307 |
| Hong Jing Tian  | 311 |
| Hou Po          | 315 |
| Huai Hua        | 319 |
| Huang Bo        | 323 |
| Huang Jing      | 327 |
| Huang Lian      | 331 |
| Huang Qi        | 335 |
| Huang Qin       | 339 |
| Huo Ma Ren      | 343 |
| Ji Li           | 347 |
| Ji Nei Jin      | 351 |
| Ji Xue Teng     | 355 |
| Jiang Huang     | 359 |
| Jiao Gu Lan     | 363 |
| Jie Geng        | 367 |
| Jin Qian Cao    | 371 |
| Jin Yin Hua     | 375 |
| Jing Jie        | 379 |
| Ju Hua          | 383 |
| Jue Ming Zi     | 387 |
| Ku Shen         | 391 |
| Kuan Dong Hua   | 395 |
| Lai Fu Zi       | 399 |
| Lian Qiao       | 403 |
| Lian Zi         | 407 |

|                |     |
|----------------|-----|
| Ling Zhi       | 411 |
| Long Dan (Cao) | 415 |
| Long Yan Rou   | 419 |
| Lu Gen         | 423 |
| Lu Jiao Shuang | 427 |
| Lu Lu Tong     | 431 |
| Ma Bian Cao    | 435 |
| Ma Huang       | 439 |
| Ma Huang Gen   | 443 |
| Mai Men Dong   | 447 |
| Mai Ya         | 451 |
| Man Jing Zi    | 455 |
| Mi Huan Jun    | 459 |
| Mo Yao         | 463 |
| Mu Dan Pi      | 467 |
| Mu Gua         | 471 |
| Mu Zei         | 475 |
| Niu Bang Zi    | 479 |
| Nü Zhen Zi     | 483 |
| Pi Pa Ye       | 487 |
| Pu Gong Ying   | 491 |
| Pu Huang       | 495 |
| Qian Hu        | 499 |
| Qiang Huo      | 503 |
| Qin Jiao       | 507 |
| Qing Pi        | 511 |
| Ren Shen       | 515 |
| Rou Cong Rong  | 519 |
| Ru Xiang       | 523 |
| San Leng       | 527 |
| San Qi         | 531 |
| Sang Bai Pi    | 535 |
| Sang Ji Shend  | 539 |
| Sang Shen      | 543 |
| Sang Ye        | 547 |
| Sang Zhi       | 551 |
| Sha Ren        | 555 |
| Sha Shen (Bei) | 559 |
| Shan Yao       | 563 |
| Shan Yu Rou    | 567 |
| Shan Zha       | 571 |
| She Gan        | 575 |
| Shen Qu        | 579 |
| Sheng Jiang    | 583 |
| Sheng Ma       | 587 |
| Shi Gao        | 591 |
| Shi Jun Zi     | 595 |
| Shi Wei        | 599 |
| Shu Di (Huang) | 603 |
| Suan Zao Ren   | 607 |
| Suo Yang       | 611 |
| Tai Zi Shen    | 615 |
| Tao Ren        | 619 |
| Tian Hua Fen   | 623 |
| Tian Men Dong  | 627 |
| Tian Nan Xing  | 631 |
| Ting Li Zi     | 635 |

|                                                                      |            |
|----------------------------------------------------------------------|------------|
| Tu Fu Ling                                                           | 639        |
| Tu Si Zi                                                             | 643        |
| Wang Bu Liu Xing                                                     | 647        |
| Wei Ling Xian                                                        | 651        |
| Wu Jia Pi                                                            | 655        |
| Wu Mei                                                               | 659        |
| Wu Wei Zi                                                            | 663        |
| Wu Yao                                                               | 667        |
| Wu Zhu Yu                                                            | 671        |
| Xi Xian Cao                                                          | 675        |
| Xi Yang Shen                                                         | 679        |
| Xia Ku Cao                                                           | 683        |
| Xian Mao                                                             | 687        |
| Xiang Fu                                                             | 691        |
| Xiao Hui Xiang                                                       | 695        |
| Xie Bai                                                              | 699        |
| Xin Yi                                                               | 703        |
| Xu Duan                                                              | 707        |
| Xuan Fu Hua                                                          | 711        |
| Xuan Shen                                                            | 715        |
| Yan Hu Suo                                                           | 719        |
| Ye Jiao Teng                                                         | 723        |
| Yi Mu Cao                                                            | 727        |
| Yi Yi Ren                                                            | 731        |
| Yi Zhi Ren                                                           | 735        |
| Yin Chen Hao                                                         | 739        |
| Yin Yang Huo                                                         | 743        |
| Yu Jin                                                               | 747        |
| Yu Xing Cao                                                          | 751        |
| Yu Zhu                                                               | 755        |
| Yuan Zhi                                                             | 759        |
| Ze Lan                                                               | 763        |
| Ze Xie                                                               | 767        |
| Zhe Bei Mu                                                           | 771        |
| Zhi Gan Cao                                                          | 775        |
| Zhi Ke                                                               | 779        |
| Zhi Mu                                                               | 783        |
| Zhi Shi                                                              | 787        |
| Zhi Zi                                                               | 791        |
| Zhu Ling                                                             | 795        |
| Zhu Ru                                                               | 799        |
| Zi Hua Di Ding                                                       | 803        |
| Zi Su Ye                                                             | 807        |
| Zi Su Zi                                                             | 811        |
| Zi Wan                                                               | 815        |
| (Bai) Dou Kou                                                        | 819        |
| (Huai) Niu Xi                                                        | 823        |
| (Ku) Xing Ren                                                        | 827        |
| (Sheng) Di Huang                                                     | 831        |
| (Shi) Chang Pu                                                       | 835        |
| <b>Appendix</b>                                                      | <b>839</b> |
| Additional calibration samples ( <i>Type A</i> )                     | 839        |
| Additional validation samples ( <i>Type B</i> )                      | 841        |
| Additional validation samples ( <i>Type C</i> )                      | 843        |
| Requirements of validation                                           | 847        |
| Conformity of <i>Apo-Ident</i> with the <i>European pharmacopeia</i> | 848        |

|                            |     |
|----------------------------|-----|
| <a href="#">References</a> | 849 |
| <a href="#">Index</a>      | 851 |





## 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.

## Validity scope of this document

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 database is exclusively established from spectra which have been recorded by *HiperScan GmbH* for traceable samples in pharmaceutical quality.
  - The samples are procured via typical pharmacy sources (*DAC III.2.: Bezugsquellennachweis für Rezepturbestandteile [reference source for prescription components]* [7]).
  - A valid manufacturer's certificate exists (content, purity and identity of the batch).
  - The identity was confirmed by a certified test laboratory or *HiperScan GmbH*.
- Each version of the reference database (every update) is validated in-full.
  - In three separately evaluated validation runs, calibration spectra, spectra from independent samples and spectra from independent field samples (described further below as *Type A*, *B* or *C*) are presented to the *IdentModule* for evaluation.
  - Here, no single *false positive* result may arise.
  - Here, the various substance classes are also tested for reciprocal rejection, where this is objectively justified (see *Summary section*).
- For each individual substance, the unambiguous identifiability with *Apo-Ident* and the demarkation against all other database substances is proven.

## Validation concept

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

1. Collection of spectra for the *calibration sample*. The results (identities) of the calibration sample must be known. The calibration samples must be representative for the samples which are to be evaluated later. Therefore, they must take the various possible (physical) compositions into account. (Therefore, sourcing calibration samples for NIR from the specialist trade is superior to the use of CRS reference substances.)

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

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

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

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

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

## Model creation procedure and validation runs

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

### 1. Collecting the reference spectra (calibration sample)

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

as the *Mahalanobis distance* to the next non-identical substance. Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

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

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

## 2. Generating the chemometric models (calibration)

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

## 3. Set of validation spectra (validation samples)

The following is provided for validation:

- a) *Type A*: The reference spectra = calibration spectra from which the database was established. These also include spectra from substances which the *chemometric model* should not identify, but were also recorded during generation in order to increase selectivity. (As a result, the model "learns" to differentiate from other substances which are actually unknown to it.)
- b) *Type B*: Spectra from independent samples not included in the generation of the respective model received but were measured by *HiperScan GmbH*. These also include reference spectra from other substance classes and spectra which are not declared as reference spectra.
- c) *Type C*: Spectra from independent field samples. These measurements were recorded under normal everyday conditions by pharmacy staff. The spectra belong both to substances of the substance class to be examined and to substances from different classes.

All manufacturers' batches from which spectra flow into the validation are listed by substance in this document: for substances included in the substance class *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 spectrum error can be proven. Here, the spectra are not deleted, but instead placed on a *blacklist* incorporating the reason, date and initials in the commentary.

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

#### 4. Validation runs and approval

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

#### Particularities of individual substance classes

Basically, *HiperScan GmbH* procures and tests the manufacturer's certificate for the batch, commissions external testing of the identity of the sample or carries it out independently and stores the certificates. As described, this process is established for the Pharmacopoeia substances, that is to say for substance classes *APIs & excipients, solid*, *APIs & excipients, liquid/semi-solid (with analysis certificate)*, *Narcotic substances, liquid/semi-solid* and *Drugs*. Therefore, *HiperScan GmbH* is able to furnish proof of the identity of the reference samples. In case of manufacturer-specific substance classes and others, individual steps are organised differently in-part:

The substance class **APIs & excipients, liquid/semi-solid (other)** (often described as cosmetics) incorporates substances for which no specification of the requirements of the pharmaceutical quality is determined, neither in a Pharmacopoeia monograph, a DAC/NRF monograph nor via a manufacturer's specification. Consequently, neither the identity nor contents can be tested independently. No certificates whatsoever exist for the reference samples. So here, merely the matching of the sample with former samples of this product is established and confusion with the other substances is ruled-out. (If the manufacturer of such a substance prepares a specification, determines testing methods and provides manufacturer's certificates in accordance with *ApBetRO* [Pharmacies Rules and Regulations] §§ 6, 11, *HiperScan GmbH* can assign the substance to the substance class *APIs & excipients, liquid/semi-solid (with analysis certificate)* again in the future).

Substance class **HCK – nutritional supplements (Hepart)** contains the HCK micro-nutrients from the Swiss company *Hepart AG*. *HiperScan GmbH* receives the reference samples directly from the manufacturer. For each reference sample, *HiperScan GmbH* also receives manufacturer's certificates and keeps these. New checking of the identity of the reference sample is not carried out by *HiperScan GmbH*. The identity of the reference samples is therefore documented by *Hepart AG*. The spectra of all batches provided by *Hepart AG* are recorded by *HiperScan GmbH* and entered in the database.

Also, the substance classes with **TCM – Granulated herbal extracts** are separated supplier-specifically. The granulates from the suppliers *HerbaSinica*, *PhytoComm* and *China-Medica* are hardly comparable with each other due to their spectra, because extracts of respectively different drug batches with different carrier materials are granulated. The spectra for all batches from these suppliers are recorded by *HiperScan GmbH* and entered in the respective database. The suppliers organise the respective tests themselves and keep the test certificates. The process implemented with *HerbaSinica* is a particularity: The reference samples are sent to a test laboratory which determines the identity of the sample and sends the container to *HiperScan GmbH* if the result is positive.

A new evaluation option was created for the class *TCM – Granulated herbal extracts (PhytoComm)* with the update 2016-01. As the risks are considerably fewer than those from chemical agents, the



pharmacist can specify a reasonable criterion for the *specificity* in accordance with internal risk estimation. The database for this is created without taking safety distances into account and no criterion is determined in advance for the *specificity*. Instead, the *specificity* for testing the identity with this concrete substance is calculated in the validation for each substance and provided with the measurement result. The pharmacist then judges himself whether this safety is reasonable with regard to the risk of the substance.

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

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

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

## Significance of testing with *Apo-Ident*

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

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

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

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

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

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

## Conclusion

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

## Explanation of terminology

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

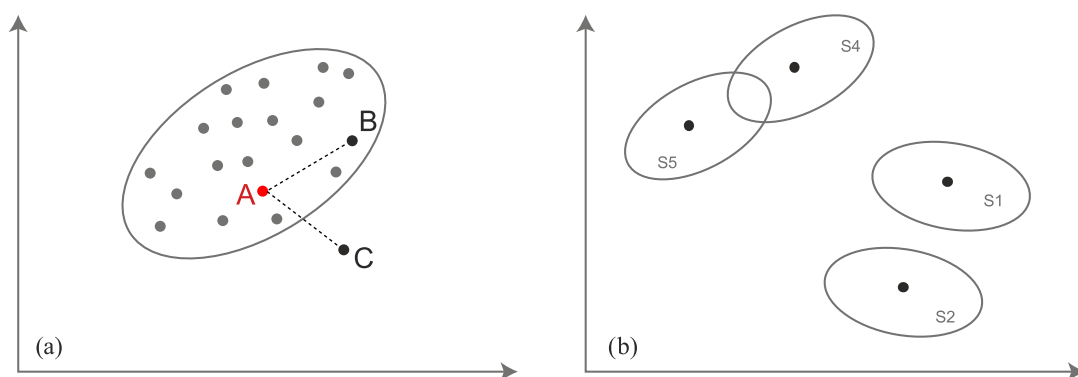


**Figure 1:** (a) The *Mahalanobis distance* from *A* to *B* is less than from *A* to *C*. However, the Euclidean distances are identical. (b) The *Mahalanobis distance* between the two measurement series *S4* and *S5* is smaller than between *S1* and *S2*. However, the Euclidean distances are identical.

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

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

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

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

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

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

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

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



## Summary

A total of 37 600 spectra from 1178 different batches for a total of 270 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) | 204        | 329     | 21 566  |

From category *A* a total of 21 566 spectra from 329 batches for a total of 204 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) | 206        | 331     | 14 053  |

From category *B* a total of 14 053 spectra from 331 batches for a total of 206 substances were taken into account for validation.

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

| Substance class                              | Substances | Batches | Spectra |
|----------------------------------------------|------------|---------|---------|
| TCM - Granulated herbal extracts (PhytoComm) | 268        | 965     | 1981    |

From category *C* a total of 1981 spectra from 965 batches for a total of 268 substances were taken into account for validation.

## Validation results

The validation runs checked whether the substances/substance groups in the substance class *TCM - Granulated herbal extracts (PhytoComm)* can be distinguished from other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, the matching of all relevant spectra of various substances with the substances/substance groups in the substance class *TCM - Granulated herbal extracts (PhytoComm)* was checked and the correctness of the results was evaluated. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|        | False positive | True positive | False negative | True negative |
|--------|----------------|---------------|----------------|---------------|
| Type A | 25             | 21 541        | 25             | 4 377 873     |
| Type B | 87             | 13 745        | 92             | 2 852 888     |
| Type C | 700            | 436           | 1294           | 401 694       |

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

|        | Specificity                 | Recognition rate            |
|--------|-----------------------------|-----------------------------|
| Type A | 99.999 31 % (> 99.999 22 %) | 99.859 68 % (> 99.840 29 %) |
| Type B | 99.997 24 % (> 99.997 07 %) | 99.406 84 % (> 99.371 84 %) |
| Type C | 99.834 12 % (> 99.832 75 %) | 22.115 03 % (> 21.851 81 %) |

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

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

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ai Ye**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60407-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Ai Ye; Artemisiae argyi folium

### Special notes

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

*no information*

### Applicable documents

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

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

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

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

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Ai Ye*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Ai Ye     | G033H0613621 | 62017 <sup>†</sup> | 20      |
| PhytoComm | Ai Ye     | G033H0613621 | 62018 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Ai Ye*.

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

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



- 1976 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 4              | 0             | 5              | 1972          |

The substance/substance group *Ai 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.8094 % (> 99.5304 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 62017     | 62017               | 0.00                         | 14.24                           |
| 62018     | 62018               | 0.00                         | 14.40                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ba Ji Tian**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60138-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

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

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

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Ba Ji Tian | G165H0445621 | 61937 <sup>†</sup> | 20      |
| PhytoComm | Ba Ji Tian | G165H0445621 | 61938 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Ba Ji Tian*.

| Supplier  | Substance  | Batch        | Spectra |
|-----------|------------|--------------|---------|
| phytoComm | Ba Ji Tian | G165H0445021 | 2       |
| PhytoComm | Ba Ji Tian | G165H0445021 | 2       |
| PhytoComm | Ba Ji Tian | G165H0445222 | 1       |
| PhytoComm | Ba Ji Tian | H0445921     | 1       |

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

- 1975 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 4              | 0             | 6              | 1971          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.8430 % (> 99.5639 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61937     | 61937               | 0.00                         | 6.23                            |
| 61938     | 61938               | 0.00                         | 6.41                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bai Guo**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60455-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Bai Guo; Ginkgonis bilobae semen

### Special notes

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

*no information*

### Applicable documents

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

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Guo*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Bai Guo   | G114H0509521 | 61685     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

**Type A** All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Bai Guo*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Bai Guo   | G114H0509521 | 61685 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Bai Guo*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Bai Guo   | G114H0509521 | 1       |
| phytocomm | Bai Guo   | G114H0509022 | 1       |
| Phytocomm | Bai Guo   | G114H0509321 | 2       |
| Caelo     | Bai Guo   | g114h0509022 | 1       |

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



- 1976 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Bai Guo* can be 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 Guo* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 1             | 4              | 1976          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4420 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61685     | 61685               | 0.00                         | 7.59                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bai He**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60093-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G139H0607421 | 61355     | 40      | from supplier |
| PhytoComm | Bai He    | G139H0607421 | 61691     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Bai He    | G139H0607421 | 61355 <sup>†</sup> | 20      |
| PhytoComm | Bai He    | G139H0607421 | 61691 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 8 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Bai He*.

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

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Bai He    | G139H0607321 | 1       |
| phytoComm | Bai He    | H0607021     | 1       |
| PhytoComm | Bai He    | H0607021     | 2       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 79            | 1              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 5              | 3             | 5              | 1968          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 98.7500 % (> 95.0000 %)  |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.7441 % (> 99.4648 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61355     | 61355               | 0.00                         | 9.05                            |
| 61691     | 61691               | 0.00                         | 9.35                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bai Hua She She Cao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60039-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 ... | G173H1153421 | 61089     | 40      | from supplier |
| PhytoComm | Bai Hua She She ... | G173H1153421 | 61629     | 40      | from supplier |
| PhytoComm | Bai Hua She She ... | G173H1153421 | 61689     | 40      | from supplier |
| PhytoComm | Bai Hua She She ... | G173H1153522 | 61967     | 40      | from supplier |
| PhytoComm | Bai Hua She She ... | G173H1153522 | 61968     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Bai Hua She She Cao*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 139 spectra of 5 reference samples from the substance/substance group *Bai Hua She She Cao*.

| Supplier  | Substance           | Batch        | Sample ID          | Spectra |
|-----------|---------------------|--------------|--------------------|---------|
| PhytoComm | Bai Hua She She Cao | G173H1153421 | 61089 <sup>†</sup> | 19      |
| PhytoComm | Bai Hua She She Cao | G173H1153421 | 61338              | 60      |
| PhytoComm | Bai Hua She She Cao | G173H1153421 | 61689 <sup>†</sup> | 20      |
| PhytoComm | Bai Hua She She Cao | G173H1153522 | 61967 <sup>†</sup> | 20      |
| PhytoComm | Bai Hua She She Cao | G173H1153522 | 61968 <sup>†</sup> | 20      |

- 13 914 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

<sup>†</sup>These spectra were recorded from 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 Hua She She Cao | G173H1153421 | 3       |
| Phytocomm | Bai Hua She She Cao | G173H1153222 | 3       |
| PhytoComm | Bai Hua She She Cao | G173H1153222 | 1       |
| PhytoComm | Bai Hua She She Cao | H1153923     | 2       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 200           | 0              | 21 366        |
| <b>Type B</b> | 0              | 139           | 0              | 13 914        |
| <b>Type C</b> | 9              | 3             | 6              | 1963          |

The substance/substance group *Bai Hua She She 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.6835 %) |
| <b>Type C</b> | 99.2620 % (> 98.9827 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61089     | 61089               | 0.00                         | 15.11                           |
| 61629     | 61629               | 0.00                         | 14.80                           |
| 61689     | 61689               | 0.00                         | 16.04                           |
| 61967     | 61967               | 0.00                         | 21.88                           |
| 61968     | 61968               | 0.00                         | 22.32                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bai Jiang Cao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50319-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Bai Jiang Cao; Patriniae herba

### Special notes

When selecting the *Bai Jiang 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Jiang Cao*:

| Supplier  | Substance     | Batch        | Sample ID | Spectra | Certificate   |
|-----------|---------------|--------------|-----------|---------|---------------|
| PhytoComm | Bai Jiang Cao | G181H1180522 | 61783     | 40      | from supplier |
| PhytoComm | Bai Jiang Cao | G181H1180522 | 61825     | 40      | from supplier |

## Validation samples

A total of 37 600 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 Jiang Cao*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance     | Batch        | Sample ID          | Spectra |
|-----------|---------------|--------------|--------------------|---------|
| PhytoComm | Bai Jiang Cao | G181H1180522 | 61783 <sup>†</sup> | 20      |
| PhytoComm | Bai Jiang Cao | G181H1180522 | 61825 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Bai Jiang Cao*.

| Supplier  | Substance     | Batch          | Spectra |
|-----------|---------------|----------------|---------|
| PhytoComm | Bai Jiang Cao | (G181)H1180022 | 1       |
| PhytoComm | Bai Jiang Cao | G181H1180422   | 1       |
| PhytoComm | Bai Jiang Cao | G181H1180022   | 1       |
| PhytoComm | Bai Jiang Cao | G181H1180321   | 1       |

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

- 1977 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Bai Jiang 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 Jiang 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 4              | 1977          |

The substance/substance group *Bai Jiang 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4424 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61783     | 61783               | 0.00                         | 9.82                            |
| 61825     | 61825               | 0.00                         | 8.98                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bai Mao Gen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60654-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G125H0512521 | 61748     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

## Type A All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Bai Mao Gen*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 20 spectra of 1 reference samples from the substance/substance group *Bai Mao Gen*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Bai Mao Gen | G125H0512521 | 61748 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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       |

- 1979 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the

<sup>†</sup>These spectra were recorded from 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 2              | 1979          |

The substance/substance group *Bai Mao 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4445 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61748     | 61748               | 0.00                         | 7.12                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bai Qian**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60327-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Bai Qian; Cynanchi stauntonii rhizoma et radix

### Special notes

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

*no information*

### Applicable documents

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

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Qian*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Bai Qian  | G087HS068NW1 | 61719     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

## Type A All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Bai Qian*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Bai Qian  | G087HS068NW1 | 61719 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Bai Qian*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| phytoComm | Bai Qian  | BP010536     | 1       |
| PhytoComm | Bai Qian  | G087H0505922 | 2       |
| PhytoComm | Bai Qian  | G087H0505922 | 1       |

- 1977 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

<sup>†</sup>These spectra were recorded from 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 Qian* can be 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 Qian* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 37            | 3              | 21 526        |
| <b>Type B</b> | 4              | 20            | 0              | 14 029        |
| <b>Type C</b> | 4              | 0             | 4              | 1973          |

The substance/substance group *Bai Qian* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 92.5000 % (> 85.0000 %)  |
| <b>Type B</b> | 99.9889 % (> 99.9546 %)  | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.8516 % (> 99.5728 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61719     | 61719               | 0.00                         | 3.13                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bai Shao Yao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60007-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G179H0502422 | 61626     | 40      | from supplier |
| PhytoComm | Bai Shao Yao | G179H0502521 | 61652     | 40      | from supplier |
| PhytoComm | Bai Shao Yao | G179H0502522 | 61796     | 40      | from supplier |
| PhytoComm | Bai Shao Yao | G179H0502522 | 61813     | 40      | from supplier |
| PhytoComm | Bai Shao Yao | G179H0502621 | 61955     | 40      | from supplier |
| PhytoComm | Bai Shao Yao | G179H0502621 | 61956     | 40      | from supplier |

## Validation samples

A total of 37 600 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 Shao Yao*. These samples are listed above in the [calibration samples](#) section.
- 21 326 spectra from a total of 325 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 160 spectra of 6 reference samples from the substance/substance group *Bai Shao Yao*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Bai Shao Yao | G179H0502422 | 61335              | 60      |
| PhytoComm | Bai Shao Yao | G179H0502521 | 61652 <sup>†</sup> | 20      |
| PhytoComm | Bai Shao Yao | G179H0502522 | 61796 <sup>†</sup> | 20      |
| PhytoComm | Bai Shao Yao | G179H0502522 | 61813 <sup>†</sup> | 20      |
| PhytoComm | Bai Shao Yao | G179H0502621 | 61955 <sup>†</sup> | 20      |
| PhytoComm | Bai Shao Yao | G179H0502621 | 61956 <sup>†</sup> | 20      |

- 13 893 spectra from a total of 327 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

<sup>†</sup>These spectra were recorded from 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 | G179H0502323 | 1       |
| Phytocomm | Bai Shao Yao | G179H0502521 | 5       |
| PhytoComm | Bai Shao Yao | 1214401      | 1       |
| PhytoComm | Bai Shao Yao | G179H0502025 | 1       |
| Phytocomm | Bai Shao Yao | G179H0502025 | 3       |
| PhytoComm | Bai Shao Yao | G179H0502121 | 1       |
| Phytocomm | Bai Shao Yao | G179H0502121 | 2       |
| PhytoComm | Bai Shao Yao | G179H0502322 | 2       |
| Phytocomm | Bai Shao Yao | G179H0502322 | 1       |
| Phytocomm | Bai Shao Yao | g179h0502322 | 1       |
| Phytocomm | Bai Shao Yao | g17h0502323  | 1       |
| phythocom | Bai Shao Yao | G179H0502121 | 1       |

- 1961 spectra from 16 *Apo-Ident* customers from a total of 956 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 240           | 0              | 21 326        |
| <b>Type B</b> | 0              | 156           | 4              | 13 893        |
| <b>Type C</b> | 12             | 16            | 4              | 1949          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 97.5000 % (> 95.6250 %)  |
| <b>Type C</b> | 99.3911 % (> 99.1115 %)  | 80.0000 % (> 65.0000 %)  |

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

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

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

### Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61626     | 61626               | 0.00                         | 7.12                            |
| 61652     | 61652               | 0.00                         | 14.16                           |
| 61796     | 61796               | 0.00                         | 11.91                           |
| 61813     | 61813               | 0.00                         | 10.37                           |
| 61955     | 61955               | 0.00                         | 9.29                            |
| 61956     | 61956               | 0.00                         | 9.36                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bai Tou Weng**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60748-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Bai Tou Weng; Pulsatillae radix

### Special notes

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

*no information*

### Applicable documents

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

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Tou Weng*:

| Supplier  | Substance    | Batch        | Sample ID | Spectra | Certificate   |
|-----------|--------------|--------------|-----------|---------|---------------|
| PhytoComm | Bai Tou Weng | G207H0511521 | 61645     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

## Type A All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Bai Tou Weng*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 20 spectra of 1 reference samples from the substance/substance group *Bai Tou Weng*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Bai Tou Weng | G207H0511521 | 61645 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Bai Tou Weng*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| Phytocomm | Bai Tou Weng | G207H0511521 | 4       |
| Phytocomm | Bai Tou Weng | G207H0511221 | 1       |
| PhytoComm | Bai Tou Weng | G207H0511221 | 1       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

<sup>†</sup>These spectra were recorded from 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 Tou Weng* can be 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 Tou Weng* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 1              | 6             | 0              | 1974          |

The substance/substance group *Bai Tou Weng* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9378 % (> 99.6587 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61645     | 61645               | 0.00                         | 10.35                           |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bai Xian Pi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60208-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Bai Xian Pi; Dictamni cortex; Dictamni dasycarpi cortex radicis

### Special notes

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

*no information*

### Applicable documents

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

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

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

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

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Bai Xian Pi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Bai Xian Pi | G090H0515521 | 61707 <sup>†</sup> | 20      |
| PhytoComm | Bai Xian Pi | G090HS355PM1 | 61849 <sup>†</sup> | 20      |
| PhytoComm | Bai Xian Pi | G090HS355PM1 | 61850 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 Xian Pi*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| PhytoComm | Bai Xian Pi | G090H0515121 | 1       |
| Phytocomm | Bai Xian Pi | G090H0515121 | 3       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 Xian Pi | H0515921 | 1       |
| Phytocomm | Bai Xian Pi | H0515921 | 2       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 119           | 1              | 21 446        |
| <b>Type B</b> | 13             | 56            | 4              | 13 980        |
| <b>Type C</b> | 4              | 0             | 7              | 1970          |

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        |
|---------------|--------------------------|-------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 99.1667 % (> 96.6667 %) |
| <b>Type B</b> | 99.9211 % (> 99.8866 %)  | 93.3333 % (> 88.3333 %) |
| <b>Type C</b> | 99.7357 % (> 99.4565 %)  | n/a (n/a)               |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61707     | 61707               | 0.00                         | 7.71                            |
| 61849     | 61849               | 0.00                         | 6.32                            |
| 61850     | 61850               | 0.00                         | 6.71                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bai Zhi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60235-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Bai Zhi; Angelicae dahuricae radix

### Special notes

When selecting the *Bai 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Zhi*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Bai Zhi   | G020H0503521 | 61679     | 40      | from supplier |
| PhytoComm | Bai Zhi   | G020H0503522 | 61770     | 40      | from supplier |
| PhytoComm | Bai Zhi   | G020H0503522 | 61820     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Bai Zhi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Bai Zhi   | G020H0503521 | 61679 <sup>†</sup> | 20      |
| PhytoComm | Bai Zhi   | G020H0503522 | 61770 <sup>†</sup> | 20      |
| PhytoComm | Bai Zhi   | G020H0503522 | 61820 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Bai Zhi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Bai Zhi   | G020H0503421 | 1       |
| Phytocomm | Bai Zhi   | G020H0503024 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Bai Zhi   | G020H0503024 | 1       |
| PhytoComm | Bai Zhi   | G020H0503122 | 2       |
| PhytoComm | Bai Zhi   | G020H0503223 | 1       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Bai 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 *Bai 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 16             | 0             | 7              | 1958          |

The substance/substance group *Bai 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.0997 % (> 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 |
|-----------|---------------------|------------------------------|---------------------------------|
| 61679     | 61679               | 0.00                         | 8.69                            |
| 61770     | 61770               | 0.00                         | 11.57                           |
| 61820     | 61820               | 0.00                         | 11.63                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bai Zhu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60015-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G041H0501321 | 60966     | 40      | from supplier |
| PhytoComm | Bai Zhu   | G041H0501321 | 61596     | 40      | from supplier |
| PhytoComm | Bai Zhu   | G041H0501422 | 61598     | 40      | from supplier |
| PhytoComm | Bai Zhu   | G041H0501621 | 61837     | 40      | from supplier |

## Validation samples

A total of 37 600 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 Zhu*. These samples are listed above in the [calibration samples](#) section.
- 21 406 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Bai Zhu   | G041H0501321 | 61305              | 75      |
| PhytoComm | Bai Zhu   | G041H0501422 | 61307              | 75      |
| PhytoComm | Bai Zhu   | G041H0501621 | 61837 <sup>†</sup> | 20      |

- 13 883 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| phythocom | Bai Zhu   | G041H0501221 | 4       |
| phythocom | Bai Zhu   | g041h0501221 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 |
|-----------|-----------|--------------|---------|
| phythocom | Bai Zhu   | h0501021     | 1       |
| Phytocomm | Bai Zhu   | G041H0501422 | 2       |
| PhytoComm | Bai Zhu   | G041H0501221 | 1       |
| Phytocomm | Bai Zhu   | G041H0501221 | 3       |
| Phytocomm | Bai Zhu   | g041h0501221 | 3       |
| PhytoComm | Bai Zhu   | H0501021     | 1       |
| Phytocomm | Bai Zhu   | H0501021     | 4       |

- 1960 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 168           | 2              | 13 883        |
| <b>Type C</b> | 18             | 2             | 19             | 1942          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 98.8235 % (> 97.0588 %)  |
| <b>Type C</b> | 99.2659 % (> 98.9862 %)  | 9.5238 % (≥ 0.0000 %)    |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60966     | 60966               | 0.00                         | 7.57                            |
| 61596     | 61596               | 0.00                         | 7.94                            |
| 61598     | 61598               | 0.00                         | 6.38                            |
| 61837     | 61837               | 0.00                         | 9.90                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bai Zi Ren**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60197-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Bai Zi Ren; Biotae orientalis semen; Platycladi semen

### Special notes

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

*no information*

### Applicable documents

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

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G052HS187    | 61640     | 40      | from supplier |
| PhytoComm | Bai Zi Ren | G052HS187PG1 | 61848     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Bai Zi Ren | G052HS187    | 61640 <sup>†</sup> | 20      |
| PhytoComm | Bai Zi Ren | G052HS187PG1 | 61848 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Bai Zi Ren*.

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

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

- 1976 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 79            | 1              | 21 486        |
| <b>Type B</b> | 2              | 38            | 2              | 14 011        |
| <b>Type C</b> | 0              | 1             | 4              | 1976          |

The substance/substance group *Bai Zi 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        |
|---------------|--------------------------|-------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 98.7500 % (> 95.0000 %) |
| <b>Type B</b> | 99.9515 % (> 99.9170 %)  | 95.0000 % (> 87.5000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4420 %) | n/a (n/a)               |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61640     | 61640               | 0.00                         | 6.38                            |
| 61848     | 61848               | 0.00                         | 7.46                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ban Lan Gen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60230-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Ban Lan Gen; Isatidis radix

### Special notes

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

*no information*

### Applicable documents

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

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

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

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

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Ban Lan Gen*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Ban Lan Gen | G128H0816521 | 61993 <sup>†</sup> | 20      |
| PhytoComm | Ban Lan Gen | G128H0816521 | 61994 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Ban Lan Gen*.

| Supplier    | Substance   | Batch               | Spectra |
|-------------|-------------|---------------------|---------|
| Phytocomm   | Ban Lan Gen | G128H0816421        | 2       |
| Herbasinica | Ban Lan Gen | GENTIANAEMACROPHYLL | 1       |
| PhytoComm   | Ban Lan Gen | G128H0816221        | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Ban Lan Gen | G128H0816221 | 3       |
| PhytoComm | Ban Lan Gen | H0816922     | 1       |
| Phytocomm | Ban Lan Gen | G128H0816022 | 2       |
| PhytoComm | Ban Lan Gen | G128H0816022 | 1       |

- 1969 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 8              | 1             | 11             | 1961          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.7779 % (> 99.4984 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61993     | 61993               | 0.00                         | 9.83                            |
| 61994     | 61994               | 0.00                         | 10.75                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ban Xia (Jiang)**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60019-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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) | G191H0526322 | 61035     | 40      | from supplier |
| PhytoComm | Ban Xia (Jiang) | G191H0526421 | 61096     | 40      | from supplier |
| PhytoComm | Ban Xia (Jiang) | G191H0526322 | 61476     | 40      | from supplier |
| PhytoComm | Ban Xia (Jiang) | G191H0526322 | 61763     | 40      | from supplier |
| PhytoComm | Ban Xia (Jiang) | G191H0526521 | 61786     | 40      | from supplier |
| PhytoComm | Ban Xia (Jiang) | G191H0526521 | 61829     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Ban Xia (Jiang)*. These samples are listed above in the [calibration samples](#) section.
- 21 326 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 155 spectra of 5 reference samples from the substance/substance group *Ban Xia (Jiang)*.

| Supplier  | Substance       | Batch        | Sample ID          | Spectra |
|-----------|-----------------|--------------|--------------------|---------|
| PhytoComm | Ban Xia (Jiang) | G191H0526421 | 61096 <sup>†</sup> | 20      |
| PhytoComm | Ban Xia (Jiang) | G191H0526322 | 61184              | 75      |
| PhytoComm | Ban Xia (Jiang) | G191H0526322 | 61763 <sup>†</sup> | 20      |
| PhytoComm | Ban Xia (Jiang) | G191H0526521 | 61786 <sup>†</sup> | 20      |
| PhytoComm | Ban Xia (Jiang) | G191H0526521 | 61829 <sup>†</sup> | 20      |

- 13 898 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Ban Xia (Jiang)*.

<sup>†</sup>These spectra were recorded from 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 | Ban Xia (Jiang) | G191H0526023 | 1       |
| PhytoComm | Ban Xia (Jiang) | G191H0526023 | 1       |
| Phytocomm | Ban Xia (Jiang) | G191H0526121 | 6       |
| PhytoComm | Ban Xia (Jiang) | G191H0526121 | 1       |
| Phytocomm | Ban Xia (Jiang) | g191h0526121 | 1       |
| Phytocomm | Ban Xia (Jiang) | G191H0526322 | 1       |

- 1970 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 240           | 0              | 21 326        |
| <b>Type B</b> | 0              | 155           | 0              | 13 898        |
| <b>Type C</b> | 0              | 1             | 10             | 1970          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 100.0000 % (> 96.1290 %) |
| <b>Type C</b> | 100.0000 % (> 99.4411 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61035     | 61035               | 0.00                         | 17.79                           |
| 61096     | 61096               | 0.00                         | 15.13                           |
| 61476     | 61476               | 0.00                         | 19.37                           |
| 61763     | 61763               | 0.00                         | 11.97                           |
| 61786     | 61786               | 0.00                         | 14.93                           |
| 61829     | 61829               | 0.00                         | 13.57                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ban Zhi Lian**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60038-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

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

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

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Ban Zhi Lian*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Ban Zhi Lian | G224H0528521 | 61362 <sup>†</sup> | 20      |
| PhytoComm | Ban Zhi Lian | G224H0528522 | 61921 <sup>†</sup> | 20      |
| PhytoComm | Ban Zhi Lian | G224H0528522 | 61922 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Ban Zhi Lian*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| PhytoComm | Ban Zhi Lian | G224H0528521 | 2       |
| PhytoComm | Ban Zhi Lian | G224H0528521 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Ban Zhi Lian | G224H0528221 | 1       |
| Herbasin  | Ban Zhi Lian | G224H0528022 | 1       |
| PhytoComm | Ban Zhi Lian | H0528021     | 1       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 1              | 3             | 3              | 1974          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.9254 % (> 99.6462 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61362     | 61362               | 0.00                         | 15.08                           |
| 61921     | 61921               | 0.00                         | 9.65                            |
| 61922     | 61922               | 0.00                         | 9.72                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bo He**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60073-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Bo He; Menthae haplocalysis herba

### Special notes

When selecting the *Bo 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

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

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Bo He     | G158H1712421 | 61493     | 40      | from supplier |
| PhytoComm | Bo He     | G158H1712422 | 61766     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Bo He*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 95 spectra of 2 reference samples from the substance/substance group *Bo He*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Bo He     | G158H1712421 | 61201              | 75      |
| PhytoComm | Bo He     | G158H1712422 | 61766 <sup>†</sup> | 20      |

- 13 958 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Bo He*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Bo He     | G158H1712022 | 3       |
| PhytoComm | Bo He     | G158H1712022 | 2       |
| Phytocomm | Bo He     | g158h1712022 | 1       |
| Phytocomm | Bo He     | G158H1712121 | 1       |
| PhytoComm | Bo He     | G158H1712121 | 1       |

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

- 1973 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Bo 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 *Bo 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 95            | 0              | 13 958        |
| <b>Type C</b> | 11             | 0             | 8              | 1962          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 93.6842 %) |
| <b>Type C</b> | 99.5114 % (> 99.2321 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61493     | 61493               | 0.00                         | 9.28                            |
| 61766     | 61766               | 0.00                         | 10.76                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Bu Gu Zhi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60023-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G205H1247421 | 61461     | 40      | from supplier |
| PhytoComm | Bu Gu Zhi | G205H1247621 | 61939     | 40      | from supplier |
| PhytoComm | Bu Gu Zhi | G205H1247621 | 61940     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Bu Gu Zhi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 115 spectra of 3 reference samples from the substance/substance group *Bu Gu Zhi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Bu Gu Zhi | G205H1247421 | 61169              | 75      |
| PhytoComm | Bu Gu Zhi | G205H1247621 | 61939 <sup>†</sup> | 20      |
| PhytoComm | Bu Gu Zhi | G205H1247621 | 61940 <sup>†</sup> | 20      |

- 13 938 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 *Bu Gu Zhi*.

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

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



- 1972 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 115           | 0              | 13 938        |
| <b>Type C</b> | 1              | 2             | 7              | 1971          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 94.7826 %) |
| <b>Type C</b> | 99.6269 % (> 99.3475 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61461     | 61461               | 0.00                         | 9.49                            |
| 61939     | 61939               | 0.00                         | 3.96                            |
| 61940     | 61940               | 0.00                         | 4.09                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Cang Er Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60054-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Cang Er Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Cang Er Zi | G251H1401622 | 61897 <sup>†</sup> | 20      |
| PhytoComm | Cang Er Zi | G251H1401622 | 61898 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 7 *Apo-Ident* customers from 7 batches from the substance/substance group *Cang Er Zi*.

| Supplier  | Substance  | Batch         | Spectra |
|-----------|------------|---------------|---------|
| PhytoComm | Cang Er Zi | (251)H1401021 | 1       |
| Phytocomm | Cang Er Zi | G251H1401021  | 2       |
| PhytoComm | Cang Er Zi | G251H1401021  | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Cang Er Zi | g251h1401021 | 1       |
| Phytocomm | Cang Er Zi | G251H1401123 | 4       |
| Phytocomm | Cang Er Zi | G251H1401322 | 2       |
| Phytocomm | Cang Er Zi | G251H1401521 | 1       |
| Phytocomm | Cang Er Zi | H1401021     | 1       |
| PhytoComm | Cang Er Zi | H1401021     | 1       |

- 1967 spectra from 16 *Apo-Ident* customers from a total of 957 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 14             | 1967          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4409 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61897     | 61897               | 0.00                         | 14.67                           |
| 61898     | 61898               | 0.00                         | 14.44                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Cang Zhu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60160-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

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

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

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Cang Zhu*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Cang Zhu  | G042H1402521 | 61767 <sup>†</sup> | 20      |
| PhytoComm | Cang Zhu  | G042H1402521 | 61800 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 *Cang Zhu*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Cang Zhu  | G042H1402221 | 2       |
| PhytoComm | Cang Zhu  | G042H1402221 | 1       |
| Phytocomm | Cang Zhu  | g042h1402221 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 Zhu  | G042H1402321 | 1       |
| PhytoComm | Cang Zhu  | H1402922     | 1       |
| Phytocomm | Cang Zhu  | H1402922     | 2       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 1              | 0             | 8              | 1972          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.9254 % (> 99.6461 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61767     | 61767               | 0.00                         | 5.12                            |
| 61800     | 61800               | 0.00                         | 4.52                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ce Bai Ye**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60313-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Ce Bai Ye; Biotae orientalis cacumen

### Special notes

When selecting the *Ce Bai 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Ce Bai Ye*:

| Supplier  | Substance | Batch     | Sample ID | Spectra | Certificate   |
|-----------|-----------|-----------|-----------|---------|---------------|
| PhytoComm | Ce Bai Ye | G050HS245 | 61639     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Ce Bai Ye*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 20 spectra of 1 reference samples from the substance/substance group *Ce Bai Ye*.

| Supplier  | Substance | Batch     | Sample ID          | Spectra |
|-----------|-----------|-----------|--------------------|---------|
| PhytoComm | Ce Bai Ye | G050HS245 | 61639 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Ce Bai Ye*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Ce Bai Ye | G050HS245    | 1       |
| PhytoComm | Ce Bai Ye | G050H0975021 | 1       |
| Phytocomm | Ce Bai Ye | G050H0975021 | 1       |
| Phytocomm | Ce Bai Ye | G050H0975321 | 1       |
| phytocomm | Ce Bai Ye | g050h0975321 | 2       |

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

- 1975 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Ce Bai 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 *Ce Bai 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 1              | 20            | 0              | 14 032        |
| <b>Type C</b> | 0              | 0             | 6              | 1975          |

The substance/substance group *Ce Bai 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 99.9977 % (> 99.9634 %)  | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4417 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61639     | 61639               | 0.00                         | 5.90                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Chai Hu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60010-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G055H1055623 | 62043     | 40      | from supplier |
| PhytoComm | Chai Hu   | G055H1055623 | 62044     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Chai Hu*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Chai Hu   | G055H1055623 | 62043 <sup>†</sup> | 20      |
| PhytoComm | Chai Hu   | G055H1055623 | 62044 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Chai Hu   | G055H1055422 | 5       |
| PhytoComm | Chai Hu   | G044H1055322 | 1       |
| PhytoComm | Chai Hu   | G055H1055123 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Chai Hu   | G055H1055123 | 5       |
| Phytocomm | Chai Hu   | g055h1055123 | 1       |
| PhytoComm | Chai Hu   | H1055022     | 1       |
| PhytoComm | Chai Hu   | G055H1055322 | 1       |
| Phytocomm | Chai Hu   | H1055022     | 1       |

- 1965 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 2              | 2             | 14             | 1963          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.8534 % (> 99.5738 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 62043     | 62043               | 0.00                         | 9.10                            |
| 62044     | 62044               | 0.00                         | 9.25                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Chan Tui**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60239-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Chan Tui; Cicadae periostracum

### Special notes

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

*no information*

### Applicable documents

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

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Chan Tui*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Chan Tui  | G067H1817322 | 60888     | 40      | from supplier |
| PhytoComm | Chan Tui  | G067H1817323 | 61015     | 40      | from supplier |
| PhytoComm | Chan Tui  | G067H1817323 | 61565     | 40      | from supplier |
| PhytoComm | Chan Tui  | G067H1817322 | 61576     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Chan Tui*. These samples are listed above in the [calibration samples](#) section.
- 21 406 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 150 spectra of 2 reference samples from the substance/substance group *Chan Tui*.

| Supplier  | Substance | Batch        | Sample ID | Spectra |
|-----------|-----------|--------------|-----------|---------|
| PhytoComm | Chan Tui  | G067H1817323 | 61274     | 75      |
| PhytoComm | Chan Tui  | G067H1817322 | 61285     | 75      |

- 13 903 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Chan Tui*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Chan Tui  | G067H1817323 | 1       |
| PhytoComm | Chan Tui  | G067H1817323 | 1       |
| Phytocomm | Chan Tui  | G067H1817121 | 2       |
| PhytoComm | Chan Tui  | G067H1817322 | 1       |
| Phytocomm | Chan Tui  | G067H1817322 | 1       |
| phytocomm | Chan Tui  | g067h1817322 | 1       |
| PhytoComm | Chan Tui  | G06H1817121  | 1       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 150           | 0              | 13 903        |
| <b>Type C</b> | 2              | 5             | 3              | 1971          |

The substance/substance group *Chan Tui* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 96.0000 %) |
| <b>Type C</b> | 99.8445 % (> 99.5652 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60888     | 60888               | 0.00                         | 12.00                           |
| 61015     | 61015               | 0.00                         | 9.32                            |
| 61565     | 61565               | 0.00                         | 10.17                           |
| 61576     | 61576               | 0.00                         | 10.73                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Che Qian Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60255-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G192H0723421 | 61078     | 40      | from supplier |
| PhytoComm | Che Qian Zi | G192H0723323 | 61468     | 40      | from supplier |
| PhytoComm | Che Qian Zi | G192H0723421 | 61473     | 40      | from supplier |
| PhytoComm | Che Qian Zi | G192H0723621 | 61963     | 40      | from supplier |
| PhytoComm | Che Qian Zi | G192H0723621 | 61964     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Che Qian Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 210 spectra of 5 reference samples from the substance/substance group *Che Qian Zi*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Che Qian Zi | G192H0723421 | 61078 <sup>†</sup> | 20      |
| PhytoComm | Che Qian Zi | G192H0723323 | 61176              | 75      |
| PhytoComm | Che Qian Zi | G192H0723421 | 61181              | 75      |
| PhytoComm | Che Qian Zi | G192H0723621 | 61963 <sup>†</sup> | 20      |
| PhytoComm | Che Qian Zi | G192H0723621 | 61964 <sup>†</sup> | 20      |

- 13 843 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 7 *Apo-Ident* customers from 4 batches from the substance/substance group *Che Qian Zi*.

<sup>†</sup>These spectra were recorded from 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 | Che Qian Zi | G192H0723421 | 2       |
| PhytoComm | Che Qian Zi | G192H0723321 | 2       |
| Phytocomm | Che Qian Zi | 410704805    | 1       |
| PhytoComm | Che Qian Zi | 410704805    | 1       |
| Phytocomm | Che Qian Zi | G192H0723121 | 1       |
| PhytoComm | Che Qian Zi | G192H0723121 | 1       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 200           | 0              | 21 366        |
| <b>Type B</b> | 0              | 209           | 1              | 13 843        |
| <b>Type C</b> | 1              | 2             | 6              | 1972          |

The substance/substance group *Che Qian 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 99.5238 % (> 98.0952 %)  |
| <b>Type C</b> | 99.9378 % (> 99.6585 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61078     | 61078               | 0.00                         | 44.42                           |
| 61468     | 61468               | 0.00                         | 11.63                           |
| 61473     | 61473               | 0.00                         | 11.40                           |
| 61963     | 61963               | 0.00                         | 70.70                           |
| 61964     | 61964               | 0.00                         | 68.83                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Chen Pi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60009-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

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

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

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

**Type A** All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Chen Pi*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Chen Pi   | G073H1128621 | 61841 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Chen Pi*.

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

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

- 1971 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 1              | 38            | 2              | 21 525        |
| <b>Type B</b> | 8              | 20            | 0              | 14 025        |
| <b>Type C</b> | 2              | 0             | 10             | 1969          |

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

|               | Specificity             | Recognition rate         |
|---------------|-------------------------|--------------------------|
| <b>Type A</b> | 99.9939 % (> 99.9746 %) | 95.0000 % (> 87.5000 %)  |
| <b>Type B</b> | 99.9029 % (> 99.8686 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9212 % (> 99.6418 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61841     | 61841               | 0.00                         | 4.89                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Chi Shao (Yao)**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60014-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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) | G180H0705522 | 61779     | 40      | from supplier |
| PhytoComm | Chi Shao (Yao) | G180H0705522 | 61821     | 40      | from supplier |
| PhytoComm | Chi Shao (Yao) | G180H0705621 | 61965     | 40      | from supplier |
| PhytoComm | Chi Shao (Yao) | G180H0705621 | 61966     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 406 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance      | Batch        | Sample ID          | Spectra |
|-----------|----------------|--------------|--------------------|---------|
| PhytoComm | Chi Shao (Yao) | G180H0705522 | 61779 <sup>†</sup> | 20      |
| PhytoComm | Chi Shao (Yao) | G180H0705522 | 61821 <sup>†</sup> | 20      |
| PhytoComm | Chi Shao (Yao) | G180H0705621 | 61965 <sup>†</sup> | 20      |
| PhytoComm | Chi Shao (Yao) | G180H0705621 | 61966 <sup>†</sup> | 20      |

- 13 973 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 13 spectra from 7 *Apo-Ident* customers from 7 batches from the substance/substance group *Chi Shao (Yao)*.

| Supplier  | Substance      | Batch        | Spectra |
|-----------|----------------|--------------|---------|
| Phytocomm | Chi Shao (Yao) | G180H0705422 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Chi Shao (Yao) | G180H0705121 | 2       |
| Gehe      | Chi Shao (Yao) | G180H0705121 | 1       |
| PhytoComm | Chi Shao (Yao) | G180H0705122 | 2       |
| Phytocomm | Chi Shao (Yao) | G180H0705122 | 2       |
| Phytocomm | Chi Shao (Yao) | g180h0705122 | 1       |
| Phytocomm | Chi Shao (Yao) | G180H0705321 | 1       |
| PhytoComm | Chi Shao (Yao) | G180H0705321 | 1       |
| Phytocomm | Chi Shao (Yao) | G180H0705121 | 1       |
| Phytocomm | Chi Shao (Yao) | G189H0705321 | 1       |

- 1968 spectra from 16 *Apo-Ident* customers from a total of 957 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 80            | 0              | 13 973        |
| <b>Type C</b> | 3              | 1             | 12             | 1965          |

The substance/substance group *Chi 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.5000 %) |
| <b>Type C</b> | 99.8632 % (> 99.5837 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61779     | 61779               | 0.00                         | 13.20                           |
| 61821     | 61821               | 0.00                         | 12.75                           |
| 61965     | 61965               | 0.00                         | 13.86                           |
| 61966     | 61966               | 0.00                         | 13.66                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Chuan Lian Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60078-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G157H0306421 | 61357     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Chuan Lian Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 20 spectra of 1 reference samples from the substance/substance group *Chuan Lian Zi*.

| Supplier  | Substance     | Batch        | Sample ID          | Spectra |
|-----------|---------------|--------------|--------------------|---------|
| PhytoComm | Chuan Lian Zi | G157H0306421 | 61357 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Chuan Lian Zi*.

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

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

- 1972 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 1              | 3             | 6              | 1971          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9534 % (> 99.6740 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61357     | 61357               | 0.00                         | 8.49                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Chuan Mu Tong**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60173-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Chuan Mu Tong; Clematidis armandii caulis

### Special notes

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

*no information*

### Applicable documents

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

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Mu Tong*:

| Supplier  | Substance     | Batch        | Sample ID | Spectra | Certificate   |
|-----------|---------------|--------------|-----------|---------|---------------|
| PhytoComm | Chuan Mu Tong | G009H0310521 | 61732     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Chuan Mu Tong*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 20 spectra of 1 reference samples from the substance/substance group *Chuan Mu Tong*.

| Supplier  | Substance     | Batch        | Sample ID          | Spectra |
|-----------|---------------|--------------|--------------------|---------|
| PhytoComm | Chuan Mu Tong | G009H0310521 | 61732 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Chuan Mu Tong*.

| Supplier  | Substance     | Batch        | Spectra |
|-----------|---------------|--------------|---------|
| Phytocomm | Chuan Mu Tong | G009H0310321 | 1       |
| PhytoComm | Chuan Mu Tong | G009H0310521 | 1       |
| phytoComm | Chuan Mu Tong | G009H0310121 | 3       |
| PhytoComm | Chuan Mu Tong | G009H0310121 | 2       |
| Phytocomm | Chuan Mu Tong | g009h0310321 | 1       |
| PhytoComm | Chuan Mu Tong | H0310021     | 1       |

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



- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 1              | 1             | 8              | 1971          |

The substance/substance group *Chuan Mu Tong* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9254 % (> 99.6460 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61732     | 61732               | 0.00                         | 7.71                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Chuan Niu Xi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60122-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Chuan Niu Xi; Cyathulae radix

### Special notes

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

*no information*

### Applicable documents

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

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

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

| Supplier  | Substance    | Batch        | Sample ID | Spectra | Certificate   |
|-----------|--------------|--------------|-----------|---------|---------------|
| PhytoComm | Chuan Niu Xi | G318H0431522 | 61788     | 40      | from supplier |
| PhytoComm | Chuan Niu Xi | G318H0431522 | 61802     | 40      | from supplier |
| PhytoComm | Chuan Niu Xi | G318H0431621 | 61883     | 40      | from supplier |
| PhytoComm | Chuan Niu Xi | G318H0431621 | 61884     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *Chuan Niu Xi*. These samples are listed above in the [calibration samples](#) section.
- 21 406 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Chuan Niu Xi*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Chuan Niu Xi | G318H0431522 | 61788 <sup>†</sup> | 20      |
| PhytoComm | Chuan Niu Xi | G318H0431522 | 61802 <sup>†</sup> | 20      |
| PhytoComm | Chuan Niu Xi | G318H0431621 | 61883 <sup>†</sup> | 20      |
| PhytoComm | Chuan Niu Xi | G318H0431621 | 61884 <sup>†</sup> | 20      |

- 13 973 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Chuan Niu Xi*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| PhytoComm | Chuan Niu Xi | G318H0431321 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Chuan Niu Xi | g318h0431321 | 1       |
| PhytoComm | Chuan Niu Xi | H0431923     | 3       |

- 1976 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 159           | 1              | 21 406        |
| <b>Type B</b> | 0              | 80            | 0              | 13 973        |
| <b>Type C</b> | 2              | 0             | 5              | 1974          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 99.3750 % (> 97.5000 %)  |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.5000 %) |
| <b>Type C</b> | 99.8964 % (> 99.6174 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61788     | 61788               | 0.00                         | 5.61                            |
| 61802     | 61802               | 0.00                         | 5.14                            |
| 61883     | 61883               | 0.00                         | 4.57                            |
| 61884     | 61884               | 0.00                         | 4.72                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Chuan Xin Lian**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60137-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Chuan Xin Lian; Andrographitis herba

### Special notes

When selecting the *Chuan Xin 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Xin Lian*:

| Supplier  | Substance      | Batch         | Sample ID | Spectra | Certificate   |
|-----------|----------------|---------------|-----------|---------|---------------|
| PhytoComm | Chuan Xin Lian | G321FB0963421 | 61636     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Chuan Xin Lian*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 15 spectra of 1 reference samples from the substance/substance group *Chuan Xin Lian*.

| Supplier  | Substance      | Batch         | Sample ID          | Spectra |
|-----------|----------------|---------------|--------------------|---------|
| PhytoComm | Chuan Xin Lian | G321FB0963421 | 61636 <sup>†</sup> | 15      |

- 14 038 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Chuan Xin Lian*.

| Supplier  | Substance      | Batch         | Spectra |
|-----------|----------------|---------------|---------|
| PhytoComm | Chuan Xin Lian | G321FB0963321 | 1       |
| PhytoComm | Chuan Xin Lian | H0963921      | 1       |

- 1979 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the

<sup>†</sup>These spectra were recorded from 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 *Chuan Xin 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 *Chuan Xin 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 15            | 0              | 14 038        |
| <b>Type C</b> | 1              | 2             | 0              | 1978          |

The substance/substance group *Chuan Xin 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9317 %) | n/a (n/a)                |
| <b>Type C</b> | 99.9378 % (> 99.6601 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61636     | 61636               | 0.00                         | 11.57                           |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Chuan Xiong**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60013-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Chuan Xiong; Ligustici chuanxiong rhizoma; Ligustici wallichii radix

### Special notes

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

*no information*

### Applicable documents

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

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G136H0305421 | 61521     | 40      | from supplier |
| PhytoComm | Chuan Xiong | G136H0305321 | 61558     | 40      | from supplier |
| PhytoComm | Chuan Xiong | G136H0305621 | 61975     | 40      | from supplier |
| PhytoComm | Chuan Xiong | G136H0305621 | 61976     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *Chuan Xiong*. These samples are listed above in the [calibration samples](#) section.
- 21 406 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 190 spectra of 4 reference samples from the substance/substance group *Chuan Xiong*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Chuan Xiong | G136H0305421 | 61230              | 75      |
| PhytoComm | Chuan Xiong | G136H0305321 | 61267              | 75      |
| PhytoComm | Chuan Xiong | G136H0305621 | 61975 <sup>†</sup> | 20      |
| PhytoComm | Chuan Xiong | G136H0305621 | 61976 <sup>†</sup> | 20      |

- 13 863 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 6 batches from the substance/substance group *Chuan Xiong*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| Phytocomm | Chuan Xiong | G136H0305421 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Chuan Xiong | G135H0305121 | 1       |
| phytocomm | Chuan Xiong | G136H0305121 | 1       |
| PhytoComm | Chuan Xiong | G136H0305121 | 1       |
| Phytocomm | Chuan Xiong | G136H0305121 | 3       |
| Phytocomm | Chuan Xiong | g136h0305121 | 1       |
| PhytoComm | Chuan Xiong | G136H0305221 | 2       |
| Phytocomm | Chuan Xiong | G136H305121  | 1       |
| Phytocomm | Chuan Xiong | G136H0305221 | 1       |

- 1969 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 1              | 160           | 0              | 21 405        |
| <b>Type B</b> | 0              | 189           | 1              | 13 863        |
| <b>Type C</b> | 15             | 4             | 8              | 1954          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 99.9969 % (> 99.9775 %)  | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 99.4737 % (> 97.8947 %)  |
| <b>Type C</b> | 98.8294 % (> 98.5499 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61521     | 61521               | 0.00                         | 5.26                            |
| 61558     | 61558               | 0.00                         | 8.53                            |
| 61975     | 61975               | 0.00                         | 6.32                            |
| 61976     | 61976               | 0.00                         | 6.86                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Chuang Mu Xiang**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50323-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G219H0309521 | 61661     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Chuang Mu Xiang*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 20 spectra of 1 reference samples from the substance/substance group *Chuang Mu Xiang*.

| Supplier  | Substance       | Batch        | Sample ID          | Spectra |
|-----------|-----------------|--------------|--------------------|---------|
| PhytoComm | Chuang Mu Xiang | G219H0309521 | 61661 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 5 batches from the substance/substance group *Chuang Mu Xiang*.

| Supplier  | Substance       | Batch        | Spectra |
|-----------|-----------------|--------------|---------|
| Phytocomm | Chuang Mu Xiang | g219h0309321 | 1       |
| Phytocomm | Chuang Mu Xiang | G219H0309521 | 2       |
| PhytoComm | Chuang Mu Xiang | G219H0309021 | 1       |
| phytocomm | Chuang Mu Xiang | G219H0309021 | 1       |
| Phytocomm | Chuang Mu Xiang | G219H0309322 | 1       |
| Phytocomm | Chuang Mu Xiang | g219h0309322 | 1       |

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



- 1974 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 19            | 1              | 14 033        |
| <b>Type C</b> | 4              | 1             | 6              | 1970          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 95.0000 % (> 80.0000 %)  |
| <b>Type C</b> | 99.8134 % (> 99.5342 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61661     | 61661               | 0.00                         | 6.39                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

|                                     |                                                                 |
|-------------------------------------|-----------------------------------------------------------------|
| Validated substance/substance group | <b>Ci Wu Jia</b>                                                |
| Substance class                     | TCM - Granulated herbal extracts (PhytoComm)                    |
| Report date                         | 01/06/2017                                                      |
| Report number                       | 60354-2017-06-01                                                |
| Executing company                   | HiperScan GmbH<br>Weißeritzstraße 3<br>01067 Dresden<br>Germany |

### Relevant substance names

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

### Special notes

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

*no information*

### Applicable documents

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

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G302H0856521 | 61784     | 40      | from supplier |
| PhytoComm | Ci Wu Jia | G302H0856521 | 61812     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Ci Wu Jia | G302H0856521 | 61784 <sup>†</sup> | 20      |
| PhytoComm | Ci Wu Jia | G302H0856521 | 61812 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Ci Wu Jia*.

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

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

- 1979 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 1              | 0             | 2              | 1978          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.9661 % (> 99.6883 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61784     | 61784               | 0.00                         | 6.58                            |
| 61812     | 61812               | 0.00                         | 6.70                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Cong Bai**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60467-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Cong Bai; Allii fistulosi bulbus

### Special notes

When selecting the *Cong 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

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

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Cong Bai  | G012H1255521 | 61708     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Cong Bai*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Cong Bai  | G012H1255521 | 61708 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Cong Bai*.

| Supplier | Substance | Batch  | Spectra |
|----------|-----------|--------|---------|
| Bios     | Cong Bai  | 424348 | 2       |

- 1979 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the

<sup>†</sup>These spectra were recorded from 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 *Cong 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 *Cong 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 2              | 1979          |

The substance/substance group *Cong 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4445 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61708     | 61708               | 0.00                         | 14.37                           |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Da Qing Ye**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60256-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Da Qing Ye; Isatidis folium

### Special notes

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

*no information*

### Applicable documents

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

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

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

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

## Validation samples

A total of 37 600 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 *Da Qing Ye*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Da Qing Ye | G127H0318621 | 62003 <sup>†</sup> | 20      |
| PhytoComm | Da Qing Ye | G127H0318621 | 62004 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Da Qing Ye*.

| Supplier  | Substance  | Batch        | Spectra |
|-----------|------------|--------------|---------|
| PhytoComm | Da Qing Ye | 4103167001   | 1       |
| PhytoComm | Da Qing Ye | G127H0318121 | 1       |
| Herbasin  | Da Qing Ye | G127H0318121 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 Qing Ye | 410316901    | 1       |
| PhytoComm | Da Qing Ye | G127H0318121 | 1       |
| Phytocomm | Da Qing Ye | G127H0318421 | 2       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 1              | 0             | 7              | 1973          |

The substance/substance group *Da Qing 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.9067 % (> 99.6275 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 62003     | 62003               | 0.00                         | 13.26                           |
| 62004     | 62004               | 0.00                         | 14.32                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Da Zao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60055-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G129H0316321 | 61034     | 50      | from supplier |
| PhytoComm | Da Zao    | G129H0316321 | 61526     | 40      | from supplier |
| PhytoComm | Da Zao    | G129H0316521 | 61730     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 130 spectra of 3 reference samples from the substance/substance group *Da Zao*. These samples are listed above in the [calibration samples](#) section.
- 21 436 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Da Zao    | G129H0316321 | 61034 <sup>†</sup> | 10      |
| PhytoComm | Da Zao    | G129H0316321 | 61235              | 75      |
| PhytoComm | Da Zao    | G129H0316521 | 61730 <sup>†</sup> | 20      |

- 13 948 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Da Zao    | G129H0316521 | 3       |
| phytocomm | Da Zao    | G129H0316121 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 Zao    | G129H0316121 | 1       |
| Phytocomm | Da Zao    | G129H0316121 | 5       |
| PhytoComm | Da Zao    | G129H0316221 | 1       |
| Phytocomm | Da Zao    | G129H0316221 | 3       |
| Phytocomm | Da Zao    | g129h0316221 | 1       |

- 1965 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 130           | 0              | 21 436        |
| <b>Type B</b> | 0              | 105           | 0              | 13 948        |
| <b>Type C</b> | 22             | 8             | 8              | 1943          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.3846 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 94.2857 %) |
| <b>Type C</b> | 99.1338 % (> 98.8542 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61034     | 61034               | 0.00                         | 10.76                           |
| 61526     | 61526               | 0.00                         | 9.35                            |
| 61730     | 61730               | 0.00                         | 10.86                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Dan Dou Chi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60794-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G232HS239    | 61641     | 40      | from supplier |
| PhytoComm | Dan Dou Chi | G232H1106621 | 61909     | 40      | from supplier |
| PhytoComm | Dan Dou Chi | G232H1106621 | 61910     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Dan Dou Chi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 60 spectra of 3 reference samples from the substance/substance group *Dan Dou Chi*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Dan Dou Chi | G232HS239    | 61641 <sup>†</sup> | 20      |
| PhytoComm | Dan Dou Chi | G232H1106621 | 61909 <sup>†</sup> | 20      |
| PhytoComm | Dan Dou Chi | G232H1106621 | 61910 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Dan Dou Chi*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| PhytoComm | Dan Dou Chi | G232HS239    | 1       |
| PhytoComm | Dan Dou Chi | G232H1106321 | 1       |

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

- 1979 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 0              | 1             | 1              | 1979          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4445 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61641     | 61641               | 0.00                         | 19.44                           |
| 61909     | 61909               | 0.00                         | 50.09                           |
| 61910     | 61910               | 0.00                         | 51.92                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Dan Shen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60030-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G214H0441324 | 61007     | 20      | from supplier |
| PhytoComm | Dan Shen  | G214H0441422 | 61367     | 40      | from supplier |
| PhytoComm | Dan Shen  | G214H0441324 | 61448     | 40      | from supplier |
| PhytoComm | Dan Shen  | G214H0441522 | 61731     | 40      | from supplier |
| PhytoComm | Dan Shen  | G214H0441522 | 62063     | 40      | from supplier |
| PhytoComm | Dan Shen  | G214H0441522 | 62064     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

**Type A** All calibration spectra.

- 220 spectra of 6 reference samples from the substance/substance group *Dan Shen*. These samples are listed above in the [calibration samples](#) section.
- 21 346 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 155 spectra of 5 reference samples from the substance/substance group *Dan Shen*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Dan Shen  | G214H0441324 | 61156              | 75      |
| PhytoComm | Dan Shen  | G214H0441422 | 61367 <sup>†</sup> | 20      |
| PhytoComm | Dan Shen  | G214H0441522 | 61731 <sup>†</sup> | 20      |
| PhytoComm | Dan Shen  | G214H0441522 | 62063 <sup>†</sup> | 20      |
| PhytoComm | Dan Shen  | G214H0441522 | 62064 <sup>†</sup> | 20      |

- 13 898 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

<sup>†</sup>These spectra were recorded from 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 | Dan Shen  | G214H0441522 | 1       |
| PhytoComm | Dan Shen  | G214H0441522 | 1       |
| Phytocomm | Dan Shen  | G214H0441121 | 5       |
| PhytoComm | Dan Shen  | G214H0441121 | 2       |
| Phytocomm | Dan Shen  | g214h0441121 | 1       |
| PhytoComm | Dan Shen  | G214H0441221 | 2       |
| Phytocomm | Dan Shen  | G214H0441221 | 1       |
| Phytocomm | Dan Shen  | G214H0441322 | 1       |
| PhytoComm | Dan Shen  | G214H0441322 | 2       |

- 1965 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

### Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 220           | 0              | 21 346        |
| <b>Type B</b> | 0              | 155           | 0              | 13 898        |
| <b>Type C</b> | 3              | 12            | 4              | 1962          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.2727 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 100.0000 % (> 96.1290 %) |
| <b>Type C</b> | 99.8756 % (> 99.5961 %)  | n/a (n/a)                |

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

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

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

### Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61007     | 61007               | 0.00                         | 9.66                            |
| 61367     | 61367               | 0.00                         | 5.78                            |
| 61448     | 61448               | 0.00                         | 8.07                            |
| 61731     | 61731               | 0.00                         | 9.23                            |
| 62063     | 62063               | 0.00                         | 11.49                           |
| 62064     | 62064               | 0.00                         | 11.82                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Dang Gui**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60003-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G022H1306621 | 61835     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Dang Gui*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 20 spectra of 1 reference samples from the substance/substance group *Dang Gui*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Dang Gui  | G022H1306621 | 61835 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 19 spectra from 9 *Apo-Ident* customers from 8 batches from the substance/substance group *Dang Gui*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Dang Gui  | G022H1306422 | 2       |
| PhytoComm | Dang Gui  | G022H1306621 | 2       |
| PhytoComm | Dang Gui  | G022H1306022 | 2       |
| Phytocomm | Dang Gui  | G022H1306022 | 5       |
| Phytocomm | Dang Gui  | G022H1306121 | 1       |
| Phytocomm | Dang Gui  | G022H1306023 | 1       |
| PhytoComm | Dang Gui  | G022H1306121 | 1       |
| Phytocomm | Dang Gui  | g022h1306121 | 3       |
| PhytoComm | Dang Gui  | G022H1306321 | 1       |
| PhytoComm | Dang Gui  | G13-0784     | 1       |

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

- 1962 spectra from 16 *Apo-Ident* customers from a total of 956 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 1              | 20            | 0              | 14 032        |
| <b>Type C</b> | 3              | 0             | 19             | 1959          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 99.9974 % (> 99.9632 %)  | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.8653 % (> 99.5856 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61835     | 61835               | 0.00                         | 9.32                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Dang Gui Wei**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60308-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G312H1307522 | 61676     | 40      | from supplier |
| PhytoComm | Dang Gui Wei | G312H1307621 | 61885     | 40      | from supplier |
| PhytoComm | Dang Gui Wei | G312H1307621 | 61886     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Dang Gui Wei*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 60 spectra of 3 reference samples from the substance/substance group *Dang Gui Wei*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Dang Gui Wei | G312H1307522 | 61676 <sup>†</sup> | 20      |
| PhytoComm | Dang Gui Wei | G312H1307621 | 61885 <sup>†</sup> | 20      |
| PhytoComm | Dang Gui Wei | G312H1307621 | 61886 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 8 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Dang Gui Wei*.

| Supplier  | Substance    | Batch          | Spectra |
|-----------|--------------|----------------|---------|
| PhytoComm | Dang Gui Wei | (G312)H1307021 | 1       |
| PhytoComm | Dang Gui Wei | G312H1307021   | 2       |
| Phytocomm | Dang Gui Wei | G312H1307021   | 5       |

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



- 1973 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 119           | 1              | 21 446        |
| <b>Type B</b> | 0              | 59            | 1              | 13 993        |
| <b>Type C</b> | 4              | 1             | 7              | 1969          |

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        |
|---------------|--------------------------|-------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 99.1667 % (> 96.6667 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 98.3333 % (> 93.3333 %) |
| <b>Type C</b> | 99.8818 % (> 99.6025 %)  | n/a (n/a)               |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61676     | 61676               | 0.00                         | 7.37                            |
| 61885     | 61885               | 0.00                         | 6.00                            |
| 61886     | 61886               | 0.00                         | 5.77                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Dang Shen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60000-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G077H2001521 | 61710     | 40      | from supplier |
| PhytoComm | Dang Shen | G077H2001621 | 62021     | 40      | from supplier |
| PhytoComm | Dang Shen | G077H2001621 | 62022     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Dang Shen*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 60 spectra of 3 reference samples from the substance/substance group *Dang Shen*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Dang Shen | G077H2001521 | 61710 <sup>†</sup> | 20      |
| PhytoComm | Dang Shen | G077H2001621 | 62021 <sup>†</sup> | 20      |
| PhytoComm | Dang Shen | G077H2001621 | 62022 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 9 *Apo-Ident* customers from 6 batches from the substance/substance group *Dang Shen*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Dang Shen | G077H2001521 | 2       |
| PhytoComm | Dang Shen | G077H2001521 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Dang Shen | G077H2001022 | 1       |
| PhytoComm | Dang Shen | G077H2001022 | 1       |
| Phytocomm | Dang Shen | G077H2001222 | 1       |
| PhytoComm | Dang Shen | G077H2001222 | 1       |
| PhytoComm | Dang Shen | g077H2001222 | 1       |
| EuRho     | Dang Shen | g077h2001222 | 2       |
| PhytoComm | Dang Shen | H2001021     | 2       |
| Phytocomm | Dang Shen | H2001021     | 1       |

- 1967 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Dang 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 2              | 60            | 0              | 13 991        |
| <b>Type C</b> | 13             | 6             | 8              | 1954          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 99.9838 % (> 99.9493 %)  | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.4377 % (> 99.1582 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61710     | 61710               | 0.00                         | 6.81                            |
| 62021     | 62021               | 0.00                         | 7.65                            |
| 62022     | 62022               | 0.00                         | 7.39                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Di Fu Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60043-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Di Fu Zi; Kochiae scopariae fructus

### Special notes

When selecting the *Di 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Fu Zi*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Di Fu Zi  | G131H0605522 | 61667     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Di Fu Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 20 spectra of 1 reference samples from the substance/substance group *Di Fu Zi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Di Fu Zi  | G131H0605522 | 61667 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 2 batches from the substance/substance group *Di Fu Zi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| PhytoComm | Di Fu Zi  | G131H0605021 | 1       |
| PhytoComm | Di Fu Zi  | G131H0605122 | 2       |
| Phytocomm | Di Fu Zi  | G131H0605122 | 2       |

- 1976 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

<sup>†</sup>These spectra were recorded from 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 *Di 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 *Di 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 5              | 1976          |

The substance/substance group *Di 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4420 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61667     | 61667               | 0.00                         | 69.96                           |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Di Gu Pi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60036-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G149H0601421 | 61499     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Di Gu Pi*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 75 spectra of 1 reference samples from the substance/substance group *Di Gu Pi*.

| Supplier  | Substance | Batch        | Sample ID | Spectra |
|-----------|-----------|--------------|-----------|---------|
| PhytoComm | Di Gu Pi  | G149H0601421 | 61207     | 75      |

- 13 978 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 9 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Di Gu Pi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Di Gu Pi  | G149H0601421 | 1       |
| PhytoComm | Di Gu Pi  | G149H0601421 | 2       |
| Phytocomm | Di Gu Pi  | g149h060112  | 1       |
| Phytocomm | Di Gu Pi  | G149H0601122 | 1       |
| PhytoComm | Di Gu Pi  | G149H0601122 | 2       |
| Phytocomm | Di Gu Pi  | G149H0601822 | 1       |
| PhytoComm | Di Gu Pi  | H0601821     | 1       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 75            | 0              | 13 978        |
| <b>Type C</b> | 3              | 3             | 6              | 1969          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.0000 %) |
| <b>Type C</b> | 99.8653 % (> 99.5859 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61499     | 61499               | 0.00                         | 10.20                           |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Di Long**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60061-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Di Long; Lumbricus

### Special notes

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

*no information*

### Applicable documents

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

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Long*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Di Long   | G148H0603421 | 61653     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Di Long*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 20 spectra of 1 reference samples from the substance/substance group *Di Long*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Di Long   | G148H0603421 | 61653 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 5 batches from the substance/substance group *Di Long*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Di Long   | G148H0603421 | 1       |
| PhytoComm | Di Long   | G148H0603421 | 1       |
| Phytocomm | Di Long   | G148H0603022 | 1       |
| PhytoComm | Di Long   | G148H0603022 | 2       |
| Phytocomm | Di Long   | G148H0603321 | 2       |
| PhytoComm | Di Long   | G148H0603321 | 1       |
| phytocomm | Di Long   | g148h603321  | 1       |

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



- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Di Long* can be 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 Long* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 4             | 5              | 1972          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4413 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61653     | 61653               | 0.00                         | 23.86                           |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Dong Gua Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60202-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Dong Gua Zi*:

| Supplier  | Substance   | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-------------|--------------|-----------|---------|---------------|
| PhytoComm | Dong Gua Zi | G049H0551622 | 62015     | 40      | from supplier |
| PhytoComm | Dong Gua Zi | G049H0551622 | 62016     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Dong Gua Zi | G049H0551622 | 62015 <sup>†</sup> | 20      |
| PhytoComm | Dong Gua Zi | G049H0551622 | 62016 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Dong Gua Zi*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| Phytocomm | Dong Gua Zi | G049H0551221 | 5       |
| Phytocomm | Dong Gua Zi | G049H0551021 | 1       |
| PhytoComm | Dong Gua Zi | G049H0551221 | 1       |

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

- 1974 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 1             | 6              | 1974          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4415 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 62015     | 62015               | 0.00                         | 13.63                           |
| 62016     | 62016               | 0.00                         | 13.37                           |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Du Huo**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50259-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G021H1610421 | 61616     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Du Huo*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 75 spectra of 1 reference samples from the substance/substance group *Du Huo*.

| Supplier  | Substance | Batch        | Sample ID | Spectra |
|-----------|-----------|--------------|-----------|---------|
| PhytoComm | Du Huo    | G021H1610421 | 61325     | 75      |

- 13 978 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Du Huo    | 421605602    | 2       |
| Phytocomm | Du Huo    | G021H1610421 | 2       |
| PhytoComm | Du Huo    | G021H1610221 | 1       |
| Phytocomm | Du Huo    | g021h610221  | 1       |
| PhytoComm | Du Huo    | H1610922     | 1       |
| Phytocomm | Du Huo    | H1610922     | 2       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented



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

## Validation results

The validation runs checked whether the substance/substance group *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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 75            | 0              | 13 978        |
| <b>Type C</b> | 5              | 2             | 7              | 1967          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.0000 %) |
| <b>Type C</b> | 99.7217 % (> 99.4423 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61616     | 61616               | 0.00                         | 11.51                           |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Du Zhong**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60214-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G101H0736522 | 61722     | 40      | from supplier |
| PhytoComm | Du Zhong  | G101H0736621 | 61997     | 40      | from supplier |
| PhytoComm | Du Zhong  | G101H0736621 | 61998     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Du Zhong*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 60 spectra of 3 reference samples from the substance/substance group *Du Zhong*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Du Zhong  | G101H0736522 | 61722 <sup>†</sup> | 20      |
| PhytoComm | Du Zhong  | G101H0736621 | 61997 <sup>†</sup> | 20      |
| PhytoComm | Du Zhong  | G101H0736621 | 61998 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 15 spectra from 8 *Apo-Ident* customers from 7 batches from the substance/substance group *Du Zhong*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Du Zhong  | G101H0736522 | 5       |
| PhytoComm | Du Zhong  | G101H0736021 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Du Zhong  | g101h0736021 | 1       |
| Phytocomm | Du Zhong  | G101H0736021 | 1       |
| Phytocomm | Du Zhong  | G101H0736321 | 1       |
| PhytoComm | Du Zhong  | G101H0736321 | 1       |
| Phytocomm | Du Zhong  | g101h076521  | 1       |
| PhytoComm | Du Zhong  | H0736021     | 3       |
| Phytocomm | Du Zhong  | H0736923     | 1       |

- 1966 spectra from 16 *Apo-Ident* customers from a total of 957 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 3              | 8             | 7              | 1963          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.9067 % (> 99.6272 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61722     | 61722               | 0.00                         | 7.21                            |
| 61997     | 61997               | 0.00                         | 8.25                            |
| 61998     | 61998               | 0.00                         | 8.16                            |

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

# VALIDATION REPORT

IdentModul 1.3-2017-03

Validated substance/substance group **E Zhu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50344-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

## Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

## Calibration samples

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

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | E Zhu     | G083H1110521 | 61741     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

**Type A** All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *E Zhu*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 20 spectra of 1 reference samples from the substance/substance group *E Zhu*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | E Zhu     | G083H1110521 | 61741 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 5 batches from the substance/substance group *E Zhu*.

| Supplier  | Substance | Batch         | Spectra |
|-----------|-----------|---------------|---------|
| PhytoComm | E Zhu     | (083)H1110021 | 1       |
| Phytocomm | E Zhu     | G083H111022   | 1       |
| Phytocomm | E Zhu     | H1110021      | 2       |
| PhytoComm | E Zhu     | H1110021      | 2       |
| PhytoComm | E Zhu     | G083H1110222  | 1       |
| Phytocomm | E Zhu     | h1110021      | 1       |

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



- 1973 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 1              | 0             | 8              | 1972          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9661 % (> 99.6868 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61741     | 61741               | 0.00                         | 9.71                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Fang Feng**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50261-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Fang Feng; Saposhnikovia 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G217H0728421 | 61446     | 40      | from supplier |
| PhytoComm | Fang Feng | G217H0728521 | 61657     | 40      | from supplier |
| PhytoComm | Fang Feng | G217H0728521 | 62053     | 40      | from supplier |
| PhytoComm | Fang Feng | G217H0728521 | 62054     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Fang Feng*. These samples are listed above in the [calibration samples](#) section.
- 21 406 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 135 spectra of 4 reference samples from the substance/substance group *Fang Feng*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Fang Feng | G217H0728421 | 61154              | 75      |
| PhytoComm | Fang Feng | G217H0728521 | 61657 <sup>†</sup> | 20      |
| PhytoComm | Fang Feng | G217H0728521 | 62053 <sup>†</sup> | 20      |
| PhytoComm | Fang Feng | G217H0728521 | 62054 <sup>†</sup> | 20      |

- 13 918 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 19 spectra from 9 *Apo-Ident* customers from 8 batches from the substance/substance group *Fang Feng*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Fang Feng | G217H0728521 | 3       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Fang Feng | G217H0728521 | 2       |
| Phytocomm | Fang Feng | G217H0728221 | 1       |
| Phytocomm | Fang Feng | g217h0728221 | 1       |
| PhytoComm | Fang Feng | G217H0728221 | 1       |
| Phytocomm | Fang Feng | G217H0728923 | 4       |
| PhytoComm | Fang Feng | G217H0728923 | 1       |
| Phytocomm | Fang Feng | g217h0728923 | 1       |
| Phytocomm | Fang Feng | G217H728923  | 1       |
| Phytocomm | Fang Feng | G21H0728923  | 1       |
| phytocomm | Fang Feng | H0728922     | 1       |
| Phytocomm | Fang Feng | H0728922     | 1       |
| phythocom | Fang Feng | G217H0728923 | 1       |

- 1962 spectra from 16 *Apo-Ident* customers from a total of 956 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 134           | 1              | 13 918        |
| <b>Type C</b> | 37             | 5             | 14             | 1925          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 99.2593 % (> 97.0370 %)  |
| <b>Type C</b> | 98.6709 % (> 98.3913 %)  | n/a (n/a)                |

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

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

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

### Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61446     | 61446               | 0.00                         | 7.89                            |
| 61657     | 61657               | 0.00                         | 6.86                            |
| 62053     | 62053               | 0.00                         | 8.04                            |
| 62054     | 62054               | 0.00                         | 8.19                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Fo Shou**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60119-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Fo Shou*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Fo Shou   | G307HS159PM1 | 61865     | 40      | from supplier |
| PhytoComm | Fo Shou   | G307HS159PM1 | 61866     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Fo Shou   | G307HS159PM1 | 61865 <sup>†</sup> | 20      |
| PhytoComm | Fo Shou   | G307HS159PM1 | 61866 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| phytocomm | Fo Shou   | 44503        | 1       |
| Phytocomm | Fo Shou   | G307H0888321 | 1       |
| phytocomm | Fo Shou   | H0888021     | 1       |
| PhytoComm | Fo Shou   | H0888021     | 1       |

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



- 1977 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 4              | 1977          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4424 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61865     | 61865               | 0.00                         | 8.71                            |
| 61866     | 61866               | 0.00                         | 9.21                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Fu Ling**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50260-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G200H1019522 | 61675     | 40      | from supplier |
| PhytoComm | Fu Ling   | G200HS211    | 61869     | 40      | from supplier |
| PhytoComm | Fu Ling   | G200HS211    | 61870     | 40      | from supplier |
| PhytoComm | Fu Ling   | G200H1019622 | 61961     | 40      | from supplier |
| PhytoComm | Fu Ling   | G200H1019622 | 61962     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Fu Ling*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 100 spectra of 5 reference samples from the substance/substance group *Fu Ling*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Fu Ling   | G200H1019522 | 61675 <sup>†</sup> | 20      |
| PhytoComm | Fu Ling   | G200HS211    | 61869 <sup>†</sup> | 20      |
| PhytoComm | Fu Ling   | G200HS211    | 61870 <sup>†</sup> | 20      |
| PhytoComm | Fu Ling   | G200H1019622 | 61961 <sup>†</sup> | 20      |
| PhytoComm | Fu Ling   | G200H1019622 | 61962 <sup>†</sup> | 20      |

- 13 953 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 18 spectra from 11 *Apo-Ident* customers from 5 batches from the substance/substance group *Fu Ling*.

<sup>†</sup>These spectra were recorded from 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  | Fu Ling   | 421001902    | 1       |
| Phyto Comm | Fu Ling   | G200H1019522 | 1       |
| Phytocomm  | Fu Ling   | G200H1019522 | 2       |
| PhytoComm  | Fu Ling   | G200H1019522 | 1       |
| PhytoComm  | Fu Ling   | G200H1019221 | 3       |
| Phytocomm  | Fu Ling   | G200H1019221 | 4       |
| Phytocomm  | Fu Ling   | G200H1019321 | 1       |
| PhytoComm  | Fu Ling   | G200H1019321 | 2       |
| Phytocomm  | Fu Ling   | g200h1019321 | 3       |

- 1963 spectra from 15 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

### Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 200           | 0              | 21 366        |
| <b>Type B</b> | 0              | 100           | 0              | 13 953        |
| <b>Type C</b> | 7              | 17            | 1              | 1956          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 94.0000 %) |
| <b>Type C</b> | 99.7130 % (> 99.4334 %)  | n/a (n/a)                |

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

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

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

### Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61675     | 61675               | 0.00                         | 13.85                           |
| 61869     | 61869               | 0.00                         | 10.04                           |
| 61870     | 61870               | 0.00                         | 10.21                           |
| 61961     | 61961               | 0.00                         | 12.47                           |
| 61962     | 61962               | 0.00                         | 12.20                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Fu Pen Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60044-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Fu Pen Zi; Rubi chingii fructus

### Special notes

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

*no information*

### Applicable documents

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

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Fu Pen Zi*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Fu Pen Zi | G213H1813422 | 61449     | 40      | from supplier |
| PhytoComm | Fu Pen Zi | G213H1813621 | 61780     | 40      | from supplier |
| PhytoComm | Fu Pen Zi | G213H1813621 | 61803     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Fu Pen Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 115 spectra of 3 reference samples from the substance/substance group *Fu Pen Zi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Fu Pen Zi | G213H1813422 | 61157              | 75      |
| PhytoComm | Fu Pen Zi | G213H1813621 | 61780 <sup>†</sup> | 20      |
| PhytoComm | Fu Pen Zi | G213H1813621 | 61803 <sup>†</sup> | 20      |

- 13 938 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Fu Pen Zi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Fu Pen Zi | g213h1813122 | 1       |
| Phytocomm | Fu Pen Zi | G213H1813122 | 1       |
| PhytoComm | Fu Pen Zi | H1813021     | 1       |

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



- 1978 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 115           | 0              | 13 938        |
| <b>Type C</b> | 3              | 1             | 2              | 1975          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 94.7826 %) |
| <b>Type C</b> | 99.8756 % (> 99.5972 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61449     | 61449               | 0.00                         | 11.06                           |
| 61780     | 61780               | 0.00                         | 16.86                           |
| 61803     | 61803               | 0.00                         | 15.41                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Fu Shen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60004-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G201HS212 | 61638     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Fu Shen*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 20 spectra of 1 reference samples from the substance/substance group *Fu Shen*.

| Supplier  | Substance | Batch     | Sample ID          | Spectra |
|-----------|-----------|-----------|--------------------|---------|
| PhytoComm | Fu Shen   | G201HS212 | 61638 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 8 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Fu Shen*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| PhytoComm | Fu Shen   | G201F110526  | 1       |
| Phytocomm | Fu Shen   | G201H1021422 | 2       |
| Phytocomm | Fu Shen   | G201H1021321 | 2       |
| Phytocomm | Fu Shen   | G201F110526  | 1       |
| Phytocomm | Fu Shen   | g201h1021321 | 1       |
| phythocom | Fu Shen   | G201H1021321 | 1       |

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

- 1973 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Fu 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 1              | 40            | 0              | 21 525        |
| <b>Type B</b> | 2              | 18            | 2              | 14 031        |
| <b>Type C</b> | 0              | 0             | 8              | 1973          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 99.9939 % (> 99.9746 %)  | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 99.9757 % (> 99.9415 %)  | 90.0000 % (> 75.0000 %)  |
| <b>Type C</b> | 100.0000 % (> 99.4414 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61638     | 61638               | 0.00                         | 4.28                            |

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



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Fu Xiao Mai**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60081-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G244H1078421 | 61428     | 40      | from supplier |
| PhytoComm | Fu Xiao Mai | G244HS0210V1 | 61855     | 40      | from supplier |
| PhytoComm | Fu Xiao Mai | G244HS0210V1 | 61856     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Fu Xiao Mai*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 115 spectra of 3 reference samples from the substance/substance group *Fu Xiao Mai*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Fu Xiao Mai | G244H1078421 | 61136              | 75      |
| PhytoComm | Fu Xiao Mai | G244HS0210V1 | 61855 <sup>†</sup> | 20      |
| PhytoComm | Fu Xiao Mai | G244HS0210V1 | 61856 <sup>†</sup> | 20      |

- 13 938 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Fu Xiao Mai*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| Phytocomm | Fu Xiao Mai | G244H1078121 | 1       |
| Phytocomm | Fu Xiao Mai | H1078021     | 1       |
| phytocomm | Fu Xiao Mai | H1078021     | 1       |

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



- 1978 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 115           | 0              | 13 938        |
| <b>Type C</b> | 0              | 0             | 3              | 1978          |

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

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 94.7826 %) |
| <b>Type C</b> | 100.0000 % (> 99.4431 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61428     | 61428               | 0.00                         | 16.26                           |
| 61855     | 61855               | 0.00                         | 8.46                            |
| 61856     | 61856               | 0.00                         | 6.04                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Fu Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50884-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Fu Zi; Aconiti lateralis radix praeparata; Aconiti radix lateralis praep.

### Special notes

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

*no information*

### Applicable documents

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

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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     | G005H0801123 | 61342     | 40      | from supplier |
| PhytoComm | Fu Zi     | G005H0801123 | 61621     | 40      | from supplier |
| PhytoComm | Fu Zi     | G005H0801524 | 61728     | 40      | from supplier |
| PhytoComm | Fu Zi     | G005H0801524 | 62071     | 40      | from supplier |
| PhytoComm | Fu Zi     | G005H0801524 | 62072     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

**Type A** All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Fu Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 155 spectra of 5 reference samples from the substance/substance group *Fu Zi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Fu Zi     | G005H0801123 | 61330              | 75      |
| PhytoComm | Fu Zi     | G005H0801123 | 61342 <sup>†</sup> | 20      |
| PhytoComm | Fu Zi     | G005H0801524 | 61728 <sup>†</sup> | 20      |
| PhytoComm | Fu Zi     | G005H0801524 | 62071 <sup>†</sup> | 20      |
| PhytoComm | Fu Zi     | G005H0801524 | 62072 <sup>†</sup> | 20      |

- 13 898 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 13 spectra from 7 *Apo-Ident* customers from 7 batches from the substance/substance group *Fu Zi*.

<sup>†</sup>These spectra were recorded from 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 |
|-----------|-----------|--------------|---------|
| phythocom | Fu Zi     | goo5h0801122 | 1       |
| Phytocomm | Fu Zi     | 161213fz     | 1       |
| Phytocomm | Fu Zi     | G005H0801524 | 1       |
| Phytocomm | Fu Zi     | G005H0801122 | 6       |
| PhytoComm | Fu Zi     | G005H0801122 | 1       |
| Phytocomm | Fu Zi     | g005h0801122 | 1       |
| Phytocomm | Fu Zi     | G005H0801322 | 1       |
| phytocomm | Fu Zi     | g005h0801322 | 1       |

- 1968 spectra from 16 *Apo-Ident* customers from a total of 957 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 1              | 200           | 0              | 21 365        |
| <b>Type B</b> | 0              | 155           | 0              | 13 898        |
| <b>Type C</b> | 2              | 2             | 11             | 1966          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 99.9877 % (> 99.9683 %)  | 100.0000 % (> 97.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 100.0000 % (> 96.1290 %) |
| <b>Type C</b> | 99.7388 % (> 99.4593 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61342     | 61342               | 0.00                         | 8.43                            |
| 61621     | 61621               | 0.00                         | 6.97                            |
| 61728     | 61728               | 0.00                         | 9.49                            |
| 62071     | 62071               | 0.00                         | 11.94                           |
| 62072     | 62072               | 0.00                         | 12.15                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Gan Cao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60011-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G119H0521522 | 61656     | 40      | from supplier |
| PhytoComm | Gan Cao   | G119H0521524 | 61977     | 40      | from supplier |
| PhytoComm | Gan Cao   | G119H0521524 | 61978     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Gan Cao*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 60 spectra of 3 reference samples from the substance/substance group *Gan Cao*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Gan Cao   | G119H0521522 | 61656 <sup>†</sup> | 20      |
| PhytoComm | Gan Cao   | G119H0521524 | 61977 <sup>†</sup> | 20      |
| PhytoComm | Gan Cao   | G119H0521524 | 61978 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 13 spectra from 8 *Apo-Ident* customers from 4 batches from the substance/substance group *Gan Cao*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Gan Cao   | G119H0521522 | 7       |
| Phytocomm | Gan Cao   | G119H0521121 | 3       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | 1       |
| PhytoComm | Gan Cao   | H0521923     | 1       |

- 1968 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 0              | 7             | 6              | 1968          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4410 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61656     | 61656               | 0.00                         | 16.86                           |
| 61977     | 61977               | 0.00                         | 15.73                           |
| 61978     | 61978               | 0.00                         | 15.96                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Gan Jiang**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60077-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G252H1145521 | 61743     | 40      | from supplier |
| PhytoComm | Gan Jiang | G252H1145621 | 61895     | 40      | from supplier |
| PhytoComm | Gan Jiang | G252H1145621 | 61896     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Gan Jiang*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 60 spectra of 3 reference samples from the substance/substance group *Gan Jiang*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Gan Jiang | G252H1145521 | 61743 <sup>†</sup> | 20      |
| PhytoComm | Gan Jiang | G252H1145621 | 61895 <sup>†</sup> | 20      |
| PhytoComm | Gan Jiang | G252H1145621 | 61896 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 8 *Apo-Ident* customers from 7 batches from the substance/substance group *Gan Jiang*.

| Supplier  | Substance | Batch         | Spectra |
|-----------|-----------|---------------|---------|
| Phytocomm | Gan Jiang | g252h01145221 | 1       |
| Phytocomm | Gan Jiang | G252H1145521  | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 Jiang | G252H1145221 | 1       |
| Caelo     | Gan Jiang | G252H1145221 | 1       |
| Phytocomm | Gan Jiang | G252H1145221 | 2       |
| Phytocomm | Gan Jiang | H1145021     | 1       |
| PhytoComm | Gan Jiang | H1145021     | 1       |
| phythocom | Gan Jiang | G252H1145221 | 1       |
| phythocom | Gan Jiang | 252h1145021  | 1       |
| phythocom | Gan Jiang | G25H1145221  | 1       |
| phythocom | Gan Jiang | g252h1145221 | 1       |

- 1969 spectra from 16 *Apo-Ident* customers from a total of 957 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 119           | 1              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 6              | 1             | 11             | 1963          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 99.1667 % (> 96.6667 %)  |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.7550 % (> 99.4755 %)  | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61743     | 61743               | 0.00                         | 4.74                            |
| 61895     | 61895               | 0.00                         | 6.28                            |
| 61896     | 61896               | 0.00                         | 6.91                            |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ge Gen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60050-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G206H1301422 | 61086     | 40      | from supplier |
| PhytoComm | Ge Gen    | G206H1301422 | 61457     | 40      | from supplier |
| PhytoComm | Ge Gen    | G206H1301621 | 61949     | 40      | from supplier |
| PhytoComm | Ge Gen    | G206H1301621 | 61950     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 406 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 135 spectra of 4 reference samples from the substance/substance group *Ge Gen*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Ge Gen    | G206H1301422 | 61086 <sup>†</sup> | 20      |
| PhytoComm | Ge Gen    | G206H1301422 | 61165              | 75      |
| PhytoComm | Ge Gen    | G206H1301621 | 61949 <sup>†</sup> | 20      |
| PhytoComm | Ge Gen    | G206H1301621 | 61950 <sup>†</sup> | 20      |

- 13 918 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 9 spectra from 7 *Apo-Ident* customers from 4 batches from the substance/substance group *Ge Gen*.

| Supplier  | Substance | Batch    | Spectra |
|-----------|-----------|----------|---------|
| Phytocomm | Ge Gen    | 161213gg | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Ge Gen    | G206H1301422 | 2       |
| phytocomm | Ge Gen    | FA1301902    | 1       |
| PhytoComm | Ge Gen    | FA1301902    | 3       |
| Phytocomm | Ge Gen    | G206H1301221 | 2       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 135           | 0              | 13 918        |
| <b>Type C</b> | 0              | 2             | 7              | 1972          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.5556 %) |
| <b>Type C</b> | 100.0000 % (> 99.4413 %) | n/a (n/a)                |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61086     | 61086               | 0.00                         | 16.00                           |
| 61457     | 61457               | 0.00                         | 17.61                           |
| 61949     | 61949               | 0.00                         | 25.72                           |
| 61950     | 61950               | 0.00                         | 27.24                           |

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

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Gou Qi Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60094-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

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

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G150H0913422 | 61383     | 40      | from supplier |
| PhytoComm | Gou Qi Zi | G150H0913621 | 61840     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Gou Qi Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Gou Qi Zi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Gou Qi Zi | G150H0913422 | 61383 <sup>†</sup> | 20      |
| PhytoComm | Gou Qi Zi | G150H0913621 | 61840 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 6 batches from the substance/substance group *Gou Qi Zi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Gou Qi Zi | G150H0913422 | 3       |
| PhytoComm | Gou Qi Zi | G150H0913023 | 2       |
| phytocomm | Gou Qi Zi | G150H0913023 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Gou Qi Zi | G150H0913121 | 1       |
| PhytoComm | Gou Qi Zi | G150H0913121 | 1       |
| PhytoComm | Gou Qi Zi | G150H0913221 | 2       |
| PhytoComm | Gou Qi Zi | G150H0913123 | 1       |
| PhytoComm | Gou Qi Zi | g150h0913221 | 1       |

- 1969 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

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

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 1              | 79            | 1              | 21 485        |
| <b>Type B</b> | 1              | 32            | 8              | 14 012        |
| <b>Type C</b> | 11             | 3             | 9              | 1958          |

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        |
|---------------|-------------------------|-------------------------|
| <b>Type A</b> | 99.9877 % (> 99.9684 %) | 98.7500 % (> 95.0000 %) |
| <b>Type B</b> | 99.9964 % (> 99.9620 %) | 80.0000 % (> 72.5000 %) |
| <b>Type C</b> | 99.4861 % (> 99.2066 %) | n/a (n/a)               |

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

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

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

## Identity according to identity test using NIR spectroscopy

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

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61383     | 61383               | 0.00                         | 7.89                            |
| 61840     | 61840               | 0.00                         | 4.74                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Gou Teng**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60097-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G247H1210621 | 61798     | 40      | from supplier |
| PhytoComm | Gou Teng  | G247H1210621 | 61811     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Gou Teng*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Gou Teng*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Gou Teng  | G247H1210621 | 61798 <sup>†</sup> | 20      |
| PhytoComm | Gou Teng  | G247H1210621 | 61811 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Gou Teng*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Gou Teng  | G247H1210422 | 2       |
| Phytocomm | Gou Teng  | 612gt        | 1       |
| Phytocomm | Gou Teng  | G247H1210122 | 3       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Gou Teng  | G247H1210122 | 1       |
| PhytoComm | Gou Teng  | g247h1210122 | 1       |
| PhytoComm | Gou Teng  | H1210021     | 1       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Gou 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 1              | 0             | 9              | 1971          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.9751 % (> 99.6958 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61798     | 61798               | 0.00                         | 18.76                           |
| 61811     | 61811               | 0.00                         | 18.54                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Gu Sui Bu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60225-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Gu Sui Bu; Drynariae rhizoma

### Special notes

When selecting the *Gu Sui Bu* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Gu Sui Bu*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Gu Sui Bu | G094H1011422 | 61350     | 40      | from supplier |
| PhytoComm | Gu Sui Bu | G094H1011522 | 61714     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Gu Sui Bu*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Gu Sui Bu*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Gu Sui Bu | G094H1011422 | 61350 <sup>†</sup> | 20      |
| PhytoComm | Gu Sui Bu | G094H1011522 | 61714 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 *Gu Sui Bu*.

| Supplier  | Substance | Batch          | Spectra |
|-----------|-----------|----------------|---------|
| PhytoComm | Gu Sui Bu | (G094)H1011221 | 1       |
| PhytoComm | Gu Sui Bu | G094H1011023   | 2       |
| Phytocomm | Gu Sui Bu | G094H1011023   | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Gu Sui Bu | g094h1011023 | 1       |
| Phytocomm | Gu Sui Bu | G094H1011221 | 2       |
| Phytocomm | Gu Sui Bu | g094h1011221 | 1       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Gu Sui Bu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gu Sui Bu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 14             | 0             | 8              | 1959          |

The substance/substance group *Gu Sui Bu* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.3363 % (> 99.0570 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61350     | 61350               | 0.00                         | 8.08                            |
| 61714     | 61714               | 0.00                         | 19.72                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Gua Lou**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60128-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Gua Lou*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Gua Lou   | G241H1096521 | 61379     | 40      | from supplier |
| PhytoComm | Gua Lou   | G241H1096523 | 61787     | 40      | from supplier |
| PhytoComm | Gua Lou   | G241H1096523 | 61801     | 40      | from supplier |
| PhytoComm | Gua Lou   | G241H1096523 | 61877     | 40      | from supplier |
| PhytoComm | Gua Lou   | G241H1096523 | 61878     | 29      | from supplier |
| PhytoComm | Gua Lou   | G241H1096621 | 61913     | 40      | from supplier |
| PhytoComm | Gua Lou   | G241H1096621 | 61914     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 269 spectra of 7 reference samples from the substance/substance group *Gua Lou*. These samples are listed above in the [calibration samples](#) section.
- 21 297 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 139 spectra of 7 reference samples from the substance/substance group *Gua Lou*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Gua Lou   | G241H1096521 | 61379 <sup>†</sup> | 20      |
| PhytoComm | Gua Lou   | G241H1096523 | 61787 <sup>†</sup> | 20      |
| PhytoComm | Gua Lou   | G241H1096523 | 61801 <sup>†</sup> | 20      |
| PhytoComm | Gua Lou   | G241H1096523 | 61877 <sup>†</sup> | 19      |
| PhytoComm | Gua Lou   | G241H1096523 | 61878 <sup>†</sup> | 20      |
| PhytoComm | Gua Lou   | G241H1096621 | 61913 <sup>†</sup> | 20      |
| PhytoComm | Gua Lou   | G241H1096621 | 61914 <sup>†</sup> | 20      |

- 13 914 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Gua Lou*.

<sup>†</sup>These spectra were recorded from 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   | G241H1096521 | 1       |
| PhytoComm | Gua Lou   | G241H1096121 | 2       |
| phytocomm | Gua Lou   | G241H1096121 | 1       |
| Phytocomm | Gua Lou   | G241H1096121 | 1       |
| Phytocomm | Gua Lou   | G241H1096321 | 1       |
| PhytoComm | Gua Lou   | G241H1096321 | 1       |
| Phytocomm | Gua Lou   | g241h1096321 | 1       |
| PhytoComm | Gua Lou   | G241H1096322 | 2       |
| Phytocomm | Gua Lou   | H1096922     | 1       |

- 1970 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Gua Lou* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gua Lou* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 269           | 0              | 21 297        |
| <b>Type B</b> | 1              | 139           | 0              | 13 913        |
| <b>Type C</b> | 1              | 5             | 6              | 1969          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.7695 %) |
| <b>Type B</b> | 99.9757 % (> 99.9412 %)  | 100.0000 % (> 95.6835 %) |
| <b>Type C</b> | 99.9733 % (> 99.6939 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61379     | 61379               | 0.00                         | 14.25                           |
| 61787     | 61787               | 0.00                         | 12.21                           |
| 61801     | 61801               | 0.00                         | 12.10                           |
| 61877     | 61877               | 0.00                         | 11.31                           |
| 61878     | 61878               | 0.00                         | 11.57                           |
| 61913     | 61913               | 0.00                         | 8.92                            |
| 61914     | 61914               | 0.00                         | 8.60                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Gua Lou Ren**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60052-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Gua Lou Ren; Trichosanthis semen

### Special notes

When selecting the *Gua Lou Ren* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Gua Lou Ren*:

| Supplier  | Substance   | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-------------|--------------|-----------|---------|---------------|
| PhytoComm | Gua Lou Ren | G243H1095421 | 61041     | 50      | from supplier |
| PhytoComm | Gua Lou Ren | G243H1095421 | 61424     | 40      | from supplier |
| PhytoComm | Gua Lou Ren | G243H1095621 | 61775     | 40      | from supplier |
| PhytoComm | Gua Lou Ren | G243H1095621 | 61809     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 170 spectra of 4 reference samples from the substance/substance group *Gua Lou Ren*. These samples are listed above in the [calibration samples](#) section.
- 21 396 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 125 spectra of 4 reference samples from the substance/substance group *Gua Lou Ren*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Gua Lou Ren | G243H1095421 | 61041 <sup>†</sup> | 10      |
| PhytoComm | Gua Lou Ren | G243H1095421 | 61132              | 75      |
| PhytoComm | Gua Lou Ren | G243H1095621 | 61775 <sup>†</sup> | 20      |
| PhytoComm | Gua Lou Ren | G243H1095621 | 61809 <sup>†</sup> | 20      |

- 13 928 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Gua Lou Ren*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| Phytocomm | Gua Lou Ren | G243H1095123 | 1       |
| Phytocomm | Gua Lou Ren | g243h1095123 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1979 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Gua Lou Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gua Lou Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 170           | 0              | 21 396        |
| <b>Type B</b> | 0              | 125           | 0              | 13 928        |
| <b>Type C</b> | 3              | 0             | 2              | 1976          |

The substance/substance group *Gua Lou 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.4706 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.2000 %) |
| <b>Type C</b> | 99.8728 % (> 99.5951 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61041     | 61041               | 0.00                         | 11.09                           |
| 61424     | 61424               | 0.00                         | 11.01                           |
| 61775     | 61775               | 0.00                         | 13.06                           |
| 61809     | 61809               | 0.00                         | 13.01                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Guang Huo Xiang**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 61079-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G007H2005521 | 61709     | 40      | from supplier |
| PhytoComm | Guang Huo Xiang | G007H2005621 | 62037     | 40      | from supplier |
| PhytoComm | Guang Huo Xiang | G007H2005621 | 62038     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Guang Huo Xiang*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Guang Huo Xiang*.

| Supplier  | Substance       | Batch        | Sample ID          | Spectra |
|-----------|-----------------|--------------|--------------------|---------|
| PhytoComm | Guang Huo Xiang | G007H2005521 | 61709 <sup>†</sup> | 20      |
| PhytoComm | Guang Huo Xiang | G007H2005621 | 62037 <sup>†</sup> | 20      |
| PhytoComm | Guang Huo Xiang | G007H2005621 | 62038 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1979 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Guang Huo Xiang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Guang Huo Xiang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 0              | 2             | 0              | 1979          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4445 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61709     | 61709               | 0.00                         | 9.56                            |
| 62037     | 62037               | 0.00                         | 20.52                           |
| 62038     | 62038               | 0.00                         | 20.79                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Gui Ban Jiao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60126-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Gui Ban Jiao; Colla carapax et plastrum chrysemys

### Special notes

When selecting the *Gui Ban Jiao* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Gui Ban Jiao*:

| Supplier  | Substance    | Batch        | Sample ID | Spectra | Certificate   |
|-----------|--------------|--------------|-----------|---------|---------------|
| PhytoComm | Gui Ban Jiao | G326HS3300V1 | 61725     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

## Type A All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Gui Ban Jiao*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Gui Ban Jiao*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Gui Ban Jiao | G326HS3300V1 | 61725 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Gui Ban Jiao*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| PhytoComm | Gui Ban Jiao | G326H2205221 | 1       |

- 1980 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the

<sup>†</sup>These spectra were recorded from 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 *Gui Ban Jiao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gui Ban Jiao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 1              | 1980          |

The substance/substance group *Gui Ban Jiao* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4487 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61725     | 61725               | 0.00                         | 21.16                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Gui Zhi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60189-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G070H1001422 | 61057     | 40      | from supplier |
| PhytoComm | Gui Zhi   | G070H1001422 | 61570     | 40      | from supplier |
| PhytoComm | Gui Zhi   | G070H1001523 | 61698     | 40      | from supplier |
| PhytoComm | Gui Zhi   | G070H1001621 | 61777     | 40      | from supplier |
| PhytoComm | Gui Zhi   | G070H1001621 | 61815     | 40      | from supplier |
| PhytoComm | Gui Zhi   | G070H1001621 | 61873     | 40      | from supplier |
| PhytoComm | Gui Zhi   | G070H1001621 | 61874     | 40      | from supplier |
| PhytoComm | Gui Zhi   | G070H1001621 | 62065     | 40      | from supplier |
| PhytoComm | Gui Zhi   | G070H1001621 | 62066     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

**Type A** All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Gui Zhi*. These samples are listed above in the [calibration samples](#) section.
- 21 206 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 235 spectra of 9 reference samples from the substance/substance group *Gui Zhi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Gui Zhi   | G070H1001422 | 61057 <sup>†</sup> | 20      |
| PhytoComm | Gui Zhi   | G070H1001422 | 61279              | 75      |
| PhytoComm | Gui Zhi   | G070H1001523 | 61698 <sup>†</sup> | 20      |
| PhytoComm | Gui Zhi   | G070H1001621 | 61777 <sup>†</sup> | 20      |
| PhytoComm | Gui Zhi   | G070H1001621 | 61815 <sup>†</sup> | 20      |
| PhytoComm | Gui Zhi   | G070H1001621 | 61873 <sup>†</sup> | 20      |
| PhytoComm | Gui Zhi   | G070H1001621 | 61874 <sup>†</sup> | 20      |
| PhytoComm | Gui Zhi   | G070H1001621 | 62065 <sup>†</sup> | 20      |
| PhytoComm | Gui Zhi   | G070H1001621 | 62066 <sup>†</sup> | 20      |

- 13 818 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 15 spectra from 8 *Apo-Ident* customers from 5 batches from the substance/substance group *Gui Zhi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Gui Zhi   | G070H1001523 | 2       |
| PhytoComm | Gui Zhi   | G070H1001221 | 1       |
| Phytocomm | Gui Zhi   | G070H1001221 | 2       |
| Phytocomm | Gui Zhi   | g070h1001422 | 1       |
| Phytocomm | Gui Zhi   | G070H100422  | 1       |
| PhytoComm | Gui Zhi   | H1001022     | 3       |
| Phytocomm | Gui Zhi   | H1001022     | 5       |

- 1966 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Gui Zhi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gui Zhi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 360           | 0              | 21 206        |
| <b>Type B</b> | 0              | 235           | 0              | 13 818        |
| <b>Type C</b> | 8              | 4             | 11             | 1958          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 98.3333 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 100.0000 % (> 97.4468 %) |
| <b>Type C</b> | 99.4362 % (> 99.1566 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

### Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61057     | 61057               | 0.00                         | 9.68                            |
| 61570     | 61570               | 0.00                         | 10.84                           |
| 61698     | 61698               | 0.00                         | 10.03                           |
| 61777     | 61777               | 0.00                         | 8.35                            |
| 61815     | 61815               | 0.00                         | 9.84                            |
| 61873     | 61873               | 0.00                         | 9.32                            |
| 61874     | 61874               | 0.00                         | 9.35                            |
| 62065     | 62065               | 0.00                         | 10.61                           |
| 62066     | 62066               | 0.00                         | 10.63                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **He Huan Pi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60175-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

He Huan Pi; Albiziae cortex; Albiziae julibrissini cortex

### Special notes

When selecting the *He Huan Pi* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G010H0635523 | 61795     | 40      | from supplier |
| PhytoComm | He Huan Pi | G010H0635523 | 61816     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *He Huan Pi*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *He Huan Pi*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | He Huan Pi | G010H0635523 | 61795 <sup>†</sup> | 20      |
| PhytoComm | He Huan Pi | G010H0635523 | 61816 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 *He Huan Pi*.

| Supplier  | Substance  | Batch        | Spectra |
|-----------|------------|--------------|---------|
| Phytocomm | He Huan Pi | G010H0635221 | 1       |
| PhytoComm | He Huan Pi | G010H0635221 | 2       |
| Phytocomm | He Huan Pi | g010h0635221 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | He Huan Pi | G010H0635321 | 1       |
| PhytoComm | He Huan Pi | H0635021     | 2       |
| Phytocomm | He Huan Pi | G010H0635423 | 1       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *He Huan Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *He Huan Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 1              | 1             | 7              | 1972          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.9627 % (> 99.6834 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61795     | 61795               | 0.00                         | 11.65                           |
| 61816     | 61816               | 0.00                         | 11.87                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **He Shou Wu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60101-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G198H0718421 | 61463     | 40      | from supplier |
| PhytoComm | He Shou Wu | G198H0718421 | 62059     | 40      | from supplier |
| PhytoComm | He Shou Wu | G198H0718421 | 62060     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *He Shou Wu*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 115 spectra of 3 reference samples from the substance/substance group *He Shou Wu*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | He Shou Wu | G198H0718421 | 61171              | 75      |
| PhytoComm | He Shou Wu | G198H0718421 | 62059 <sup>†</sup> | 20      |
| PhytoComm | He Shou Wu | G198H0718421 | 62060 <sup>†</sup> | 20      |

- 13 938 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 8 *Apo-Ident* customers from 5 batches from the substance/substance group *He Shou Wu*.

| Supplier  | Substance  | Batch          | Spectra |
|-----------|------------|----------------|---------|
| PhytoComm | He Shou Wu | (G198)H0718222 | 1       |
| Phytocomm | He Shou Wu | g198h0718222   | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | He Shou Wu | G198H0718222 | 1       |
| PhytoComm | He Shou Wu | G198H0718222 | 1       |
| Phytocomm | He Shou Wu | G198H0718421 | 2       |
| Phytocomm | He Shou Wu | H0718021     | 1       |
| PhytoComm | He Shou Wu | G198H0718421 | 1       |
| PhytoComm | He Shou Wu | H0718021     | 1       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *He 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 106           | 9              | 13 938        |
| <b>Type C</b> | 3              | 3             | 6              | 1969          |

The substance/substance group *He Shou Wu* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 92.1739 % (> 89.5652 %)  |
| <b>Type C</b> | 99.9097 % (> 99.6303 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61463     | 61463               | 0.00                         | 7.85                            |
| 62059     | 62059               | 0.00                         | 7.27                            |
| 62060     | 62060               | 0.00                         | 7.32                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **He Ye**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60512-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

He Ye; Nelumbinis nuciferae folium

### Special notes

When selecting the *He 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Ye*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | He Ye     | G170H1170521 | 61646     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *He Ye*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *He Ye*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | He Ye     | G170H1170521 | 61646 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *He Ye*.

| Supplier  | Substance | Batch    | Spectra |
|-----------|-----------|----------|---------|
| PhytoComm | He Ye     | H1170922 | 1       |

- 1980 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the

<sup>†</sup>These spectra were recorded from 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 *He 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 *He 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 11             | 0             | 1              | 1969          |

The substance/substance group *He 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.4202 % (> 99.1445 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61646     | 61646               | 0.00                         | 6.54                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Hei Zhi Ma**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 61724-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Hei Zhi Ma; Sesami indicii semen; Sesami semen nigrum

### Special notes

When selecting the *Hei Zhi 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Hei Zhi Ma*:

| Supplier  | Substance  | Batch        | Sample ID | Spectra | Certificate   |
|-----------|------------|--------------|-----------|---------|---------------|
| PhytoComm | Hei Zhi Ma | G228H1178521 | 61724     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Hei Zhi Ma*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Hei Zhi Ma*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Hei Zhi Ma | G228H1178521 | 61724 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Hei Zhi Ma*.
- 1981 spectra from 16 *Apo-Ident* customers from a total of 964 batches from a further 268 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

### Validation results

The validation runs checked whether the substance/substance group *Hei Zhi Ma* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant

<sup>†</sup>These spectra were recorded from 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 *Hei Zhi 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 0              | 1981          |

The substance/substance group *Hei Zhi Ma* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4403 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

### Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61724     | 61724               | 0.00                         | 35.67                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Hong Hua**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60206-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G057H0901621 | 61768     | 40      | from supplier |
| PhytoComm | Hong Hua  | G057H0901621 | 61845     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Hong Hua*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Hong Hua  | G057H0901621 | 61768 <sup>†</sup> | 20      |
| PhytoComm | Hong Hua  | G057H0901621 | 61845 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Hong Hua*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| phythocom | Hong Hua  | g057h0901121 | 1       |
| Phytocomm | Hong Hua  | 41024032/2   | 1       |
| PhytoComm | Hong Hua  | G057H0901121 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Hong Hua  | G057H0901121 | 1       |
| Phytocomm | Hong Hua  | g057h0901121 | 1       |
| Phytocomm | Hong Hua  | G057H0901221 | 1       |
| PhytoComm | Hong Hua  | G057H0901221 | 1       |
| Phytocomm | Hong Hua  | G057H0901322 | 1       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Hong 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 5              | 2             | 7              | 1967          |

The substance/substance group *Hong 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.6642 % (> 99.3848 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61768     | 61768               | 0.00                         | 9.81                            |
| 61845     | 61845               | 0.00                         | 10.13                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Hong Jing Tian**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60031-2017-06-01  
Executing company HiperScan GmbH  
Weiskeritzstraße 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G237H0906421 | 61097     | 40      | from supplier |
| PhytoComm | Hong Jing Tian | G237H0906421 | 61430     | 40      | from supplier |
| PhytoComm | Hong Jing Tian | G237H0906621 | 61911     | 40      | from supplier |
| PhytoComm | Hong Jing Tian | G237H0906621 | 61912     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Hong Jing Tian*. These samples are listed above in the [calibration samples](#) section.
- 21 406 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 134 spectra of 4 reference samples from the substance/substance group *Hong Jing Tian*.

| Supplier  | Substance      | Batch        | Sample ID          | Spectra |
|-----------|----------------|--------------|--------------------|---------|
| PhytoComm | Hong Jing Tian | G237H0906421 | 61097 <sup>†</sup> | 19      |
| PhytoComm | Hong Jing Tian | G237H0906421 | 61138              | 75      |
| PhytoComm | Hong Jing Tian | G237H0906621 | 61911 <sup>†</sup> | 20      |
| PhytoComm | Hong Jing Tian | G237H0906621 | 61912 <sup>†</sup> | 20      |

- 13 919 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Hong Jing Tian*.

| Supplier  | Substance      | Batch        | Spectra |
|-----------|----------------|--------------|---------|
| PhytoComm | Hong Jing Tian | G237H0906221 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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   | Hong Jing Tian | G237H0906221 | 2       |
| Phytocomm   | Hong Jing Tian | G237H0906321 | 1       |
| Herbasinica | Hong Jing Tian | H0906021     | 1       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Hong Jing Tian* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hong Jing Tian* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 134           | 0              | 13 919        |
| <b>Type C</b> | 0              | 1             | 5              | 1975          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.5224 %) |
| <b>Type C</b> | 100.0000 % (> 99.4417 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61097     | 61097               | 0.00                         | 14.02                           |
| 61430     | 61430               | 0.00                         | 13.00                           |
| 61911     | 61911               | 0.00                         | 15.33                           |
| 61912     | 61912               | 0.00                         | 15.42                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Hou Po**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50289-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Hou Po*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Hou Po    | G154H0917423 | 61387     | 40      | from supplier |
| PhytoComm | Hou Po    | G154H0917421 | 61501     | 40      | from supplier |
| PhytoComm | Hou Po    | G154H0917521 | 61782     | 40      | from supplier |
| PhytoComm | Hou Po    | G154H0917521 | 61826     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 406 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 160 spectra of 4 reference samples from the substance/substance group *Hou Po*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Hou Po    | G154H0917421 | 61209              | 100     |
| PhytoComm | Hou Po    | G154H0917423 | 61387 <sup>†</sup> | 20      |
| PhytoComm | Hou Po    | G154H0917521 | 61782 <sup>†</sup> | 20      |
| PhytoComm | Hou Po    | G154H0917521 | 61826 <sup>†</sup> | 20      |

- 13 893 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 2 batches from the substance/substance group *Hou Po*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| PhytoComm | Hou Po    | G154H0917222 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Hou Po    | G154H0917222 | 1       |
| phytocomm | Hou Po    | H0917022     | 1       |
| PhytoComm | Hou Po    | H0917022     | 1       |
| Phytocomm | Hou Po    | H0917022     | 2       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Hou Po* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hou Po* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 160           | 0              | 13 893        |
| <b>Type C</b> | 10             | 2             | 4              | 1965          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 100.0000 % (> 96.2500 %) |
| <b>Type C</b> | 99.5854 % (> 99.3063 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61387     | 61387               | 0.00                         | 15.06                           |
| 61501     | 61501               | 0.00                         | 13.10                           |
| 61782     | 61782               | 0.00                         | 9.72                            |
| 61826     | 61826               | 0.00                         | 8.74                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Huai Hua**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60120-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Huai Hua; Sophorae japonicae flos

### Special notes

When selecting the *Huai Hua* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Huai Hua*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Huai Hua  | G263H1423421 | 61631     | 40      | from supplier |
| PhytoComm | Huai Hua  | G263H1423521 | 61891     | 40      | from supplier |
| PhytoComm | Huai Hua  | G263H1423521 | 61892     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Huai Hua*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Huai Hua*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Huai Hua  | G263H1423421 | 61631 <sup>†</sup> | 20      |
| PhytoComm | Huai Hua  | G263H1423521 | 61891 <sup>†</sup> | 20      |
| PhytoComm | Huai Hua  | G263H1423521 | 61892 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Huai Hua*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Huai Hua  | G263H1423421 | 1       |
| Phytocomm | Huai Hua  | G263H1423121 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Huai Hua  | G263H1423121 | 2       |
| PhytoComm | Huai Hua  | G263H143121  | 1       |
| phythocom | Huai Hua  | g263h1423121 | 1       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Huai Hua* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Huai Hua* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 2              | 1             | 5              | 1973          |

The substance/substance group *Huai Hua* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.7512 % (> 99.4721 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61631     | 61631               | 0.00                         | 19.13                           |
| 61891     | 61891               | 0.00                         | 22.50                           |
| 61892     | 61892               | 0.00                         | 22.21                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Huang Bo**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60057-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Huang Bo*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Huang Bo  | G188H1203622 | 61953     | 40      | from supplier |
| PhytoComm | Huang Bo  | G188H1203622 | 61954     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Huang Bo*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Huang Bo  | G188H1203622 | 61953 <sup>†</sup> | 20      |
| PhytoComm | Huang Bo  | G188H1203622 | 61954 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 9 *Apo-Ident* customers from 5 batches from the substance/substance group *Huang Bo*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| PhytoComm | Huang Bo  | G188H1203123 | 2       |
| Phytocomm | Huang Bo  | G188H1203321 | 4       |
| Phytocomm | Huang Bo  | 161213hb     | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 Bo  | G188H1203123 | 4       |
| Phytocomm | Huang Bo  | g188h1203123 | 1       |
| PhytoComm | Huang Bo  | G188H1203321 | 2       |
| Phytocomm | Huang Bo  | h1203022     | 1       |

- 1966 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Huang Bo* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Huang Bo* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 15             | 1966          |

The substance/substance group *Huang Bo* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4409 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61953     | 61953               | 0.00                         | 11.89                           |
| 61954     | 61954               | 0.00                         | 11.46                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Huang Jing**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60108-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G196H1206521 | 61746     | 40      | from supplier |
| PhytoComm | Huang Jing | G196H1206522 | 61951     | 40      | from supplier |
| PhytoComm | Huang Jing | G196H1206522 | 61952     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Huang Jing*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Huang Jing*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Huang Jing | G196H1206521 | 61746 <sup>†</sup> | 20      |
| PhytoComm | Huang Jing | G196H1206522 | 61951 <sup>†</sup> | 20      |
| PhytoComm | Huang Jing | G196H1206522 | 61952 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 Jing*.

| Supplier    | Substance  | Batch        | Spectra |
|-------------|------------|--------------|---------|
| ChinaMedica | Huang Jing | G196H1206121 | 1       |
| phytoComm   | Huang Jing | FA1206822    | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Huang Jing | G196H1206121 | 2       |
| PhytoComm | Huang Jing | G196H1206121 | 1       |
| Phytocomm | Huang Jing | g196h1206121 | 1       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Huang Jing* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Huang Jing* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 5              | 0             | 6              | 1970          |

The substance/substance group *Huang Jing* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.6212 % (> 99.3421 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61746     | 61746               | 0.00                         | 17.64                           |
| 61951     | 61951               | 0.00                         | 8.84                            |
| 61952     | 61952               | 0.00                         | 8.73                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Huang Lian**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60219-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G079H1205421 | 61045     | 40      | from supplier |
| PhytoComm | Huang Lian | G079H1205421 | 61523     | 40      | from supplier |
| PhytoComm | Huang Lian | G079H1205521 | 61729     | 40      | from supplier |
| PhytoComm | Huang Lian | G079H1205621 | 61776     | 40      | from supplier |
| PhytoComm | Huang Lian | G079H1205621 | 61819     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Huang Lian*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 155 spectra of 5 reference samples from the substance/substance group *Huang Lian*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Huang Lian | G079H1205421 | 61045 <sup>†</sup> | 20      |
| PhytoComm | Huang Lian | G079H1205421 | 61232              | 75      |
| PhytoComm | Huang Lian | G079H1205521 | 61729 <sup>†</sup> | 20      |
| PhytoComm | Huang Lian | G079H1205621 | 61776 <sup>†</sup> | 20      |
| PhytoComm | Huang Lian | G079H1205621 | 61819 <sup>†</sup> | 20      |

- 13 898 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 6 batches from the substance/substance group *Huang Lian*.

<sup>†</sup>These spectra were recorded from 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 | Huang Lian | FA1205702    | 1       |
| Phytocomm | Huang Lian | G079H1205321 | 2       |
| Phytocomm | Huang Lian | G079H1205021 | 1       |
| PhytoComm | Huang Lian | G079H1205321 | 2       |
| Phytocomm | Huang Lian | G079H1205521 | 2       |
| Phytocomm | Huang Lian | g079h1205321 | 1       |
| PhytoComm | Huang Lian | G079H1205521 | 2       |
| PhytoComm | Huang Lian | H1205021     | 2       |
| Phytocomm | Huang Lian | H1205021     | 1       |

- 1967 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Huang Lian* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Huang Lian* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 200           | 0              | 21 366        |
| <b>Type B</b> | 0              | 155           | 0              | 13 898        |
| <b>Type C</b> | 0              | 11            | 3              | 1967          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 100.0000 % (> 96.1290 %) |
| <b>Type C</b> | 100.0000 % (> 99.4409 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61045     | 61045               | 0.00                         | 39.01                           |
| 61523     | 61523               | 0.00                         | 37.09                           |
| 61729     | 61729               | 0.00                         | 39.86                           |
| 61776     | 61776               | 0.00                         | 39.63                           |
| 61819     | 61819               | 0.00                         | 39.61                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Huang Qi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60154-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G040H1202420 | 61595     | 40      | from supplier |
| PhytoComm | Huang Qi  | G040H1202621 | 61769     | 40      | from supplier |
| PhytoComm | Huang Qi  | G040H1202621 | 61824     | 40      | from supplier |
| PhytoComm | Huang Qi  | G040H1202621 | 62075     | 40      | from supplier |
| PhytoComm | Huang Qi  | G040H1202621 | 62076     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Huang Qi*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 155 spectra of 5 reference samples from the substance/substance group *Huang Qi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Huang Qi  | G040H1202420 | 61304              | 75      |
| PhytoComm | Huang Qi  | G040H1202621 | 61769 <sup>†</sup> | 20      |
| PhytoComm | Huang Qi  | G040H1202621 | 61824 <sup>†</sup> | 20      |
| PhytoComm | Huang Qi  | G040H1202621 | 62075 <sup>†</sup> | 20      |
| PhytoComm | Huang Qi  | G040H1202621 | 62076 <sup>†</sup> | 20      |

- 13 898 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 24 spectra from 8 *Apo-Ident* customers from 8 batches from the substance/substance group *Huang Qi*.

<sup>†</sup>These spectra were recorded from 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 | Huang Qi  | G040H1202423 | 1       |
| Phytocomm | Huang Qi  | G040H1202521 | 2       |
| PhytoComm | Huang Qi  | G040H1202621 | 1       |
| PhytoComm | Huang Qi  | G040H1202222 | 3       |
| Phytocomm | Huang Qi  | G040H1202222 | 5       |
| Phytocomm | Huang Qi  | G040H1202321 | 2       |
| Caelo     | Huang Qi  | g040h1202222 | 1       |
| PhytoComm | Huang Qi  | G040H1202321 | 2       |
| Phytocomm | Huang Qi  | g040h1202321 | 2       |
| PhytoComm | Huang Qi  | H1202021     | 1       |
| Phytocomm | Huang Qi  | H1202021     | 4       |

- 1957 spectra from 16 *Apo-Ident* customers from a total of 956 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Huang Qi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Huang Qi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 1              | 200           | 0              | 21 365        |
| <b>Type B</b> | 0              | 155           | 0              | 13 898        |
| <b>Type C</b> | 21             | 3             | 21             | 1936          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 99.9959 % (> 99.9765 %)  | 100.0000 % (> 97.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 100.0000 % (> 96.1290 %) |
| <b>Type C</b> | 99.2174 % (> 98.9378 %)  | 12.5000 % (≥ 0.0000 %)   |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61595     | 61595               | 0.00                         | 10.84                           |
| 61769     | 61769               | 0.00                         | 6.53                            |
| 61824     | 61824               | 0.00                         | 6.04                            |
| 62075     | 62075               | 0.00                         | 5.49                            |
| 62076     | 62076               | 0.00                         | 6.12                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Huang Qin**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60012-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G225H1204322 | 60930     | 35      | from supplier |
| PhytoComm | Huang Qin | G225H1204322 | 61440     | 40      | from supplier |
| PhytoComm | Huang Qin | G225H1204522 | 61669     | 40      | from supplier |
| PhytoComm | Huang Qin | G225H1204622 | 61919     | 40      | from supplier |
| PhytoComm | Huang Qin | G225H1204622 | 61920     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 195 spectra of 5 reference samples from the substance/substance group *Huang Qin*. These samples are listed above in the [calibration samples](#) section.
- 21 371 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 135 spectra of 4 reference samples from the substance/substance group *Huang Qin*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Huang Qin | G225H1204322 | 61148              | 75      |
| PhytoComm | Huang Qin | G225H1204522 | 61669 <sup>†</sup> | 20      |
| PhytoComm | Huang Qin | G225H1204622 | 61919 <sup>†</sup> | 20      |
| PhytoComm | Huang Qin | G225H1204622 | 61920 <sup>†</sup> | 20      |

- 13 918 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 25 spectra from 10 *Apo-Ident* customers from 8 batches from the substance/substance group *Huang Qin*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| PhytoComm | Huang Qin | G225H1204322 | 4       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Huang Qin | G225H1204522 | 3       |
| Phytocomm | Huang Qin | 161213hq     | 1       |
| PhytoComm | Huang Qin | G225H1204022 | 1       |
| Phytocomm | Huang Qin | G225H1204022 | 4       |
| Phytocomm | Huang Qin | G225H1204121 | 3       |
| PhytoComm | Huang Qin | G225H1204121 | 2       |
| Phytocomm | Huang Qin | G225H1204221 | 2       |
| Phytocomm | Huang Qin | g225h1204121 | 1       |
| PhytoComm | Huang Qin | G225H1204221 | 2       |
| Herbasin  | Huang Qin | g225h120442  | 1       |
| phytocomm | Huang Qin | G225H1204022 | 1       |

- 1956 spectra from 16 *Apo-Ident* customers from a total of 956 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Huang 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 195           | 0              | 21 371        |
| <b>Type B</b> | 0              | 135           | 0              | 13 918        |
| <b>Type C</b> | 0              | 17            | 8              | 1956          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.9231 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.5556 %) |
| <b>Type C</b> | 100.0000 % (> 99.4407 %) | 68.0000 % (> 56.0000 %)  |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60930     | 60930               | 0.00                         | 19.94                           |
| 61440     | 61440               | 0.00                         | 19.34                           |
| 61669     | 61669               | 0.00                         | 23.91                           |
| 61919     | 61919               | 0.00                         | 23.60                           |
| 61920     | 61920               | 0.00                         | 24.67                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Huo Ma Ren**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60234-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Huo Ma Ren; Cannabis semen; 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G141H0449321 | 61066     | 40      | from supplier |
| PhytoComm | Huo Ma Ren | G141H0449321 | 61630     | 40      | from supplier |
| PhytoComm | Huo Ma Ren | G141HS061    | 61642     | 40      | from supplier |
| PhytoComm | Huo Ma Ren | G141H0449621 | 61846     | 40      | from supplier |
| PhytoComm | Huo Ma Ren | G141H0449621 | 61847     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Huo Ma Ren*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 155 spectra of 5 reference samples from the substance/substance group *Huo Ma Ren*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Huo Ma Ren | G141H0449321 | 61066 <sup>†</sup> | 20      |
| PhytoComm | Huo Ma Ren | G141H0449321 | 61214              | 75      |
| PhytoComm | Huo Ma Ren | G141HS061    | 61642 <sup>†</sup> | 20      |
| PhytoComm | Huo Ma Ren | G141H0449621 | 61846 <sup>†</sup> | 20      |
| PhytoComm | Huo Ma Ren | G141H0449621 | 61847 <sup>†</sup> | 20      |

- 13 898 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Huo Ma Ren*.

<sup>†</sup>These spectra were recorded from 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 | Huo Ma Ren | G141H0449121 | 2       |
| Phytocomm | Huo Ma Ren | G141HS061    | 1       |

- 1978 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 194           | 6              | 21 366        |
| <b>Type B</b> | 0              | 135           | 20             | 13 898        |
| <b>Type C</b> | 2              | 1             | 2              | 1976          |

The substance/substance group *Huo Ma 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        |
|---------------|--------------------------|-------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 97.0000 % (> 95.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 87.0968 % (> 85.1613 %) |
| <b>Type C</b> | 99.5896 % (> 99.3111 %)  | n/a (n/a)               |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61066     | 61066               | 0.00                         | 2.95                            |
| 61630     | 61630               | 0.00                         | 4.71                            |

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| <b>Sample ID</b> | <b>Reference sample ID</b> | <b>Distance to reference sample</b> | <b>Distance to next foreign sample</b> |
|------------------|----------------------------|-------------------------------------|----------------------------------------|
| 61642            | 61642                      | 0.00                                | 5.26                                   |
| 61846            | 61846                      | 0.00                                | 10.50                                  |
| 61847            | 61847                      | 0.00                                | 9.87                                   |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ji Li**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60110-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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     | G240H1410522 | 61917     | 40      | from supplier |
| PhytoComm | Ji Li     | G240H1410522 | 61918     | 40      | from supplier |

## Validation samples

A total of 37 600 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 Li*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Ji Li*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Ji Li     | G240H1410522 | 61917 <sup>†</sup> | 20      |
| PhytoComm | Ji Li     | G240H1410522 | 61918 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Ji Li*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| PhytoComm | Ji Li     | G240H1410221 | 1       |
| Phytocomm | Ji Li     | H0858021     | 2       |
| Phytocomm | Ji Li     | G240H1410421 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1977 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 4              | 0             | 4              | 1973          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.8290 % (> 99.5502 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61917     | 61917               | 0.00                         | 5.97                            |
| 61918     | 61918               | 0.00                         | 6.29                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ji Nei Jin**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50329-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Ji Nei Jin; Endothelium corneum gigeriae galli

### Special notes

When selecting the *Ji Nei 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Nei Jin*:

| Supplier  | Substance  | Batch        | Sample ID | Spectra | Certificate   |
|-----------|------------|--------------|-----------|---------|---------------|
| PhytoComm | Ji Nei Jin | G259H2102321 | 60850     | 40      | from supplier |
| PhytoComm | Ji Nei Jin | G259H2102321 | 61418     | 40      | from supplier |
| PhytoComm | Ji Nei Jin | G259H2102421 | 61654     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Ji Nei Jin*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 95 spectra of 2 reference samples from the substance/substance group *Ji Nei Jin*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Ji Nei Jin | G259H2102321 | 61126              | 75      |
| PhytoComm | Ji Nei Jin | G259H2102421 | 61654 <sup>†</sup> | 20      |

- 13 958 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Ji Nei Jin*.

| Supplier  | Substance  | Batch        | Spectra |
|-----------|------------|--------------|---------|
| PhytoComm | Ji Nei Jin | G259H2102023 | 2       |
| Phytocomm | Ji Nei Jin | G259H2102023 | 1       |
| PhytoComm | Ji Nei Jin | G259H2102321 | 1       |

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<sup>†</sup>These spectra were recorded from 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 | Ji Nei Jin | G259H2102321 | 1       |
| Phytocomm | Ji Nei Jin | g259h2102321 | 1       |
| PhytoComm | Ji Nei Jin | H2102021     | 1       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Ji Nei 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 *Ji Nei 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 95            | 0              | 13 958        |
| <b>Type C</b> | 1              | 3             | 4              | 1973          |

The substance/substance group *Ji Nei 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 93.6842 %) |
| <b>Type C</b> | 99.9067 % (> 99.6275 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60850     | 60850               | 0.00                         | 18.90                           |
| 61418     | 61418               | 0.00                         | 19.44                           |
| 61654     | 61654               | 0.00                         | 14.03                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ji Xue Teng**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60099-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G159H2101622 | 61999     | 40      | from supplier |
| PhytoComm | Ji Xue Teng | G159H2101622 | 62000     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Ji Xue Teng*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Ji Xue Teng | G159H2101622 | 61999 <sup>†</sup> | 20      |
| PhytoComm | Ji Xue Teng | G159H2101622 | 62000 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 10 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Ji Xue Teng*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| Phytocomm | Ji Xue Teng | G159H2101423 | 3       |
| Phytocomm | Ji Xue Teng | G159H2101122 | 2       |
| PhytoComm | Ji Xue Teng | G159H2101122 | 3       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Ji Xue Teng | g159h2101122 | 1       |
| Phytocomm | Ji Xue Teng | H2101923     | 1       |

- 1971 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 1              | 0             | 10             | 1970          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.9585 % (> 99.6791 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61999     | 61999               | 0.00                         | 16.02                           |
| 62000     | 62000               | 0.00                         | 15.98                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Jiang Huang**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60181-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G085H1716321 | 60884     | 40      | from supplier |
| PhytoComm | Jiang Huang | G085H1716321 | 61562     | 40      | from supplier |
| PhytoComm | Jiang Huang | G085H1716422 | 61683     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Jiang Huang*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 95 spectra of 2 reference samples from the substance/substance group *Jiang Huang*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Jiang Huang | G085H1716321 | 61271              | 75      |
| PhytoComm | Jiang Huang | G085H1716422 | 61683 <sup>†</sup> | 20      |

- 13 958 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 8 *Apo-Ident* customers from 4 batches from the substance/substance group *Jiang Huang*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| PhytoComm | Jiang Huang | G085H1716422 | 3       |
| PhytoComm | Jiang Huang | G085H1716321 | 2       |
| PhytoComm | Jiang Huang | G085H1716422 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Jiang Huang | G085H1716022 | 1       |
| PhytoComm | Jiang Huang | G085H1716022 | 1       |
| Phytocomm | Jiang Huang | G085H1716022 | 1       |
| PhytoComm | Jiang Huang | G085H1716122 | 2       |
| Phytocomm | Jiang Huang | G085H1716122 | 1       |

- 1969 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Jiang Huang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Jiang Huang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 95            | 0              | 13 958        |
| <b>Type C</b> | 0              | 7             | 5              | 1969          |

The substance/substance group *Jiang 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 93.6842 %) |
| <b>Type C</b> | 100.0000 % (> 99.4410 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60884     | 60884               | 0.00                         | 12.56                           |
| 61562     | 61562               | 0.00                         | 12.30                           |
| 61683     | 61683               | 0.00                         | 13.41                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Jiao Gu Lan**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60332-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Jiao Gu Lan*:

| Supplier  | Substance   | Batch         | Sample ID | Spectra | Certificate   |
|-----------|-------------|---------------|-----------|---------|---------------|
| PhytoComm | Jiao Gu Lan | G065FB1276621 | 62013     | 40      | from supplier |
| PhytoComm | Jiao Gu Lan | G065FB1276621 | 62014     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Jiao Gu Lan*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Jiao Gu Lan*.

| Supplier  | Substance   | Batch         | Sample ID          | Spectra |
|-----------|-------------|---------------|--------------------|---------|
| PhytoComm | Jiao Gu Lan | G065FB1276621 | 62013 <sup>†</sup> | 20      |
| PhytoComm | Jiao Gu Lan | G065FB1276621 | 62014 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Jiao Gu Lan*.

| Supplier    | Substance   | Batch          | Spectra |
|-------------|-------------|----------------|---------|
| Phytocomm   | Jiao Gu Lan | G065FB1276421  | 3       |
| Phytocomm   | Jiao Gu Lan | G065F-B1276121 | 1       |
| Herbasin    | Jiao Gu Lan | G065FB1276121  | 1       |
| PhytoComm   | Jiao Gu Lan | G065H1276922   | 1       |
| Herbasinica | Jiao Gu Lan | G065F-B1276121 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1974 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Jiao Gu Lan* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Jiao Gu Lan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 2              | 0             | 7              | 1972          |

The substance/substance group *Jiao Gu Lan* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.9160 % (> 99.6368 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 62013     | 62013               | 0.00                         | 9.71                            |
| 62014     | 62014               | 0.00                         | 10.04                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Jie Geng**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60034-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G193H1015521 | 61378     | 40      | from supplier |
| PhytoComm | Jie Geng  | G193H1015621 | 61931     | 40      | from supplier |
| PhytoComm | Jie Geng  | G193H1015621 | 61932     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Jie Geng*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Jie Geng*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Jie Geng  | G193H1015521 | 61378 <sup>†</sup> | 20      |
| PhytoComm | Jie Geng  | G193H1015621 | 61931 <sup>†</sup> | 20      |
| PhytoComm | Jie Geng  | G193H1015621 | 61932 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Jie Geng*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Jie Geng  | G193H1015521 | 3       |
| PhytoComm | Jie Geng  | G193H1015024 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Jie Geng  | G193H1015024 | 3       |
| phytocomm | Jie Geng  | G193H1015025 | 1       |
| Phytocomm | Jie Geng  | G193H1015025 | 2       |
| Phytocomm | Jie Geng  | G193H1015221 | 3       |
| Phytocomm | Jie Geng  | g193h1015221 | 1       |

- 1966 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Jie Geng* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Jie Geng* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 4              | 3             | 12             | 1962          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.8828 % (> 99.6033 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61378     | 61378               | 0.00                         | 9.03                            |
| 61931     | 61931               | 0.00                         | 6.17                            |
| 61932     | 61932               | 0.00                         | 6.64                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Jin Qian Cao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50293-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G151HS368 | 61861     | 40      | from supplier |
| PhytoComm | Jin Qian Cao | G151HS368 | 61862     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Jin Qian Cao*.

| Supplier  | Substance    | Batch     | Sample ID          | Spectra |
|-----------|--------------|-----------|--------------------|---------|
| PhytoComm | Jin Qian Cao | G151HS368 | 61861 <sup>†</sup> | 20      |
| PhytoComm | Jin Qian Cao | G151HS368 | 61862 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Jin Qian Cao*.

| Supplier  | Substance    | Batch         | Spectra |
|-----------|--------------|---------------|---------|
| Phytocomm | Jin Qian Cao | G1514H0847122 | 1       |
| PhytoComm | Jin Qian Cao | G151H0847122  | 1       |
| Phytocomm | Jin Qian Cao | G151H0847122  | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Jin Qian Cao | g151h0847122 | 1       |
| PhytoComm | Jin Qian Cao | G151H0847922 | 2       |
| Phytocomm | Jin Qian Cao | G151H0847922 | 1       |
| PhytoComm | Jin Qian Cao | H0847921     | 1       |
| Phytocomm | Jin Qian Cao | H0847921     | 1       |

- 1971 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Jin 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 10             | 1971          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4412 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61861     | 61861               | 0.00                         | 29.65                           |
| 61862     | 61862               | 0.00                         | 30.05                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Jin Yin Hua**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60350-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G145H0845621 | 61778     | 40      | from supplier |
| PhytoComm | Jin Yin Hua | G145H0845621 | 61822     | 40      | from supplier |
| PhytoComm | Jin Yin Hua | G145H0845621 | 61871     | 40      | from supplier |
| PhytoComm | Jin Yin Hua | G145H0845621 | 61872     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 406 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 80 spectra of 4 reference samples from the substance/substance group *Jin Yin Hua*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Jin Yin Hua | G145H0845621 | 61778 <sup>†</sup> | 20      |
| PhytoComm | Jin Yin Hua | G145H0845621 | 61822 <sup>†</sup> | 20      |
| PhytoComm | Jin Yin Hua | G145H0845621 | 61871 <sup>†</sup> | 20      |
| PhytoComm | Jin Yin Hua | G145H0845621 | 61872 <sup>†</sup> | 20      |

- 13 973 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Jin Yin Hua*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| Phytocomm | Jin Yin Hua | G145H0845021 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Jin Yin Hua | G145H0845022 | 4       |
| Phytocomm | Jin Yin Hua | G145H0845321 | 1       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Jin Yin Hua* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Jin Yin Hua* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 80            | 0              | 13 973        |
| <b>Type C</b> | 17             | 0             | 6              | 1958          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.5000 %) |
| <b>Type C</b> | 99.2956 % (> 99.0165 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61778     | 61778               | 0.00                         | 9.13                            |
| 61822     | 61822               | 0.00                         | 8.62                            |
| 61871     | 61871               | 0.00                         | 10.11                           |
| 61872     | 61872               | 0.00                         | 9.70                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Jing Jie**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60088-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G221HS218    | 61857     | 40      | from supplier |
| PhytoComm | Jing Jie  | G221HS218    | 61858     | 40      | from supplier |
| PhytoComm | Jing Jie  | G221H1038621 | 61923     | 40      | from supplier |
| PhytoComm | Jing Jie  | G221H1038621 | 61924     | 40      | from supplier |
| PhytoComm | Jing Jie  | G221H1038621 | 62055     | 40      | from supplier |
| PhytoComm | Jing Jie  | G221H1038621 | 62056     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Jing Jie*. These samples are listed above in the [calibration samples](#) section.
- 21 326 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 120 spectra of 6 reference samples from the substance/substance group *Jing Jie*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Jing Jie  | G221HS218    | 61857 <sup>†</sup> | 20      |
| PhytoComm | Jing Jie  | G221HS218    | 61858 <sup>†</sup> | 20      |
| PhytoComm | Jing Jie  | G221H1038621 | 61923 <sup>†</sup> | 20      |
| PhytoComm | Jing Jie  | G221H1038621 | 61924 <sup>†</sup> | 20      |
| PhytoComm | Jing Jie  | G221H1038621 | 62055 <sup>†</sup> | 20      |
| PhytoComm | Jing Jie  | G221H1038621 | 62056 <sup>†</sup> | 20      |

- 13 933 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Jing Jie*.

<sup>†</sup>These spectra were recorded from 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  | Jing Jie  | G221H1038121 | 2       |
| PhytoComm  | Jing Jie  | G221H1038121 | 1       |
| Sino Phyto | Jing Jie  | G221H1038121 | 1       |
| Phytocomm  | Jing Jie  | G221H1038221 | 4       |
| PhytoComm  | Jing Jie  | G221H1038221 | 1       |
| Phytocomm  | Jing Jie  | g221h1038221 | 1       |
| PhytoComm  | Jing Jie  | H1038021     | 1       |

- 1970 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Jing Jie* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Jing Jie* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 1              | 239           | 1              | 21 325        |
| <b>Type B</b> | 1              | 120           | 0              | 13 932        |
| <b>Type C</b> | 7              | 0             | 11             | 1963          |

The substance/substance group *Jing Jie* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

|               | Specificity             | Recognition rate         |
|---------------|-------------------------|--------------------------|
| <b>Type A</b> | 99.9959 % (> 99.9765 %) | 99.5833 % (> 98.3333 %)  |
| <b>Type B</b> | 99.9919 % (> 99.9573 %) | 100.0000 % (> 95.0000 %) |
| <b>Type C</b> | 99.3159 % (> 99.0365 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61857     | 61857               | 0.00                         | 7.21                            |
| 61858     | 61858               | 0.00                         | 7.32                            |
| 61923     | 61923               | 0.00                         | 5.72                            |
| 61924     | 61924               | 0.00                         | 5.61                            |
| 62055     | 62055               | 0.00                         | 5.59                            |
| 62056     | 62056               | 0.00                         | 5.76                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ju Hua**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60232-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G064H1231301 | 60988     | 40      | from supplier |
| PhytoComm | Ju Hua    | G064H1231321 | 61572     | 40      | from supplier |
| PhytoComm | Ju Hua    | G064H1231421 | 61697     | 40      | from supplier |
| PhytoComm | Ju Hua    | G064H1231521 | 62023     | 40      | from supplier |
| PhytoComm | Ju Hua    | G064H1231521 | 62024     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Ju Hua*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 325 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 135 spectra of 4 reference samples from the substance/substance group *Ju Hua*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Ju Hua    | G064H1231321 | 61281              | 75      |
| PhytoComm | Ju Hua    | G064H1231421 | 61697 <sup>†</sup> | 20      |
| PhytoComm | Ju Hua    | G064H1231521 | 62023 <sup>†</sup> | 20      |
| PhytoComm | Ju Hua    | G064H1231521 | 62024 <sup>†</sup> | 20      |

- 13 918 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 2 batches from the substance/substance group *Ju Hua*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Ju Hua    | G064H1231421 | 2       |

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<sup>†</sup>These spectra were recorded from 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 | Ju Hua    | G064H1231421 | 1       |
| PhytoComm | Ju Hua    | G064H1231021 | 2       |

- 1976 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Ju Hua* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ju Hua* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 200           | 0              | 21 366        |
| <b>Type B</b> | 0              | 135           | 0              | 13 918        |
| <b>Type C</b> | 12             | 5             | 0              | 1964          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.5556 %) |
| <b>Type C</b> | 99.3306 % (> 99.0516 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60988     | 60988               | 0.00                         | 10.70                           |

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| <b>Sample ID</b> | <b>Reference sample ID</b> | <b>Distance to reference sample</b> | <b>Distance to next foreign sample</b> |
|------------------|----------------------------|-------------------------------------|----------------------------------------|
| 61572            | 61572                      | 0.00                                | 10.80                                  |
| 61697            | 61697                      | 0.00                                | 11.67                                  |
| 62023            | 62023                      | 0.00                                | 15.89                                  |
| 62024            | 62024                      | 0.00                                | 15.82                                  |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Jue Ming Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60312-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Jue Ming Zi; Cassiae torae semen

### Special notes

When selecting the *Jue Ming 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Jue Ming Zi*:

| Supplier  | Substance   | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-------------|--------------|-----------|---------|---------------|
| PhytoComm | Jue Ming Zi | G059H1097521 | 61867     | 40      | from supplier |
| PhytoComm | Jue Ming Zi | G059H1097521 | 61868     | 40      | from supplier |
| PhytoComm | Jue Ming Zi | G059H1097521 | 61875     | 40      | from supplier |
| PhytoComm | Jue Ming Zi | G059H1097521 | 61876     | 40      | from supplier |
| PhytoComm | Jue Ming Zi | G059H1097621 | 62033     | 40      | from supplier |
| PhytoComm | Jue Ming Zi | G059H1097621 | 62034     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Jue Ming Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 326 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 115 spectra of 6 reference samples from the substance/substance group *Jue Ming Zi*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Jue Ming Zi | G059H1097521 | 61867 <sup>†</sup> | 20      |
| PhytoComm | Jue Ming Zi | G059H1097521 | 61868 <sup>†</sup> | 20      |
| PhytoComm | Jue Ming Zi | G059H1097521 | 61875 <sup>†</sup> | 20      |
| PhytoComm | Jue Ming Zi | G059H1097521 | 61876 <sup>†</sup> | 15      |
| PhytoComm | Jue Ming Zi | G059H1097621 | 62033 <sup>†</sup> | 20      |
| PhytoComm | Jue Ming Zi | G059H1097621 | 62034 <sup>†</sup> | 20      |

- 13 938 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Jue Ming Zi*.

<sup>†</sup>These spectra were recorded from 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 | Jue Ming Zi | G059H1097221 | 1       |
| Phytocomm | Jue Ming Zi | G059H1097023 | 1       |
| phytocomm | Jue Ming Zi | G059H1097121 | 1       |
| PhytoComm | Jue Ming Zi | G059H1097221 | 2       |
| PhytoComm | Jue Ming Zi | G059H1097121 | 1       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Jue Ming 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 *Jue Ming 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 240           | 0              | 21 326        |
| <b>Type B</b> | 0              | 115           | 0              | 13 938        |
| <b>Type C</b> | 0              | 2             | 4              | 1975          |

The substance/substance group *Jue Ming 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 94.7826 %) |
| <b>Type C</b> | 100.0000 % (> 99.4417 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61867     | 61867               | 0.00                         | 16.63                           |
| 61868     | 61868               | 0.00                         | 16.37                           |
| 61875     | 61875               | 0.00                         | 15.29                           |
| 61876     | 61876               | 0.00                         | 14.81                           |
| 62033     | 62033               | 0.00                         | 8.05                            |
| 62034     | 62034               | 0.00                         | 8.01                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ku Shen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60112-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Ku Shen; Sophorae flavescentis radix

### Special notes

When selecting the *Ku Shen* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Ku Shen*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Ku Shen   | G233H0908521 | 61927     | 40      | from supplier |
| PhytoComm | Ku Shen   | G233H0908521 | 61928     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Ku Shen*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Ku Shen*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Ku Shen   | G233H0908521 | 61927 <sup>†</sup> | 20      |
| PhytoComm | Ku Shen   | G233H0908521 | 61928 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Ku Shen*.

| Supplier                | Substance | Batch        | Spectra |
|-------------------------|-----------|--------------|---------|
| china medica 14.06.2013 | Ku Shen   | 210013       | 1       |
| Phytocomm               | Ku Shen   | FA0908901    | 1       |
| Phytocomm               | Ku Shen   | G233H0908121 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Ku Shen   | G233H0908121 | 1       |
| Defektur  | Ku Shen   | G233H0908121 | 2       |
| Phytocomm | Ku Shen   | h0908121     | 1       |

- 1973 spectra from 15 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Ku Shen* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ku Shen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 8              | 1973          |

The substance/substance group *Ku Shen* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4414 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61927     | 61927               | 0.00                         | 18.62                           |
| 61928     | 61928               | 0.00                         | 19.78                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Kuan Dong Hua**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60035-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Kuan Dong Hua; Farfarae flos; Tussilaginis farfarae flos

### Special notes

When selecting the *Kuan Dong Hua* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Kuan Dong Hua*:

| Supplier  | Substance     | Batch        | Sample ID | Spectra | Certificate   |
|-----------|---------------|--------------|-----------|---------|---------------|
| PhytoComm | Kuan Dong Hua | G276H1219421 | 61073     | 40      | from supplier |
| PhytoComm | Kuan Dong Hua | G276H1219521 | 61660     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Kuan Dong Hua*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Kuan Dong Hua*.

| Supplier  | Substance     | Batch        | Sample ID          | Spectra |
|-----------|---------------|--------------|--------------------|---------|
| PhytoComm | Kuan Dong Hua | G276H1219421 | 61073 <sup>†</sup> | 20      |
| PhytoComm | Kuan Dong Hua | G276H1219521 | 61660 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Kuan Dong Hua*.

| Supplier  | Substance     | Batch    | Spectra |
|-----------|---------------|----------|---------|
| PhytoComm | Kuan Dong Hua | H1219921 | 2       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1979 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Kuan Dong Hua* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Kuan Dong Hua* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 6              | 0             | 2              | 1973          |

The substance/substance group *Kuan Dong Hua* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.8001 % (> 99.5224 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61073     | 61073               | 0.00                         | 10.44                           |
| 61660     | 61660               | 0.00                         | 9.82                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Lai Fu Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60067-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Lai Fu Zi*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Lai Fu Zi | G209H1220621 | 61959     | 40      | from supplier |
| PhytoComm | Lai Fu Zi | G209H1220621 | 61960     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Lai Fu Zi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Lai Fu Zi | G209H1220621 | 61959 <sup>†</sup> | 20      |
| PhytoComm | Lai Fu Zi | G209H1220621 | 61960 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 *Lai Fu Zi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Lai Fu Zi | G209H1220022 | 2       |
| PhytoComm | Lai Fu Zi | G209H1220022 | 1       |
| Phytocomm | Lai Fu Zi | G209H1220221 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Lai Fu Zi | G209H1220321 | 1       |
| PhytoComm | Lai Fu Zi | G209H1220321 | 1       |
| Herbasin  | Lai Fu Zi | g209h1220321 | 1       |
| PhytoComm | Lai Fu Zi | H1220922     | 2       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Lai Fu Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lai Fu Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 9              | 1972          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4413 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61959     | 61959               | 0.00                         | 26.57                           |
| 61960     | 61960               | 0.00                         | 26.58                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Lian Qiao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60146-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Lian Qiao; Forsythiae fructus; Forsythiae suspensae fructus

### Special notes

When selecting the *Lian Qiao* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G105H1132521 | 61716     | 40      | from supplier |
| PhytoComm | Lian Qiao | G105H1132621 | 61979     | 40      | from supplier |
| PhytoComm | Lian Qiao | G105H1132621 | 61980     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Lian Qiao*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Lian Qiao*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Lian Qiao | G105H1132521 | 61716 <sup>†</sup> | 20      |
| PhytoComm | Lian Qiao | G105H1132621 | 61979 <sup>†</sup> | 20      |
| PhytoComm | Lian Qiao | G105H1132621 | 61980 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Lian Qiao*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Lian Qiao | G105H1132521 | 1       |
| Phytocomm | Lian Qiao | G105H1132221 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Lian Qiao | G105H1132221 | 1       |
| PhytoComm | Lian Qiao | H1132022     | 1       |
| Phytocomm | Lian Qiao | H1132022     | 1       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Lian Qiao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lian Qiao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 5              | 1             | 5              | 1970          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.7668 % (> 99.4877 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61716     | 61716               | 0.00                         | 12.23                           |
| 61979     | 61979               | 0.00                         | 14.59                           |
| 61980     | 61980               | 0.00                         | 15.10                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Lian Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60248-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G171H1501421 | 61480     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Lian Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 75 spectra of 1 reference samples from the substance/substance group *Lian Zi*.

| Supplier  | Substance | Batch        | Sample ID | Spectra |
|-----------|-----------|--------------|-----------|---------|
| PhytoComm | Lian Zi   | G171H1501421 | 61188     | 75      |

- 13 978 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Lian Zi*.

| Supplier  | Substance | Batch     | Spectra |
|-----------|-----------|-----------|---------|
| Phytocomm | Lian Zi   | 411502701 | 1       |

- 1980 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).



## Validation results

The validation runs checked whether the substance/substance group *Lian Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lian Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 75            | 0              | 13 978        |
| <b>Type C</b> | 0              | 0             | 1              | 1980          |

The substance/substance group *Lian 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4487 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61480     | 61480               | 0.00                         | 23.97                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ling Zhi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60187-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G109FB2405521 | 61713     | 40      | from supplier |
| PhytoComm | Ling Zhi  | G109FB2405621 | 62005     | 40      | from supplier |
| PhytoComm | Ling Zhi  | G109FB2405621 | 62006     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Ling Zhi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Ling Zhi*.

| Supplier  | Substance | Batch         | Sample ID          | Spectra |
|-----------|-----------|---------------|--------------------|---------|
| PhytoComm | Ling Zhi  | G109FB2405521 | 61713 <sup>†</sup> | 20      |
| PhytoComm | Ling Zhi  | G109FB2405621 | 62005 <sup>†</sup> | 20      |
| PhytoComm | Ling Zhi  | G109FB2405621 | 62006 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 2 *Apo-Ident* customers from 4 batches from the substance/substance group *Ling Zhi*.

| Supplier  | Substance | Batch          | Spectra |
|-----------|-----------|----------------|---------|
| PhytoComm | Ling Zhi  | G109FB2405321  | 1       |
| PhytoComm | Ling Zhi  | G109F-B2405221 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Ling Zhi  | FA2405901     | 1       |
| Phytocomm | Ling Zhi  | g109fb2405321 | 1       |

- 1976 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 9              | 0             | 5              | 1967          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.6973 % (> 99.4184 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61713     | 61713               | 0.00                         | 6.56                            |
| 62005     | 62005               | 0.00                         | 8.43                            |
| 62006     | 62006               | 0.00                         | 8.50                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Long Dan (Cao)**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60227-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Long Dan (Cao); Gentianae longdanco radix; Gentianae scabrae radix

### Special notes

When selecting the *Long Dan (Cao)* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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) | G112H1705321 | 60907     | 40      | from supplier |
| PhytoComm | Long Dan (Cao) | G112H1705321 | 61527     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Long Dan (Cao)*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 75 spectra of 1 reference samples from the substance/substance group *Long Dan (Cao)*.

| Supplier  | Substance      | Batch        | Sample ID | Spectra |
|-----------|----------------|--------------|-----------|---------|
| PhytoComm | Long Dan (Cao) | G112H1705321 | 61236     | 75      |

- 13 978 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Long Dan (Cao)*.

| Supplier  | Substance      | Batch        | Spectra |
|-----------|----------------|--------------|---------|
| Phytocomm | Long Dan (Cao) | G112H1705321 | 3       |
| Phytocomm | Long Dan (Cao) | g112h1705022 | 1       |
| PhytoComm | Long Dan (Cao) | G112H1705022 | 3       |
| Phytocomm | Long Dan (Cao) | G112H1705022 | 1       |



- 1973 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Long Dan (Cao)* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Long Dan (Cao)* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 1              | 80            | 0              | 21 485        |
| <b>Type B</b> | 0              | 75            | 0              | 13 978        |
| <b>Type C</b> | 19             | 4             | 4              | 1954          |

The substance/substance group *Long Dan (Cao)* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 99.9877 % (> 99.9684 %)  | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.0000 %) |
| <b>Type C</b> | 99.3650 % (> 99.0857 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60907     | 60907               | 0.00                         | 7.74                            |
| 61527     | 61527               | 0.00                         | 6.81                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Long Yan Rou**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60463-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G144H1708421 | 61508     | 40      | from supplier |
| PhytoComm | Long Yan Rou | G144H1708421 | 61853     | 40      | from supplier |
| PhytoComm | Long Yan Rou | G144H1708421 | 61854     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Long Yan Rou*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 115 spectra of 3 reference samples from the substance/substance group *Long Yan Rou*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Long Yan Rou | G144H1708421 | 61217              | 75      |
| PhytoComm | Long Yan Rou | G144H1708421 | 61853 <sup>†</sup> | 20      |
| PhytoComm | Long Yan Rou | G144H1708421 | 61854 <sup>†</sup> | 20      |

- 13 938 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 2 batches from the substance/substance group *Long Yan Rou*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| Phytocomm | Long Yan Rou | G144H1708221 | 1       |
| PhytoComm | Long Yan Rou | G144H1708221 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Long Yan Rou | H1708922 | 2       |
| PhytoComm | Long Yan Rou | H1708922 | 2       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Long Yan Rou* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Long Yan Rou* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 115           | 0              | 13 938        |
| <b>Type C</b> | 14             | 2             | 4              | 1961          |

The substance/substance group *Long Yan 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 94.7826 %) |
| <b>Type C</b> | 99.1456 % (> 98.8664 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61508     | 61508               | 0.00                         | 6.80                            |
| 61853     | 61853               | 0.00                         | 7.38                            |
| 61854     | 61854               | 0.00                         | 7.59                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Lu Gen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60259-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G189H2014521 | 61663     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Lu Gen*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Lu Gen*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Lu Gen    | G189H2014521 | 61663 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 10 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Lu Gen*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Lu Gen    | G189H2014521 | 1       |
| PhytoComm | Lu Gen    | G189H2014521 | 2       |
| Phytocomm | Lu Gen    | F100708      | 2       |
| PhytoComm | Lu Gen    | F100708      | 1       |
| Phytocomm | Lu Gen    | G189H2014221 | 3       |
| PhytoComm | Lu Gen    | G189H2014221 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1971 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Lu 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 3             | 7              | 1971          |

The substance/substance group *Lu 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4412 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61663     | 61663               | 0.00                         | 12.21                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Lu Jiao Shuang**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50328-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Lu Jiao Shuang; Cervi corni degelatinatum

### Special notes

When selecting the *Lu Jiao Shuang* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Jiao Shuang*:

| Supplier  | Substance      | Batch        | Sample ID | Spectra | Certificate   |
|-----------|----------------|--------------|-----------|---------|---------------|
| PhytoComm | Lu Jiao Shuang | G062H1415522 | 61678     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Lu Jiao Shuang*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Lu Jiao Shuang*.

| Supplier  | Substance      | Batch        | Sample ID          | Spectra |
|-----------|----------------|--------------|--------------------|---------|
| PhytoComm | Lu Jiao Shuang | G062H1415522 | 61678 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Lu Jiao Shuang*.

| Supplier  | Substance      | Batch        | Spectra |
|-----------|----------------|--------------|---------|
| phythocom | Lu Jiao Shuang | G062H1419321 | 1       |
| Phytocomm | Lu Jiao Shuang | FB1419901    | 2       |
| Phytocomm | Lu Jiao Shuang | G062H1419421 | 1       |

- 1977 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

<sup>†</sup>These spectra were recorded from 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 Jiao Shuang* can be 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 Jiao Shuang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 4              | 1977          |

The substance/substance group *Lu Jiao Shuang* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4424 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61678     | 61678               | 0.00                         | 160.22                          |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Lu Lu Tong**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60240-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Lu Lu Tong; Liquidambaris fructus

### Special notes

When selecting the *Lu Lu Tong* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Lu Lu Tong*:

| Supplier  | Substance  | Batch        | Sample ID | Spectra | Certificate   |
|-----------|------------|--------------|-----------|---------|---------------|
| PhytoComm | Lu Lu Tong | G142H1336622 | 62001     | 40      | from supplier |
| PhytoComm | Lu Lu Tong | G142H1336622 | 62002     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Lu Lu Tong*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Lu Lu Tong*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Lu Lu Tong | G142H1336622 | 62001 <sup>†</sup> | 20      |
| PhytoComm | Lu Lu Tong | G142H1336622 | 62002 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Lu Lu Tong*.

| Supplier    | Substance  | Batch         | Spectra |
|-------------|------------|---------------|---------|
| PhytoComm   | Lu Lu Tong | G142GH1336022 | 1       |
| PhytoComm   | Lu Lu Tong | G142H1336122  | 1       |
| Herbasinica | Lu Lu Tong | G142H1336122  | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Lu Lu Tong | g142h1336122 | 1       |
| PhytoComm | Lu Lu Tong | G142H1336122 | 1       |
| PhytoComm | Lu Lu Tong | G142H1336521 | 2       |
| PhytoComm | Lu Lu Tong | G142H1336321 | 1       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Lu Lu Tong* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lu Lu Tong* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 1             | 8              | 1972          |

The substance/substance group *Lu Lu Tong* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4413 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 62001     | 62001               | 0.00                         | 14.57                           |
| 62002     | 62002               | 0.00                         | 14.61                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ma Bian Cao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60479-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G248H1085621 | 61833     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

## Type A All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Ma Bian Cao*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Ma Bian Cao*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Ma Bian Cao | G248H1085621 | 61833 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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       |

- 1980 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the

<sup>†</sup>These spectra were recorded from 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 1              | 1980          |

The substance/substance group *Ma Bian 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4487 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61833     | 61833               | 0.00                         | 7.21                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ma Huang**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50283-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G097H1101422 | 61542     | 40      | from supplier |
| PhytoComm | Ma Huang  | G097H1101522 | 61684     | 40      | from supplier |
| PhytoComm | Ma Huang  | G097H1101422 | 61692     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Ma Huang*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 115 spectra of 3 reference samples from the substance/substance group *Ma Huang*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Ma Huang  | G097H1101422 | 61251              | 75      |
| PhytoComm | Ma Huang  | G097H1101522 | 61684 <sup>†</sup> | 20      |
| PhytoComm | Ma Huang  | G097H1101422 | 61692 <sup>†</sup> | 20      |

- 13 938 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Ma Huang*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Ma Huang  | G097H1101522 | 2       |
| Phytocomm | Ma Huang  | G097H1101223 | 3       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Ma Huang  | H1101023 | 2       |
| Phytocomm | Ma Huang  | H1101023 | 1       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Ma Huang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ma Huang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 115           | 0              | 13 938        |
| <b>Type C</b> | 0              | 5             | 3              | 1973          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 94.7826 %) |
| <b>Type C</b> | 100.0000 % (> 99.4414 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61542     | 61542               | 0.00                         | 40.87                           |
| 61684     | 61684               | 0.00                         | 36.21                           |
| 61692     | 61692               | 0.00                         | 39.45                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ma Huang Gen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60063-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G278HS3930V1 | 61727     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Ma Huang Gen*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Ma Huang Gen*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Ma Huang Gen | G278HS3930V1 | 61727 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Ma Huang Gen*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| phythocom | Ma Huang Gen | g278h1102121 | 1       |
| phytocomm | Ma Huang Gen | h1102021     | 1       |
| PhytoComm | Ma Huang Gen | G278H1102121 | 1       |
| Herbasin  | Ma Huang Gen | G278H1102121 | 2       |
| PhytoComm | Ma Huang Gen | H1102021     | 1       |
| Phytocomm | Ma Huang Gen | G278H1102121 | 2       |
| Herbasin  | Ma Huang Gen | H1102021     | 1       |
| Phytocomm | Ma Huang Gen | H1102021     | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1971 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Ma Huang Gen* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ma Huang Gen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 6              | 40            | 0              | 21 520        |
| <b>Type B</b> | 21             | 20            | 0              | 14 012        |
| <b>Type C</b> | 0              | 0             | 10             | 1971          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 99.9853 % (> 99.9660 %)  | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 99.9293 % (> 99.8950 %)  | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4412 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61727     | 61727               | 0.00                         | 2.49                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Mai Men Dong**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60024-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G176H1118521 | 61364     | 40      | from supplier |
| PhytoComm | Mai Men Dong | G176H1118521 | 61694     | 40      | from supplier |
| PhytoComm | Mai Men Dong | G176H1118621 | 61945     | 40      | from supplier |
| PhytoComm | Mai Men Dong | G176H1118621 | 61946     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *Mai Men Dong*. These samples are listed above in the [calibration samples](#) section.
- 21 406 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 80 spectra of 4 reference samples from the substance/substance group *Mai Men Dong*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Mai Men Dong | G176H1118521 | 61364 <sup>†</sup> | 20      |
| PhytoComm | Mai Men Dong | G176H1118521 | 61694 <sup>†</sup> | 20      |
| PhytoComm | Mai Men Dong | G176H1118621 | 61945 <sup>†</sup> | 20      |
| PhytoComm | Mai Men Dong | G176H1118621 | 61946 <sup>†</sup> | 20      |

- 13 973 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Mai Men Dong*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| PhytoComm | Mai Men Dong | G176H1118322 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Mai Men Dong | G176H1118521 | 3       |
| Phytocomm | Mai Men Dong | 1206mmd      | 1       |
| Phytocomm | Mai Men Dong | G176H1118221 | 1       |
| Phytocomm | Mai Men Dong | g176h1118221 | 1       |
| Phytocomm | Mai Men Dong | H1118021     | 2       |
| PhytoComm | Mai Men Dong | H1118021     | 2       |

- 1970 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Mai Men Dong* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mai Men Dong* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 80            | 0              | 13 973        |
| <b>Type C</b> | 1              | 4             | 7              | 1969          |

The substance/substance group *Mai Men Dong* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.5000 %) |
| <b>Type C</b> | 99.9585 % (> 99.6791 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61364     | 61364               | 0.00                         | 13.61                           |
| 61694     | 61694               | 0.00                         | 12.24                           |
| 61945     | 61945               | 0.00                         | 16.15                           |
| 61946     | 61946               | 0.00                         | 16.29                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Mai Ya**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60210-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G123H1119421 | 61520     | 40      | from supplier |
| PhytoComm | Mai Ya    | G123H1119521 | 61745     | 40      | from supplier |
| PhytoComm | Mai Ya    | G123H1119521 | 62069     | 40      | from supplier |
| PhytoComm | Mai Ya    | G123H1119521 | 62070     | 31      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 151 spectra of 4 reference samples from the substance/substance group *Mai Ya*. These samples are listed above in the [calibration samples](#) section.
- 21 415 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 135 spectra of 4 reference samples from the substance/substance group *Mai Ya*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Mai Ya    | G123H1119421 | 61229              | 75      |
| PhytoComm | Mai Ya    | G123H1119521 | 61745 <sup>†</sup> | 20      |
| PhytoComm | Mai Ya    | G123H1119521 | 62069 <sup>†</sup> | 20      |
| PhytoComm | Mai Ya    | G123H1119521 | 62070 <sup>†</sup> | 20      |

- 13 918 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Mai Ya*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Mai Ya    | G123H1119521 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Mai Ya    | G123H1119022 | 1       |
| PhytoComm | Mai Ya    | G123H1119022 | 1       |
| Phytocomm | Mai Ya    | g123h1119022 | 1       |
| PhytoComm | Mai Ya    | G123H1119122 | 2       |
| Phytocomm | Mai Ya    | G123H1119122 | 1       |
| PhytoComm | Mai Ya    | H1119922     | 1       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Mai Ya* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mai Ya* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 151           | 0              | 21 415        |
| <b>Type B</b> | 2              | 135           | 0              | 13 916        |
| <b>Type C</b> | 6              | 1             | 7              | 1967          |

The substance/substance group *Mai Ya* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.0265 %) |
| <b>Type B</b> | 99.9838 % (> 99.9492 %)  | 100.0000 % (> 95.5556 %) |
| <b>Type C</b> | 99.6934 % (> 99.4141 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61520     | 61520               | 0.00                         | 7.48                            |
| 61745     | 61745               | 0.00                         | 5.93                            |
| 62069     | 62069               | 0.00                         | 7.53                            |
| 62070     | 62070               | 0.00                         | 7.35                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Man Jing Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60025-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G250H1505522 | 61739     | 40      | from supplier |
| PhytoComm | Man Jing Zi | G250H1505622 | 61899     | 40      | from supplier |
| PhytoComm | Man Jing Zi | G250H1505622 | 61900     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Man Jing Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Man Jing Zi*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Man Jing Zi | G250H1505522 | 61739 <sup>†</sup> | 20      |
| PhytoComm | Man Jing Zi | G250H1505622 | 61899 <sup>†</sup> | 20      |
| PhytoComm | Man Jing Zi | G250H1505622 | 61900 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Man Jing Zi*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| Phytocomm | Man Jing Zi | G250H1505122 | 1       |
| Phytocomm | Man Jing Zi | G250H1505121 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Man Jing Zi | h1505021 | 1       |
| Phytocomm | Man Jing Zi | H1505922 | 1       |
| PhytoComm | Man Jing Zi | H150922  | 1       |

- 1976 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Man Jing Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Man Jing Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 0              | 0             | 5              | 1976          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4420 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61739     | 61739               | 0.00                         | 69.14                           |
| 61899     | 61899               | 0.00                         | 60.87                           |
| 61900     | 61900               | 0.00                         | 60.93                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Mi Huan Jun**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60556-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Mi Huan Jun; Armillariella mellea rhizoma

### Special notes

When selecting the *Mi Huan Jun* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Mi Huan Jun*:

| Supplier  | Substance   | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-------------|--------------|-----------|---------|---------------|
| PhytoComm | Mi Huan Jun | G510H0418422 | 61067     | 40      | from supplier |
| PhytoComm | Mi Huan Jun | G510H0418422 | 61393     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Mi Huan Jun*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 80 spectra of 2 reference samples from the substance/substance group *Mi Huan Jun*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Mi Huan Jun | G510H0418422 | 61067 <sup>†</sup> | 20      |
| PhytoComm | Mi Huan Jun | G510H0418422 | 61101              | 60      |

- 13 973 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Mi Huan Jun*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| Phytocomm | Mi Huan Jun | G510H0418221 | 1       |
| Phytocomm | Mi Huan Jun | G510H0418422 | 1       |
| Phytocomm | Mi Huan Jun | G510H110164  | 2       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1977 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Mi Huan Jun* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mi Huan Jun* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 65            | 15             | 13 973        |
| <b>Type C</b> | 1              | 1             | 3              | 1976          |

The substance/substance group *Mi Huan Jun* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 81.2500 % (> 77.5000 %)  |
| <b>Type C</b> | 99.9751 % (> 99.6963 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61067     | 61067               | 0.00                         | 7.86                            |
| 61393     | 61393               | 0.00                         | 8.20                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Mo Yao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50343-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Mo Yao*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Mo Yao    | G169H0732621 | 61957     | 40      | from supplier |
| PhytoComm | Mo Yao    | G169H0732621 | 61958     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Mo Yao*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Mo Yao    | G169H0732621 | 61957 <sup>†</sup> | 20      |
| PhytoComm | Mo Yao    | G169H0732621 | 61958 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Mo Yao*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Mo Yao    | G1690732222  | 1       |
| phytocomm | Mo Yao    | G169H0732023 | 1       |
| Phytocomm | Mo Yao    | G169H0732122 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Mo Yao    | G169H0732222 | 2       |
| Phytocomm | Mo Yao    | H0732922     | 1       |
| Caelo     | Mo Yao    | G169H0732222 | 1       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Mo Yao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mo Yao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 8              | 1973          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4414 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61957     | 61957               | 0.00                         | 12.69                           |
| 61958     | 61958               | 0.00                         | 13.57                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Mu Dan Pi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60113-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G166H0741421 | 61358     | 40      | from supplier |
| PhytoComm | Mu Dan Pi | G166H0741621 | 61947     | 40      | from supplier |
| PhytoComm | Mu Dan Pi | G166H0741621 | 61948     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Mu Dan Pi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Mu Dan Pi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Mu Dan Pi | G166H0741421 | 61358 <sup>†</sup> | 20      |
| PhytoComm | Mu Dan Pi | G166H0741621 | 61947 <sup>†</sup> | 20      |
| PhytoComm | Mu Dan Pi | G166H0741621 | 61948 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 21 spectra from 8 *Apo-Ident* customers from 6 batches from the substance/substance group *Mu Dan Pi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Mu Dan Pi | G166H0741321 | 2       |
| Phytocomm | Mu Dan Pi | G166H0741421 | 4       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Mu Dan Pi | G166H0741022 | 1       |
| PhytoComm | Mu Dan Pi | G166H0741121 | 2       |
| Phytocomm | Mu Dan Pi | G166H0741121 | 5       |
| Phytocomm | Mu Dan Pi | G166H0741122 | 3       |
| PhytoComm | Mu Dan Pi | G166H0741122 | 1       |
| PhytoComm | Mu Dan Pi | G166H0741321 | 2       |
| Phytocomm | Mu Dan Pi | g166j074122  | 1       |

- 1960 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Mu Dan Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mu Dan Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 1              | 0             | 21             | 1959          |

The substance/substance group *Mu Dan Pi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.9627 % (> 99.6831 %)  | 0.0000 % (≥ 0.0000 %)    |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61358     | 61358               | 0.00                         | 5.43                            |
| 61947     | 61947               | 0.00                         | 6.88                            |
| 61948     | 61948               | 0.00                         | 6.32                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Mu Gua**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60236-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Mu Gua*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Mu Gua    | G063H0424521 | 61696     | 40      | from supplier |
| PhytoComm | Mu Gua    | G063H0424321 | 61706     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Mu Gua*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Mu Gua    | G063H0424521 | 61696 <sup>†</sup> | 20      |
| PhytoComm | Mu Gua    | G063H0424321 | 61706 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Mu Gua*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Mu Gua    | G063H0424521 | 4       |
| PhytoComm | Mu Gua    | G063H0424021 | 2       |
| PhytoComm | Mu Gua    | G063H0424221 | 1       |
| Phytocomm | Mu Gua    | G063H0424221 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1973 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Mu Gua* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mu Gua* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 4              | 40            | 0              | 14 009        |
| <b>Type C</b> | 4              | 7             | 1              | 1969          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 99.9879 % (> 99.9534 %)  | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.6953 % (> 99.4160 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61696     | 61696               | 0.00                         | 9.45                            |
| 61706     | 61706               | 0.00                         | 14.13                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Mu Zei**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60123-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Mu Zei; Equiseti hiemalis herba

### Special notes

When selecting the *Mu Zei* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Zei*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Mu Zei    | G265H0427421 | 61632     | 40      | from supplier |
| PhytoComm | Mu Zei    | G265H0427421 | 62057     | 40      | from supplier |
| PhytoComm | Mu Zei    | G265H0427421 | 62058     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Mu Zei*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Mu Zei*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Mu Zei    | G265H0427421 | 61632 <sup>†</sup> | 20      |
| PhytoComm | Mu Zei    | G265H0427421 | 62057 <sup>†</sup> | 20      |
| PhytoComm | Mu Zei    | G265H0427421 | 62058 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Mu Zei*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Mu Zei    | G265H0427421 | 1       |
| Phytocomm | Mu Zei    | G265H0427823 | 1       |

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<sup>†</sup>These spectra were recorded from 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 | Mu Zei    | G265H0427823 | 1       |
| PhytoComm | Mu Zei    | H0427822     | 1       |

- 1977 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Mu Zei* can be 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 Zei* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 8              | 1             | 3              | 1969          |

The substance/substance group *Mu Zei* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.6961 % (> 99.4173 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61632     | 61632               | 0.00                         | 12.86                           |
| 62057     | 62057               | 0.00                         | 8.52                            |
| 62058     | 62058               | 0.00                         | 8.19                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Niu Bang Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60161-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Niu Bang Zi; Arctii fructus; Arctii lappae fructus

### Special notes

When selecting the *Niu Bang Zi* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Niu Bang Zi*:

| Supplier  | Substance   | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-------------|--------------|-----------|---------|---------------|
| PhytoComm | Niu Bang Zi | G026H0433521 | 61677     | 40      | from supplier |
| PhytoComm | Niu Bang Zi | G026H0433521 | 61744     | 41      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 81 spectra of 2 reference samples from the substance/substance group *Niu Bang Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 485 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Niu Bang Zi*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Niu Bang Zi | G026H0433521 | 61677 <sup>†</sup> | 20      |
| PhytoComm | Niu Bang Zi | G026H0433521 | 61744 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Niu Bang Zi*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| PhytoComm | Niu Bang Zi | G026H0433321 | 1       |
| Phytocomm | Niu Bang Zi | G026H0433321 | 1       |
| phytocomm | Niu Bang Zi | g026h0433321 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Niu Bang Zi | G026H0433521 | 3       |
| Phytocomm | Niu Bang Zi | G026H0433222 | 2       |
| PhytoComm | Niu Bang Zi | G026H0433222 | 1       |
| PhytoComm | Niu Bang Zi | H0433021     | 1       |
| Phytocomm | Niu Bang Zi | H0433021     | 3       |

- 1967 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Niu Bang Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Niu Bang Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 81            | 0              | 21 485        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 3             | 11             | 1967          |

The substance/substance group *Niu Bang Zi* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5926 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4409 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61677     | 61677               | 0.00                         | 8.75                            |
| 61744     | 61744               | 0.00                         | 10.70                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Nü Zhen Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60065-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G138H0345421 | 61510     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Nü Zhen Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 75 spectra of 1 reference samples from the substance/substance group *Nü Zhen Zi*.

| Supplier  | Substance  | Batch        | Sample ID | Spectra |
|-----------|------------|--------------|-----------|---------|
| PhytoComm | Nü Zhen Zi | G138H0345421 | 61219     | 75      |

- 13 978 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 5 batches from the substance/substance group *Nü Zhen Zi*.

| Supplier  | Substance  | Batch        | Spectra |
|-----------|------------|--------------|---------|
| Phytocomm | Nü Zhen Zi | 420319901    | 2       |
| Phytocomm | Nü Zhen Zi | G138H0345421 | 1       |
| PhytoComm | Nü Zhen Zi | G138H0345321 | 1       |
| PhytoComm | Nü Zhen Zi | H0345021     | 1       |
| PhytoComm | Nü Zhen Zi | 420319901    | 1       |
| PhytoComm | Nü Zhen Zi | h0345021     | 1       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Nü Zhen Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nü Zhen Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 75            | 0              | 13 978        |
| <b>Type C</b> | 0              | 1             | 6              | 1974          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4415 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61510     | 61510               | 0.00                         | 10.37                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Pi Pa Ye**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60201-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Pi Pa Ye*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Pi Pa Ye  | G099H0832521 | 61681     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

**Type A** All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Pi Pa Ye*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Pi Pa Ye*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Pi Pa Ye  | G099H0832521 | 61681 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 2 batches from the substance/substance group *Pi Pa Ye*.

| Supplier    | Substance | Batch        | Spectra |
|-------------|-----------|--------------|---------|
| PhytoComm   | Pi Pa Ye  | G099H0832221 | 1       |
| Phytocomm   | Pi Pa Ye  | G099H0832221 | 1       |
| Herbasinica | Pi Pa Ye  | G099H0832221 | 1       |
| PhytoComm   | Pi Pa Ye  | H0832922     | 2       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1976 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Pi Pa Ye* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pi Pa Ye* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 6              | 0             | 5              | 1970          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.7444 % (> 99.4654 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61681     | 61681               | 0.00                         | 6.57                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Pu Gong Ying**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50358-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G239H1315321 | 60854     | 40      | from supplier |
| PhytoComm | Pu Gong Ying | G239H1315321 | 61431     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Pu Gong Ying*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 75 spectra of 1 reference samples from the substance/substance group *Pu Gong Ying*.

| Supplier  | Substance    | Batch        | Sample ID | Spectra |
|-----------|--------------|--------------|-----------|---------|
| PhytoComm | Pu Gong Ying | G239H1315321 | 61139     | 75      |

- 13 978 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 2 batches from the substance/substance group *Pu Gong Ying*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| PhytoComm | Pu Gong Ying | G239H1315321 | 5       |
| PhytoComm | Pu Gong Ying | G239H1315321 | 2       |
| PhytoComm | Pu Gong Ying | H1315923     | 1       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Pu Gong Ying* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pu Gong Ying* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 74            | 1              | 13 978        |
| <b>Type C</b> | 6              | 7             | 1              | 1967          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 98.6667 % (> 94.6667 %)  |
| <b>Type C</b> | 99.7122 % (> 99.4328 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60854     | 60854               | 0.00                         | 10.23                           |
| 61431     | 61431               | 0.00                         | 12.71                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Pu Huang**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60066-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Pu Huang; Typhae pollen

### Special notes

When selecting the *Pu 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Huang*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Pu Huang  | G245H1316521 | 61794     | 40      | from supplier |
| PhytoComm | Pu Huang  | G245H1316521 | 61810     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Pu Huang*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Pu Huang*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Pu Huang  | G245H1316521 | 61794 <sup>†</sup> | 20      |
| PhytoComm | Pu Huang  | G245H1316521 | 61810 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Pu Huang*.

| Supplier  | Substance | Batch    | Spectra |
|-----------|-----------|----------|---------|
| phytocomm | Pu Huang  | H1316021 | 1       |
| Phytocomm | Pu Huang  | H1316021 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1979 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Pu 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 *Pu 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 2              | 0             | 2              | 1977          |

The substance/substance group *Pu 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.8721 % (> 99.5943 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61794     | 61794               | 0.00                         | 10.94                           |
| 61810     | 61810               | 0.00                         | 10.59                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Qian Hu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60495-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Qian Hu; Peucedani radix

### Special notes

When selecting the *Qian 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Qian Hu*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Qian Hu   | G185H0926421 | 61381     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Qian Hu*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Qian Hu*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Qian Hu   | G185H0926421 | 61381 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Qian Hu*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Qian Hu   | G185H0926322 | 2       |
| Phytocomm | Qian Hu   | G185H0926121 | 1       |
| PhytoComm | Qian Hu   | H0926021     | 1       |
| Phytocomm | Qian Hu   | H0926021     | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1976 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Qian 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 *Qian 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 5              | 1976          |

The substance/substance group *Qian Hu* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4420 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61381     | 61381               | 0.00                         | 9.77                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Qiang Huo**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60109-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G172H0840521 | 61789     | 40      | from supplier |
| PhytoComm | Qiang Huo | G172H0840521 | 61808     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Qiang Huo*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Qiang Huo*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Qiang Huo | G172H0840521 | 61789 <sup>†</sup> | 20      |
| PhytoComm | Qiang Huo | G172H0840521 | 61808 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Qiang Huo*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Qiang Huo | G172H0840321 | 1       |
| PhytoComm | Qiang Huo | G172H0840321 | 1       |
| Phytocomm | Qiang Huo | g172h0841321 | 1       |
| PhytoComm | Qiang Huo | H0840922     | 2       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1976 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Qiang Huo* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Qiang Huo* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 39            | 1              | 14 013        |
| <b>Type C</b> | 3              | 0             | 5              | 1973          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 97.5000 % (> 90.0000 %)  |
| <b>Type C</b> | 99.7886 % (> 99.5096 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61789     | 61789               | 0.00                         | 5.55                            |
| 61808     | 61808               | 0.00                         | 4.90                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Qin Jiao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60222-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Qin Jiao*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Qin Jiao  | G113H1059521 | 61772 <sup>†</sup> | 20      |
| PhytoComm | Qin Jiao  | G113H1059521 | 61814 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 *Qin Jiao*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Qin Jiao  | G113H1059022 | 2       |
| PhytoComm | Qin Jiao  | G113H1059022 | 1       |
| Phytocomm | Qin Jiao  | G113H1059121 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Qin Jiao  | G113H1059121 | 1       |
| PhytoComm | Qin Jiao  | G113H1059321 | 1       |
| PhytoComm | Qin Jiao  | H1059922     | 1       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Qin Jiao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Qin Jiao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 6              | 0             | 8              | 1967          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.7583 % (> 99.4790 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61772     | 61772               | 0.00                         | 12.90                           |
| 61814     | 61814               | 0.00                         | 13.18                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Qing Pi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50371-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Qing Pi*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Qing Pi   | G074H0809621 | 62041     | 40      | from supplier |
| PhytoComm | Qing Pi   | G074H0809621 | 62042     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Qing Pi*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Qing Pi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Qing Pi   | G074H0809621 | 62041 <sup>†</sup> | 20      |
| PhytoComm | Qing Pi   | G074H0809621 | 62042 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Qing Pi*.

| Supplier  | Substance | Batch       | Spectra |
|-----------|-----------|-------------|---------|
| PhytoComm | Qing Pi   | G074H100713 | 2       |
| Phytocomm | Qing Pi   | G074H100713 | 2       |
| Phytocomm | Qing Pi   | g074h100713 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1976 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Qing Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Qing Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 5              | 1976          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4420 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 62041     | 62041               | 0.00                         | 8.70                            |
| 62042     | 62042               | 0.00                         | 8.81                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ren Shen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60984-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Ren Shen; Ginseng radix et rhizoma

### Special notes

When selecting the *Ren 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Ren Shen*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Ren Shen  | G115H0562621 | 61839     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Ren Shen*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Ren Shen*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Ren Shen  | G115H0562621 | 61839 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Ren Shen*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| phythocom | Ren Shen  | 115h562121   | 1       |
| phythocom | Ren Shen  | g115h0562121 | 1       |
| Phytocomm | Ren Shen  | G1150562121  | 1       |
| PhytoComm | Ren Shen  | G115H0562121 | 1       |
| Phytocomm | Ren Shen  | g115ho562121 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1976 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Ren 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 *Ren 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 5              | 1976          |

The substance/substance group *Ren 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4420 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61839     | 61839               | 0.00                         | 9.32                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Rou Cong Rong**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60182-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Rou Cong Rong*:

| Supplier  | Substance     | Batch        | Sample ID | Spectra | Certificate   |
|-----------|---------------|--------------|-----------|---------|---------------|
| PhytoComm | Rou Cong Rong | G072H1460621 | 61834     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Rou Cong Rong*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Rou Cong Rong*.

| Supplier  | Substance     | Batch        | Sample ID          | Spectra |
|-----------|---------------|--------------|--------------------|---------|
| PhytoComm | Rou Cong Rong | G072H1460621 | 61834 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Rou Cong Rong*.

| Supplier  | Substance     | Batch        | Spectra |
|-----------|---------------|--------------|---------|
| PhytoComm | Rou Cong Rong | G072H1460321 | 1       |
| Bios      | Rou Cong Rong | 434550       | 1       |
| PhytoComm | Rou Cong Rong | 444151       | 1       |

- 1978 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

<sup>†</sup>These spectra were recorded from 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 *Rou Cong Rong* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Rou Cong Rong* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 1              | 0             | 3              | 1977          |

The substance/substance group *Rou Cong Rong* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9378 % (> 99.6594 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61834     | 61834               | 0.00                         | 14.77                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ru Xiang**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50370-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G174H0820421 | 61048     | 40      | from supplier |
| PhytoComm | Ru Xiang  | G174H0820421 | 61481     | 40      | from supplier |
| PhytoComm | Ru Xiang  | G174H0820421 | 61755     | 40      | from supplier |
| PhytoComm | Ru Xiang  | G174H0820621 | 61935     | 40      | from supplier |
| PhytoComm | Ru Xiang  | G174H0820621 | 61936     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Ru Xiang*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 135 spectra of 4 reference samples from the substance/substance group *Ru Xiang*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Ru Xiang  | G174H0820421 | 61189              | 75      |
| PhytoComm | Ru Xiang  | G174H0820421 | 61755 <sup>†</sup> | 20      |
| PhytoComm | Ru Xiang  | G174H0820621 | 61935 <sup>†</sup> | 20      |
| PhytoComm | Ru Xiang  | G174H0820621 | 61936 <sup>†</sup> | 20      |

- 13 918 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 5 batches from the substance/substance group *Ru Xiang*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Ru Xiang  | G174H0820421 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Ru Xiang  | G174H0820421 | 2       |
| Phytocomm | Ru Xiang  | G174H0820231 | 1       |
| PhytoComm | Ru Xiang  | G174H0820321 | 1       |
| Phytocomm | Ru Xiang  | G174H0820123 | 1       |
| PhytoComm | Ru Xiang  | H0820923     | 1       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Ru Xiang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ru Xiang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 200           | 0              | 21 366        |
| <b>Type B</b> | 0              | 135           | 0              | 13 918        |
| <b>Type C</b> | 0              | 4             | 3              | 1974          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.5556 %) |
| <b>Type C</b> | 100.0000 % (> 99.4415 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61048     | 61048               | 0.00                         | 30.51                           |
| 61481     | 61481               | 0.00                         | 29.90                           |
| 61755     | 61755               | 0.00                         | 28.71                           |
| 61935     | 61935               | 0.00                         | 71.91                           |
| 61936     | 61936               | 0.00                         | 73.02                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **San Leng**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60029-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G270H0311522 | 61889     | 40      | from supplier |
| PhytoComm | San Leng  | G270H0311522 | 61890     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *San Leng*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | San Leng  | G270H0311522 | 61889 <sup>†</sup> | 20      |
| PhytoComm | San Leng  | G270H0311522 | 61890 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *San Leng*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | San Leng  | G270H0311121 | 1       |
| PhytoComm | San Leng  | G270H0311221 | 1       |
| Phytocomm | San Leng  | g270h0311221 | 1       |
| Phytocomm | San Leng  | H0311922     | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1977 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *San Leng* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *San Leng* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 3              | 78            | 2              | 21 483        |
| <b>Type B</b> | 2              | 38            | 2              | 14 011        |
| <b>Type C</b> | 1              | 0             | 4              | 1976          |

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        |
|---------------|-------------------------|-------------------------|
| <b>Type A</b> | 99.9877 % (> 99.9684 %) | 97.5000 % (> 93.7500 %) |
| <b>Type B</b> | 99.9838 % (> 99.9494 %) | 95.0000 % (> 87.5000 %) |
| <b>Type C</b> | 99.9689 % (> 99.6901 %) | n/a (n/a)               |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61889     | 61889               | 0.00                         | 4.17                            |
| 61890     | 61890               | 0.00                         | 4.23                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **San Qi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60415-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

San Qi; Notoginseng radix; Pseudoginseng radix

### Special notes

When selecting the *San Qi* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G203H0312321 | 60916     | 40      | from supplier |
| PhytoComm | San Qi    | G203H0312321 | 61460     | 40      | from supplier |
| PhytoComm | San Qi    | G203H0312321 | 61765     | 40      | from supplier |
| PhytoComm | San Qi    | G203H0312421 | 61793     | 40      | from supplier |
| PhytoComm | San Qi    | G203H0312421 | 61805     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *San Qi*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 135 spectra of 4 reference samples from the substance/substance group *San Qi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | San Qi    | G203H0312321 | 61168              | 75      |
| PhytoComm | San Qi    | G203H0312321 | 61765 <sup>†</sup> | 20      |
| PhytoComm | San Qi    | G203H0312421 | 61793 <sup>†</sup> | 20      |
| PhytoComm | San Qi    | G203H0312421 | 61805 <sup>†</sup> | 20      |

- 13 918 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *San Qi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| phytocomm | San Qi    | G203H0312021 | 1       |

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<sup>†</sup>These spectra were recorded from 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 | San Qi    | G203H0312021 | 2       |
| Phytocomm | San Qi    | g203h0312021 | 1       |

- 1977 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *San Qi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *San Qi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 200           | 0              | 21 366        |
| <b>Type B</b> | 0              | 135           | 0              | 13 918        |
| <b>Type C</b> | 0              | 0             | 4              | 1977          |

The substance/substance group *San Qi* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.5556 %) |
| <b>Type C</b> | 100.0000 % (> 99.4424 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60916     | 60916               | 0.00                         | 9.42                            |
| 61460     | 61460               | 0.00                         | 7.83                            |

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| <b>Sample ID</b> | <b>Reference sample ID</b> | <b>Distance to reference sample</b> | <b>Distance to next foreign sample</b> |
|------------------|----------------------------|-------------------------------------|----------------------------------------|
| 61765            | 61765                      | 0.00                                | 7.74                                   |
| 61793            | 61793                      | 0.00                                | 8.71                                   |
| 61805            | 61805                      | 0.00                                | 7.55                                   |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Sang Bai Pi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50287-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G161H1042521 | 61670     | 40      | from supplier |
| PhytoComm | Sang Bai Pi | G161H1042621 | 61989     | 40      | from supplier |
| PhytoComm | Sang Bai Pi | G161H1042621 | 61990     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Sang Bai Pi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Sang Bai Pi*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Sang Bai Pi | G161H1042521 | 61670 <sup>†</sup> | 20      |
| PhytoComm | Sang Bai Pi | G161H1042621 | 61989 <sup>†</sup> | 20      |
| PhytoComm | Sang Bai Pi | G161H1042621 | 61990 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 3 batches from the substance/substance group *Sang Bai Pi*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| PhytoComm | Sang Bai Pi | G161H1042121 | 2       |
| Phytocomm | Sang Bai Pi | G161H1042321 | 1       |

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<sup>†</sup>These spectra were recorded from 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 | Sang Bai Pi | G161H1042321 | 2       |
| PhytoComm | Sang Bai Pi | G161H1042922 | 1       |
| PhytoComm | Sang Bai Pi | G161H1042922 | 1       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Sang Bai Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sang Bai Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 1              | 119           | 1              | 21 445        |
| <b>Type B</b> | 0              | 59            | 1              | 13 993        |
| <b>Type C</b> | 12             | 0             | 7              | 1962          |

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        |
|---------------|--------------------------|-------------------------|
| <b>Type A</b> | 99.9980 % (> 99.9785 %)  | 99.1667 % (> 96.6667 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 98.3333 % (> 93.3333 %) |
| <b>Type C</b> | 99.4537 % (> 99.1745 %)  | n/a (n/a)               |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61670     | 61670               | 0.00                         | 5.75                            |
| 61989     | 61989               | 0.00                         | 11.66                           |
| 61990     | 61990               | 0.00                         | 11.99                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Sang Ji Shend**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60142-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G146H1045522 | 61649     | 40      | from supplier |
| PhytoComm | Sang Ji Shend | G146H1045621 | 61991     | 40      | from supplier |
| PhytoComm | Sang Ji Shend | G146H1045621 | 61992     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Sang Ji Shend*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Sang Ji Shend*.

| Supplier  | Substance     | Batch        | Sample ID          | Spectra |
|-----------|---------------|--------------|--------------------|---------|
| PhytoComm | Sang Ji Shend | G146H1045522 | 61649 <sup>†</sup> | 20      |
| PhytoComm | Sang Ji Shend | G146H1045621 | 61991 <sup>†</sup> | 20      |
| PhytoComm | Sang Ji Shend | G146H1045621 | 61992 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 9 *Apo-Ident* customers from 5 batches from the substance/substance group *Sang Ji Shend*.

| Supplier    | Substance     | Batch        | Spectra |
|-------------|---------------|--------------|---------|
| PhytoComm   | Sang Ji Shend | G146H1045322 | 1       |
| Herbasinica | Sang Ji Shend | G146H1045322 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Sang Ji Shend | G146H1045522 | 4       |
| PhytoComm | Sang Ji Shend | G146H1045222 | 1       |
| Phytocomm | Sang Ji Shend | G146H1045222 | 1       |
| Phytocomm | Sang Ji Shend | g146h1045222 | 1       |
| Phytocomm | Sang Ji Shend | H1045021     | 2       |

- 1970 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Sang 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 2              | 4             | 7              | 1968          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.8653 % (> 99.5858 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61649     | 61649               | 0.00                         | 14.90                           |
| 61991     | 61991               | 0.00                         | 11.78                           |
| 61992     | 61992               | 0.00                         | 11.86                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Sang Shen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60022-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Sang Shen; Mori fructus

### Special notes

When selecting the *Sang 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Shen*:

| Supplier  | Substance | Batch         | Sample ID | Spectra | Certificate   |
|-----------|-----------|---------------|-----------|---------|---------------|
| PhytoComm | Sang Shen | G163FB1047621 | 61836     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Sang Shen*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Sang Shen*.

| Supplier  | Substance | Batch         | Sample ID          | Spectra |
|-----------|-----------|---------------|--------------------|---------|
| PhytoComm | Sang Shen | G163FB1047621 | 61836 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Sang Shen*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Sang Shen | G163H1047121 | 2       |
| PhytoComm | Sang Shen | G163H1047221 | 1       |
| Phytocomm | Sang Shen | G163H1047221 | 1       |
| PhytoComm | Sang Shen | H1047921     | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1976 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Sang 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 *Sang 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 5              | 1976          |

The substance/substance group *Sang 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4420 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61836     | 61836               | 0.00                         | 11.89                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Sang Ye**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60079-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G162H1043421 | 61496     | 40      | from supplier |
| PhytoComm | Sang Ye   | G162H1043621 | 61973     | 40      | from supplier |
| PhytoComm | Sang Ye   | G162H1043621 | 61974     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Sang Ye*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 115 spectra of 3 reference samples from the substance/substance group *Sang Ye*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Sang Ye   | G162H1043421 | 61204              | 75      |
| PhytoComm | Sang Ye   | G162H1043621 | 61973 <sup>†</sup> | 20      |
| PhytoComm | Sang Ye   | G162H1043621 | 61974 <sup>†</sup> | 20      |

- 13 938 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 10 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Sang Ye*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Sang Ye   | 421013801    | 1       |
| Phytocomm | Sang Ye   | G162H1043421 | 3       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Sang Ye   | G162H1043121 | 1       |
| PhytoComm | Sang Ye   | G162H1043121 | 4       |
| PhytoComm | Sang Ye   | H1043021     | 1       |

- 1971 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Sang Ye* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sang Ye* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 115           | 0              | 13 938        |
| <b>Type C</b> | 10             | 7             | 3              | 1961          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 94.7826 %) |
| <b>Type C</b> | 99.5451 % (> 99.2657 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61496     | 61496               | 0.00                         | 11.01                           |
| 61973     | 61973               | 0.00                         | 14.23                           |
| 61974     | 61974               | 0.00                         | 14.17                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Sang Zhi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60091-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G164H1044421 | 61366     | 40      | from supplier |
| PhytoComm | Sang Zhi  | G164H1044621 | 61969     | 40      | from supplier |
| PhytoComm | Sang Zhi  | G164H1044621 | 61970     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Sang Zhi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Sang Zhi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Sang Zhi  | G164H1044421 | 61366 <sup>†</sup> | 20      |
| PhytoComm | Sang Zhi  | G164H1044621 | 61969 <sup>†</sup> | 20      |
| PhytoComm | Sang Zhi  | G164H1044621 | 61970 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 3 batches from the substance/substance group *Sang Zhi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Sang Zhi  | G164H1044022 | 4       |
| PhytoComm | Sang Zhi  | G164H1044221 | 1       |

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<sup>†</sup>These spectra were recorded from 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 | Sang Zhi  | G164H1044022 | 1       |
| PhytoComm | Sang Zhi  | G164H1044221 | 1       |
| PhytoComm | Sang Zhi  | H1044921     | 2       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Sang Zhi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sang Zhi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 1              | 120           | 0              | 21 445        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 3              | 0             | 9              | 1969          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 99.9959 % (> 99.9765 %)  | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.9067 % (> 99.6274 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61366     | 61366               | 0.00                         | 7.81                            |
| 61969     | 61969               | 0.00                         | 8.16                            |
| 61970     | 61970               | 0.00                         | 8.09                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Sha Ren**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60184-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G018H0939322 | 60955     | 40      | from supplier |
| PhytoComm | Sha Ren   | G018H0939522 | 61703     | 40      | from supplier |
| PhytoComm | Sha Ren   | G018H0939523 | 61799     | 40      | from supplier |
| PhytoComm | Sha Ren   | G018H0939523 | 61818     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Sha Ren*. These samples are listed above in the [calibration samples](#) section.
- 21 406 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Sha Ren*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Sha Ren   | G018H0939522 | 61703 <sup>†</sup> | 20      |
| PhytoComm | Sha Ren   | G018H0939523 | 61799 <sup>†</sup> | 20      |
| PhytoComm | Sha Ren   | G018H0939523 | 61818 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 8 *Apo-Ident* customers from 5 batches from the substance/substance group *Sha Ren*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Sha Ren   | G018H0939522 | 1       |
| PhytoComm | Sha Ren   | G018H0939321 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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   | G018H0939523 | 1       |
| Phytocomm | Sha Ren   | g018h0939321 | 1       |
| PhytoComm | Sha Ren   | H0939022     | 4       |
| Euro OTC  | Sha Ren   | H0939022     | 1       |
| Phytocomm | Sha Ren   | H0939022     | 2       |

- 1969 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Sha Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sha Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 5              | 4             | 8              | 1964          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.7264 % (> 99.4469 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60955     | 60955               | 0.00                         | 8.40                            |
| 61703     | 61703               | 0.00                         | 10.66                           |
| 61799     | 61799               | 0.00                         | 13.52                           |
| 61818     | 61818               | 0.00                         | 14.45                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Sha Shen (Bei)**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60200-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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) | G117H0754322 | 61517     | 40      | from supplier |

### Validation samples

A total of 37 600 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.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 75 spectra of 1 reference samples from the substance/substance group *Sha Shen (Bei)*.

| Supplier  | Substance      | Batch        | Sample ID | Spectra |
|-----------|----------------|--------------|-----------|---------|
| PhytoComm | Sha Shen (Bei) | G117H0754322 | 61226     | 75      |

- 13 978 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 5 *Apo-Ident* customers from 2 batches from the substance/substance group *Sha Shen (Bei)*.

| Supplier    | Substance      | Batch        | Spectra |
|-------------|----------------|--------------|---------|
| PhytoComm   | Sha Shen (Bei) | G117H0754121 | 3       |
| Herbasin    | Sha Shen (Bei) | G117H0754121 | 4       |
| Phytocomm   | Sha Shen (Bei) | G117H0754322 | 3       |
| Herbasinica | Sha Shen (Bei) | G117H0754121 | 1       |

- 1970 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the



samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Sha 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 75            | 0              | 13 978        |
| <b>Type C</b> | 1              | 3             | 8              | 1969          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.0000 %) |
| <b>Type C</b> | 99.9689 % (> 99.6895 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61517     | 61517               | 0.00                         | 7.06                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Shan Yao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60207-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G091H0330521 | 61699     | 40      | from supplier |
| PhytoComm | Shan Yao  | G091H0330622 | 62009     | 40      | from supplier |
| PhytoComm | Shan Yao  | G091H0330622 | 62010     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Shan Yao*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Shan Yao*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Shan Yao  | G091H0330521 | 61699 <sup>†</sup> | 20      |
| PhytoComm | Shan Yao  | G091H0330622 | 62009 <sup>†</sup> | 20      |
| PhytoComm | Shan Yao  | G091H0330622 | 62010 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Shan Yao*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Shan Yao  | G091H0330521 | 2       |
| PhytoComm | Shan Yao  | G091H0330521 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Shan Yao  | G091H0330122 | 1       |
| PhytoComm | Shan Yao  | H0330021     | 2       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Shan 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 6              | 4             | 3              | 1968          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.5469 % (> 99.2677 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61699     | 61699               | 0.00                         | 8.39                            |
| 62009     | 62009               | 0.00                         | 11.07                           |
| 62010     | 62010               | 0.00                         | 11.56                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Shan Yu Rou**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60226-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G080H0333421 | 61723     | 40      | from supplier |
| PhytoComm | Shan Yu Rou | G080H0333621 | 62011     | 40      | from supplier |
| PhytoComm | Shan Yu Rou | G080H0333621 | 62012     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Shan Yu Rou*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Shan Yu Rou*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Shan Yu Rou | G080H0333421 | 61723 <sup>†</sup> | 20      |
| PhytoComm | Shan Yu Rou | G080H0333621 | 62011 <sup>†</sup> | 20      |
| PhytoComm | Shan Yu Rou | G080H0333621 | 62012 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Shan Yu Rou*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| PhytoComm | Shan Yu Rou | G080H0333421 | 1       |
| PhytoComm | Shan Yu Rou | G080H0333021 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Shan Yu Rou | G080H0333021 | 1       |
| Phytocomm | Shan Yu Rou | G080H0333121 | 2       |
| PhytoComm | Shan Yu Rou | G080H0333121 | 1       |
| PhytoComm | Shan Yu Rou | G080H033321  | 1       |
| Phytocomm | Shan Yu Rou | G080H0333221 | 1       |
| Phytocomm | Shan Yu Rou | g080h0333221 | 1       |

- 1971 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Shan Yu Rou* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Shan Yu Rou* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 1              | 60            | 0              | 13 992        |
| <b>Type C</b> | 18             | 3             | 7              | 1953          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 99.9919 % (> 99.9574 %)  | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.1921 % (> 98.9127 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61723     | 61723               | 0.00                         | 9.06                            |
| 62011     | 62011               | 0.00                         | 10.48                           |
| 62012     | 62012               | 0.00                         | 9.99                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Shan Zha**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60192-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Shan Zha; Crataegi fructus

### Special notes

When selecting the *Shan Zha* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Shan Zha*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Shan Zha  | G082H0331522 | 62029     | 40      | from supplier |
| PhytoComm | Shan Zha  | G082H0331522 | 62030     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Shan Zha*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Shan Zha*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Shan Zha  | G082H0331522 | 62029 <sup>†</sup> | 20      |
| PhytoComm | Shan Zha  | G082H0331522 | 62030 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Shan Zha*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Shan Zha  | G082H0331521 | 1       |
| phytocomm | Shan Zha  | G082H0331022 | 1       |
| PhytoComm | Shan Zha  | G082H0331022 | 4       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Shan Zha  | G082H0331022 | 1       |
| Phytocomm | Shan Zha  | G082H0331324 | 1       |
| PhytoComm | Shan Zha  | G082H0331324 | 1       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Shan Zha* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Shan Zha* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 1              | 0             | 9              | 1971          |

The substance/substance group *Shan Zha* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.9733 % (> 99.6940 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 62029     | 62029               | 0.00                         | 7.85                            |
| 62030     | 62030               | 0.00                         | 7.24                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **She Gan**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60335-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G048H1034422 | 61682     | 40      | from supplier |
| PhytoComm | She Gan   | G048H1034621 | 61771     | 40      | from supplier |
| PhytoComm | She Gan   | G048H1034621 | 61828     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *She Gan*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *She Gan*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | She Gan   | G048H1034422 | 61682 <sup>†</sup> | 20      |
| PhytoComm | She Gan   | G048H1034621 | 61771 <sup>†</sup> | 20      |
| PhytoComm | She Gan   | G048H1034621 | 61828 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *She Gan*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | She Gan   | G048H1034422 | 1       |
| PhytoComm | She Gan   | G048H1034021 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | She Gan   | G048H1034021 | 2       |
| Phytocomm | She Gan   | G048H1034122 | 2       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *She Gan* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *She Gan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 4              | 59            | 1              | 13 989        |
| <b>Type C</b> | 12             | 1             | 5              | 1963          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 99.9781 % (> 99.9436 %)  | 98.3333 % (> 93.3333 %)  |
| <b>Type C</b> | 99.6547 % (> 99.3756 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61682     | 61682               | 0.00                         | 6.18                            |
| 61771     | 61771               | 0.00                         | 5.04                            |
| 61828     | 61828               | 0.00                         | 5.78                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Shen Qu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60020-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G156H0935421 | 61025     | 40      | from supplier |
| PhytoComm | Shen Qu   | G156H0935421 | 61494     | 40      | from supplier |
| PhytoComm | Shen Qu   | G156H0935521 | 61665     | 40      | from supplier |
| PhytoComm | Shen Qu   | G156H0935522 | 61971     | 40      | from supplier |
| PhytoComm | Shen Qu   | G156H0935522 | 61972     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Shen Qu*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 135 spectra of 4 reference samples from the substance/substance group *Shen Qu*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Shen Qu   | G156H0935421 | 61202              | 75      |
| PhytoComm | Shen Qu   | G156H0935521 | 61665 <sup>†</sup> | 20      |
| PhytoComm | Shen Qu   | G156H0935522 | 61971 <sup>†</sup> | 20      |
| PhytoComm | Shen Qu   | G156H0935522 | 61972 <sup>†</sup> | 20      |

- 13 918 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 5 batches from the substance/substance group *Shen Qu*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| PhytoComm | Shen Qu   | G156H0935521 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Shen Qu   | G156H0935521 | 1       |
| phytocomm | Shen Qu   | G156H0935023 | 1       |
| Phytocomm | Shen Qu   | G156H0935023 | 1       |
| PhytoComm | Shen Qu   | G156H0935121 | 1       |
| phytocomm | Shen Qu   | g156h0935421 | 1       |
| PhytoComm | Shen Qu   | H0935021     | 2       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Shen Qu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Shen Qu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 200           | 0              | 21 366        |
| <b>Type B</b> | 0              | 135           | 0              | 13 918        |
| <b>Type C</b> | 0              | 4             | 4              | 1973          |

The substance/substance group *Shen Qu* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.5556 %) |
| <b>Type C</b> | 100.0000 % (> 99.4414 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61025     | 61025               | 0.00                         | 22.39                           |
| 61494     | 61494               | 0.00                         | 19.84                           |
| 61665     | 61665               | 0.00                         | 16.65                           |
| 61971     | 61971               | 0.00                         | 16.45                           |
| 61972     | 61972               | 0.00                         | 16.52                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Sheng Jiang**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60017-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G253H0534421 | 60991     | 40      | from supplier |
| PhytoComm | Sheng Jiang | G253H0534421 | 61414     | 40      | from supplier |
| PhytoComm | Sheng Jiang | G253H0534522 | 61650     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Sheng Jiang*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 95 spectra of 2 reference samples from the substance/substance group *Sheng Jiang*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Sheng Jiang | G253H0534421 | 61122              | 75      |
| PhytoComm | Sheng Jiang | G253H0534522 | 61650 <sup>†</sup> | 20      |

- 13 958 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Sheng Jiang*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| Phytocomm | Sheng Jiang | G253H0534522 | 1       |
| PhytoComm | Sheng Jiang | G253H0534522 | 3       |
| PhytoComm | Sheng Jiang | G253H0534221 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Sheng Jiang | G253H0534221 | 2       |
| PhytoComm | Sheng Jiang | G253H0534321 | 2       |
| PhytoComm | Sheng Jiang | H0534022     | 1       |
| Phytocomm | Sheng Jiang | H0534022     | 1       |

- 1970 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Sheng Jiang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sheng Jiang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 1              | 120           | 0              | 21 445        |
| <b>Type B</b> | 2              | 95            | 0              | 13 956        |
| <b>Type C</b> | 2              | 3             | 8              | 1968          |

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         |
|---------------|-------------------------|--------------------------|
| <b>Type A</b> | 99.9939 % (> 99.9744 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 99.9879 % (> 99.9533 %) | 100.0000 % (> 93.6842 %) |
| <b>Type C</b> | 99.9171 % (> 99.6376 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60991     | 60991               | 0.00                         | 6.09                            |
| 61414     | 61414               | 0.00                         | 6.09                            |
| 61650     | 61650               | 0.00                         | 10.70                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Sheng Ma**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60216-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G068H0437421 | 61566     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Sheng Ma*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 75 spectra of 1 reference samples from the substance/substance group *Sheng Ma*.

| Supplier  | Substance | Batch        | Sample ID | Spectra |
|-----------|-----------|--------------|-----------|---------|
| PhytoComm | Sheng Ma  | G068H0437421 | 61275     | 75      |

- 13 978 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Sheng Ma*.

| Supplier  | Substance | Batch         | Spectra |
|-----------|-----------|---------------|---------|
| Phytocomm | Sheng Ma  | G068H0437421  | 2       |
| Phytocomm | Sheng Ma  | g068h04317121 | 1       |
| Phytocomm | Sheng Ma  | G068H0437121  | 1       |
| PhytoComm | Sheng Ma  | G068H0437021  | 1       |
| PhytoComm | Sheng Ma  | G068H0437121  | 2       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the

samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Sheng Ma* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sheng Ma* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 75            | 0              | 13 978        |
| <b>Type C</b> | 4              | 4             | 3              | 1970          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.0000 %) |
| <b>Type C</b> | 99.8348 % (> 99.5555 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61566     | 61566               | 0.00                         | 12.31                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Shi Gao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50368-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G120H0541522 | 61843     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Shi Gao*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Shi Gao*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Shi Gao   | G120H0541522 | 61843 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 19 spectra from 7 *Apo-Ident* customers from 4 batches from the substance/substance group *Shi Gao*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| phythocom | Shi Gao   | G120H0541223 | 2       |
| phytocomm | Shi Gao   | g120h541024  | 1       |
| Phytocomm | Shi Gao   | G120H051024  | 1       |
| Phytocomm | Shi Gao   | G120H0541024 | 9       |
| PhytoComm | Shi Gao   | G120H0541024 | 2       |
| Phytocomm | Shi Gao   | G120H0541223 | 3       |
| PhytoComm | Shi Gao   | G120H0541223 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1962 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Shi 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 19             | 1962          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4408 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61843     | 61843               | 0.00                         | 510.93                          |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Shi Jun Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60793-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Shi Jun Zi; Quisqualis fructus

### Special notes

When selecting the *Shi Jun 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Jun Zi*:

| Supplier  | Substance  | Batch        | Sample ID | Spectra | Certificate   |
|-----------|------------|--------------|-----------|---------|---------------|
| PhytoComm | Shi Jun Zi | G208H0869521 | 61648     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Shi Jun Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Shi Jun Zi*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Shi Jun Zi | G208H0869521 | 61648 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Shi Jun Zi*.
- 1981 spectra from 16 *Apo-Ident* customers from a total of 964 batches from a further 268 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 Jun Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant

<sup>†</sup>These spectra were recorded from 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 *Shi Jun 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 1              | 0             | 0              | 1980          |

The substance/substance group *Shi Jun 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9804 % (> 99.7005 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

### Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61648     | 61648               | 0.00                         | 12.73                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Shi Wei**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50363-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Shi Wei; Pyrrosiae folium

### Special notes

When selecting the *Shi 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Wei*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Shi Wei   | G298HS0800N1 | 61672     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Shi Wei*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Shi Wei*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Shi Wei   | G298HS0800N1 | 61672 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Shi Wei*.

| Supplier  | Substance | Batch    | Spectra |
|-----------|-----------|----------|---------|
| PhytoComm | Shi Wei   | H0543021 | 2       |

- 1979 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the

<sup>†</sup>These spectra were recorded from 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 *Shi 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 *Shi 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 2              | 40            | 0              | 21 524        |
| <b>Type B</b> | 2              | 20            | 0              | 14 031        |
| <b>Type C</b> | 0              | 0             | 2              | 1979          |

The substance/substance group *Shi 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 99.9755 % (> 99.9562 %)  | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 99.9945 % (> 99.9602 %)  | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4445 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61672     | 61672               | 0.00                         | 4.54                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Shu Di (Huang)**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60006-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Shu Di (Huang); Rehmanniae praeparata radix; Rehmanniae radix praep.

### Special notes

When selecting the *Shu Di (Huang)* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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) | G210H1601421 | 61456     | 40      | from supplier |
| PhytoComm | Shu Di (Huang) | G210H1601521 | 61749     | 40      | from supplier |
| PhytoComm | Shu Di (Huang) | G210H1601521 | 62061     | 40      | from supplier |
| PhytoComm | Shu Di (Huang) | G210H1601521 | 62062     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 406 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 135 spectra of 4 reference samples from the substance/substance group *Shu Di (Huang)*.

| Supplier  | Substance      | Batch        | Sample ID          | Spectra |
|-----------|----------------|--------------|--------------------|---------|
| PhytoComm | Shu Di (Huang) | G210H1601421 | 61164              | 75      |
| PhytoComm | Shu Di (Huang) | G210H1601521 | 61749 <sup>†</sup> | 20      |
| PhytoComm | Shu Di (Huang) | G210H1601521 | 62061 <sup>†</sup> | 20      |
| PhytoComm | Shu Di (Huang) | G210H1601521 | 62062 <sup>†</sup> | 20      |

- 13 918 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 19 spectra from 9 *Apo-Ident* customers from 6 batches from the substance/substance group *Shu Di (Huang)*.

| Supplier  | Substance      | Batch        | Spectra |
|-----------|----------------|--------------|---------|
| Phytocomm | Shu Di (Huang) | G210H1601421 | 5       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Shu Di (Huang) | G210H1601521 | 3       |
| PhytoComm | Shu Di (Huang) | G210H1601221 | 1       |
| PhytoComm | Shu Di (Huang) | G210H1601121 | 3       |
| Phytocomm | Shu Di (Huang) | g210h1601221 | 4       |
| Phytocomm | Shu Di (Huang) | G210H1601221 | 1       |
| Phytocomm | Shu Di (Huang) | G210H1601121 | 1       |
| PhytoComm | Shu Di (Huang) | H1601021     | 1       |

- 1962 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Shu Di (Huang)* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Shu Di (Huang)* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 135           | 0              | 13 918        |
| <b>Type C</b> | 12             | 9             | 10             | 1950          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.5556 %) |
| <b>Type C</b> | 99.6956 % (> 99.4160 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61456     | 61456               | 0.00                         | 13.23                           |
| 61749     | 61749               | 0.00                         | 12.96                           |
| 62061     | 62061               | 0.00                         | 7.45                            |
| 62062     | 62062               | 0.00                         | 7.97                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Suan Zao Ren**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60059-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G254H1418322 | 60993     | 50      | from supplier |
| PhytoComm | Suan Zao Ren | G254H1418421 | 61071     | 40      | from supplier |
| PhytoComm | Suan Zao Ren | G254H1418421 | 61417     | 40      | from supplier |
| PhytoComm | Suan Zao Ren | G254H1418621 | 61893     | 40      | from supplier |
| PhytoComm | Suan Zao Ren | G254H1418621 | 61894     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 210 spectra of 5 reference samples from the substance/substance group *Suan Zao Ren*. These samples are listed above in the [calibration samples](#) section.
- 21 356 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 145 spectra of 5 reference samples from the substance/substance group *Suan Zao Ren*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Suan Zao Ren | G254H1418322 | 60993 <sup>†</sup> | 10      |
| PhytoComm | Suan Zao Ren | G254H1418421 | 61071 <sup>†</sup> | 20      |
| PhytoComm | Suan Zao Ren | G254H1418421 | 61125              | 75      |
| PhytoComm | Suan Zao Ren | G254H1418621 | 61893 <sup>†</sup> | 20      |
| PhytoComm | Suan Zao Ren | G254H1418621 | 61894 <sup>†</sup> | 20      |

- 13 908 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Suan Zao Ren*.

<sup>†</sup>These spectra were recorded from 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 | Suan Zao Ren | G254H1418421 | 1       |
| PhytoComm | Suan Zao Ren | G254H1418121 | 1       |
| Phytocomm | Suan Zao Ren | g254h1418121 | 2       |
| Phytocomm | Suan Zao Ren | G254H1418121 | 2       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

### Validation results

The validation runs checked whether the substance/substance group *Suan Zao Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Suan Zao Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 210           | 0              | 21 356        |
| <b>Type B</b> | 0              | 145           | 0              | 13 908        |
| <b>Type C</b> | 0              | 1             | 5              | 1975          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.1429 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.8621 %) |
| <b>Type C</b> | 100.0000 % (> 99.4417 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

### Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60993     | 60993               | 0.00                         | 25.37                           |

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| <b>Sample ID</b> | <b>Reference sample ID</b> | <b>Distance to reference sample</b> | <b>Distance to next foreign sample</b> |
|------------------|----------------------------|-------------------------------------|----------------------------------------|
| 61071            | 61071                      | 0.00                                | 26.61                                  |
| 61417            | 61417                      | 0.00                                | 24.97                                  |
| 61893            | 61893                      | 0.00                                | 18.15                                  |
| 61894            | 61894                      | 0.00                                | 18.31                                  |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Suo Yang**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60117-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Suo Yang; Cynomorii songarici herba

### Special notes

When selecting the *Suo Yang* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Suo Yang*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Suo Yang  | G260H1831521 | 61781     | 40      | from supplier |
| PhytoComm | Suo Yang  | G260H1831521 | 61807     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Suo Yang*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Suo Yang*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Suo Yang  | G260H1831521 | 61781 <sup>†</sup> | 20      |
| PhytoComm | Suo Yang  | G260H1831521 | 61807 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 *Suo Yang*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| phytoComm | Suo Yang  | G260H1439022 | 1       |
| Phytocomm | Suo Yang  | G260H1831121 | 1       |
| PhytoComm | Suo Yang  | G260H1831121 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1978 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Suo Yang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Suo Yang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 3              | 1978          |

The substance/substance group *Suo Yang* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4431 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61781     | 61781               | 0.00                         | 20.19                           |
| 61807     | 61807               | 0.00                         | 19.71                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Tai Zi Shen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60114-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G204H0446521 | 61666     | 40      | from supplier |
| PhytoComm | Tai Zi Shen | G204H0446621 | 61929     | 40      | from supplier |
| PhytoComm | Tai Zi Shen | G204H0446621 | 61930     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Tai Zi Shen*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Tai Zi Shen*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Tai Zi Shen | G204H0446521 | 61666 <sup>†</sup> | 20      |
| PhytoComm | Tai Zi Shen | G204H0446621 | 61929 <sup>†</sup> | 20      |
| PhytoComm | Tai Zi Shen | G204H0446621 | 61930 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 *Tai Zi Shen*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| Phytocomm | Tai Zi Shen | G204H0446521 | 1       |
| Phytocomm | Tai Zi Shen | G204H0446221 | 1       |
| PhytoComm | Tai Zi Shen | G204H0446221 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1978 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 5              | 1             | 2              | 1973          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.6002 % (> 99.3218 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61666     | 61666               | 0.00                         | 8.07                            |
| 61929     | 61929               | 0.00                         | 12.33                           |
| 61930     | 61930               | 0.00                         | 13.03                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Tao Ren**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60454-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G184H1007422 | 61093     | 40      | from supplier |
| PhytoComm | Tao Ren   | G184HS220    | 61643     | 40      | from supplier |
| PhytoComm | Tao Ren   | G184H1007621 | 61943     | 40      | from supplier |
| PhytoComm | Tao Ren   | G184H1007621 | 61944     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Tao Ren*. These samples are listed above in the [calibration samples](#) section.
- 21 406 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 80 spectra of 4 reference samples from the substance/substance group *Tao Ren*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Tao Ren   | G184H1007422 | 61093 <sup>†</sup> | 20      |
| PhytoComm | Tao Ren   | G184HS220    | 61643 <sup>†</sup> | 20      |
| PhytoComm | Tao Ren   | G184H1007621 | 61943 <sup>†</sup> | 20      |
| PhytoComm | Tao Ren   | G184H1007621 | 61944 <sup>†</sup> | 20      |

- 13 973 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Tao Ren*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| phytocomm | Tao Ren   | G184H1007023 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Tao Ren   | G184H1007122 | 2       |
| PhytoComm | Tao Ren   | G184H1007122 | 2       |
| Phytocomm | Tao Ren   | g184h1007122 | 1       |
| PhytoComm | Tao Ren   | G184H1007321 | 1       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Tao Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tao Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 80            | 0              | 13 973        |
| <b>Type C</b> | 0              | 0             | 7              | 1974          |

The substance/substance group *Tao Ren* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.5000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4415 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61093     | 61093               | 0.00                         | 22.93                           |
| 61643     | 61643               | 0.00                         | 7.94                            |
| 61943     | 61943               | 0.00                         | 45.90                           |
| 61944     | 61944               | 0.00                         | 46.05                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Tian Hua Fen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60139-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G242H0417522 | 61735     | 40      | from supplier |
| PhytoComm | Tian Hua Fen | G242H0417621 | 61905     | 40      | from supplier |
| PhytoComm | Tian Hua Fen | G242H0417621 | 61906     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Tian Hua Fen*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Tian Hua Fen*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Tian Hua Fen | G242H0417522 | 61735 <sup>†</sup> | 20      |
| PhytoComm | Tian Hua Fen | G242H0417621 | 61905 <sup>†</sup> | 20      |
| PhytoComm | Tian Hua Fen | G242H0417621 | 61906 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Tian Hua Fen*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| Phytocomm | Tian Hua Fen | G242H0417423 | 1       |
| Phytocomm | Tian Hua Fen | G242H0417522 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Tian Hua Fen | G242H0417522 | 1       |
| PhytoComm | Tian Hua Fen | G242H0417122 | 1       |
| PhytoComm | Tian Hua Fen | H0417022     | 2       |
| Phytocomm | Tian Hua Fen | H0417022     | 1       |
| Phytocomm | Tian Hua Fen | h0417022     | 1       |
| phytocomm | Tian Hua Fen | h0417022     | 1       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 2              | 117           | 3              | 21 444        |
| <b>Type B</b> | 2              | 58            | 2              | 13 991        |
| <b>Type C</b> | 0              | 2             | 7              | 1972          |

The substance/substance group *Tian Hua Fen* 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        |
|---------------|--------------------------|-------------------------|
| <b>Type A</b> | 99.9877 % (> 99.9683 %)  | 97.5000 % (> 95.0000 %) |
| <b>Type B</b> | 99.9757 % (> 99.9412 %)  | 96.6667 % (> 91.6667 %) |
| <b>Type C</b> | 100.0000 % (> 99.4413 %) | n/a (n/a)               |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61735     | 61735               | 0.00                         | 6.54                            |
| 61905     | 61905               | 0.00                         | 4.12                            |
| 61906     | 61906               | 0.00                         | 3.21                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Tian Men Dong**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60156-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G037H0415521 | 61701     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Tian Men Dong*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Tian Men Dong*.

| Supplier  | Substance     | Batch        | Sample ID          | Spectra |
|-----------|---------------|--------------|--------------------|---------|
| PhytoComm | Tian Men Dong | G037H0415521 | 61701 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 6 *Apo-Ident* customers from 7 batches from the substance/substance group *Tian Men Dong*.

| Supplier  | Substance     | Batch        | Spectra |
|-----------|---------------|--------------|---------|
| phythocom | Tian Men Dong | g037h0415021 | 1       |
| Phytocomm | Tian Men Dong | G037H0415321 | 1       |
| PhytoComm | Tian Men Dong | G037H0415021 | 2       |
| PhytoComm | Tian Men Dong | G037H0415121 | 1       |
| Phytocomm | Tian Men Dong | G037H0415221 | 1       |
| Phytocomm | Tian Men Dong | G037H0415121 | 1       |
| Phytocomm | Tian Men Dong | g037h0415221 | 1       |
| Phytocomm | Tian Men Dong | g03h0415521  | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1972 spectra from 16 *Apo-Ident* customers from a total of 957 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 4              | 1             | 8              | 1968          |

The substance/substance group *Tian Men Dong* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.8789 % (> 99.5995 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61701     | 61701               | 0.00                         | 8.16                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Tian Nan Xing**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60168-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Tian Nan Xing; Arisaematis rhizoma; Arisaematis rhizoma praep.

### Special notes

When selecting the *Tian Nan 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Nan Xing*:

| Supplier  | Substance     | Batch        | Sample ID | Spectra | Certificate   |
|-----------|---------------|--------------|-----------|---------|---------------|
| PhytoComm | Tian Nan Xing | G028H0420521 | 61704     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Tian Nan Xing*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Tian Nan Xing*.

| Supplier  | Substance     | Batch        | Sample ID          | Spectra |
|-----------|---------------|--------------|--------------------|---------|
| PhytoComm | Tian Nan Xing | G028H0420521 | 61704 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Tian Nan Xing*.

| Supplier  | Substance     | Batch        | Spectra |
|-----------|---------------|--------------|---------|
| Phytocomm | Tian Nan Xing | G028H0420922 | 2       |

- 1979 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the

<sup>†</sup>These spectra were recorded from 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 *Tian Nan 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 *Tian Nan 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 2              | 1979          |

The substance/substance group *Tian Nan 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4445 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61704     | 61704               | 0.00                         | 11.87                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ting Li Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50303-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Ting Li Zi; Lepidii semen

### Special notes

When selecting the *Ting Li 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Ting Li Zi*:

| Supplier  | Substance  | Batch        | Sample ID | Spectra | Certificate   |
|-----------|------------|--------------|-----------|---------|---------------|
| PhytoComm | Ting Li Zi | G135H1340521 | 61647     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Ting Li Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Ting Li Zi*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Ting Li Zi | G135H1340521 | 61647 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Ting Li Zi*.

| Supplier  | Substance  | Batch        | Spectra |
|-----------|------------|--------------|---------|
| PhytoComm | Ting Li Zi | G135H1340121 | 1       |
| Phytocomm | Ting Li Zi | H1340022     | 1       |

- 1979 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the

<sup>†</sup>These spectra were recorded from 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 *Ting Li 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 *Ting Li 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 1              | 0             | 2              | 1978          |

The substance/substance group *Ting Li 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9467 % (> 99.6690 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61647     | 61647               | 0.00                         | 7.58                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Tu Fu Ling**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50885-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G231H0325421 | 61094     | 40      | from supplier |
| PhytoComm | Tu Fu Ling | G231H0325421 | 61436     | 40      | from supplier |
| PhytoComm | Tu Fu Ling | G231H0325621 | 61915     | 40      | from supplier |
| PhytoComm | Tu Fu Ling | G231H0325621 | 61916     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Tu Fu Ling*. These samples are listed above in the [calibration samples](#) section.
- 21 406 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 135 spectra of 4 reference samples from the substance/substance group *Tu Fu Ling*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Tu Fu Ling | G231H0325421 | 61094 <sup>†</sup> | 20      |
| PhytoComm | Tu Fu Ling | G231H0325421 | 61144              | 75      |
| PhytoComm | Tu Fu Ling | G231H0325621 | 61915 <sup>†</sup> | 20      |
| PhytoComm | Tu Fu Ling | G231H0325621 | 61916 <sup>†</sup> | 20      |

- 13 918 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Tu Fu Ling*.

| Supplier  | Substance  | Batch        | Spectra |
|-----------|------------|--------------|---------|
| Phytocomm | Tu Fu Ling | G231H0325121 | 5       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Tu Fu Ling | G231H0325421 | 2       |
| PhytoComm | Tu Fu Ling | G231H0325421 | 1       |
| Phytocomm | Tu Fu Ling | G231H325121  | 1       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Tu Fu Ling* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tu Fu Ling* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 135           | 0              | 13 918        |
| <b>Type C</b> | 1              | 7             | 2              | 1971          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.5556 %) |
| <b>Type C</b> | 99.9627 % (> 99.6833 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61094     | 61094               | 0.00                         | 8.61                            |
| 61436     | 61436               | 0.00                         | 11.05                           |
| 61915     | 61915               | 0.00                         | 6.91                            |
| 61916     | 61916               | 0.00                         | 7.17                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Tu Si Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60217-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G086H1243322 | 60999     | 40      | from supplier |
| PhytoComm | Tu Si Zi  | G086H1243422 | 61046     | 40      | from supplier |
| PhytoComm | Tu Si Zi  | G086H1243422 | 61552     | 40      | from supplier |
| PhytoComm | Tu Si Zi  | G086H1243322 | 61554     | 40      | from supplier |
| PhytoComm | Tu Si Zi  | G086H1243521 | 61680     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Tu Si Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 170 spectra of 3 reference samples from the substance/substance group *Tu Si Zi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Tu Si Zi  | G086H1243422 | 61261              | 75      |
| PhytoComm | Tu Si Zi  | G086H1243322 | 61263              | 75      |
| PhytoComm | Tu Si Zi  | G086H1243521 | 61680 <sup>†</sup> | 20      |

- 13 883 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Tu Si Zi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Tu Si Zi  | G086H1243521 | 3       |
| PhytoComm | Tu Si Zi  | G086H1243521 | 1       |

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<sup>†</sup>These spectra were recorded from 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 | Tu Si Zi  | 161213tsz | 1       |
| Phytocomm | Tu Si Zi  | H1243022  | 1       |
| PhytoComm | Tu Si Zi  | H1243022  | 1       |
| Phytocomm | Tu Si Zi  | h1243022  | 1       |
| Phytocomm | Tu Si Zi  | H1243923  | 1       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Tu Si Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tu Si Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 200           | 0              | 21 366        |
| <b>Type B</b> | 0              | 170           | 0              | 13 883        |
| <b>Type C</b> | 1              | 8             | 1              | 1971          |

The substance/substance group *Tu Si 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 100.0000 % (> 96.4706 %) |
| <b>Type C</b> | 99.8134 % (> 99.5341 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60999     | 60999               | 0.00                         | 11.67                           |
| 61046     | 61046               | 0.00                         | 16.74                           |
| 61552     | 61552               | 0.00                         | 17.00                           |
| 61554     | 61554               | 0.00                         | 18.46                           |
| 61680     | 61680               | 0.00                         | 21.40                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Wang Bu Liu Xing**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50390-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G281H0456521 | 61747     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Wang Bu Liu Xing*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Wang Bu Liu Xing*.

| Supplier  | Substance        | Batch        | Sample ID          | Spectra |
|-----------|------------------|--------------|--------------------|---------|
| PhytoComm | Wang Bu Liu Xing | G281H0456521 | 61747 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Wang Bu Liu Xing*.

| Supplier  | Substance        | Batch        | Spectra |
|-----------|------------------|--------------|---------|
| PhytoComm | Wang Bu Liu Xing | G281H0456221 | 1       |
| Phytocomm | Wang Bu Liu Xing | G281H0456521 | 1       |
| Phytocomm | Wang Bu Liu Xing | G281H0456221 | 2       |
| PhytoComm | Wang Bu Liu Xing | H0456021     | 1       |
| Phytocomm | Wang Bu Liu Xing | H0456021     | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1975 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Wang Bu Liu Xing* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wang Bu Liu Xing* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 1             | 5              | 1975          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4417 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61747     | 61747               | 0.00                         | 12.27                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Wei Ling Xian**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60543-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Wei Ling Xian*:

| Supplier  | Substance     | Batch        | Sample ID | Spectra | Certificate   |
|-----------|---------------|--------------|-----------|---------|---------------|
| PhytoComm | Wei Ling Xian | G075H0943521 | 62031     | 40      | from supplier |
| PhytoComm | Wei Ling Xian | G075H0943521 | 62032     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Wei Ling Xian*.

| Supplier  | Substance     | Batch        | Sample ID          | Spectra |
|-----------|---------------|--------------|--------------------|---------|
| PhytoComm | Wei Ling Xian | G075H0943521 | 62031 <sup>†</sup> | 20      |
| PhytoComm | Wei Ling Xian | G075H0943521 | 62032 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 *Wei Ling Xian*.

| Supplier  | Substance     | Batch        | Spectra |
|-----------|---------------|--------------|---------|
| Phytocomm | Wei Ling Xian | G075H0943223 | 2       |
| PhytoComm | Wei Ling Xian | G075H0943223 | 2       |
| Phytocomm | Wei Ling Xian | g075h0943223 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Wei Ling Xian | 420905402    | 2       |
| Phytocomm | Wei Ling Xian | G075H0943422 | 1       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Wei Ling Xian* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wei Ling Xian* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 8              | 1973          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4414 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 62031     | 62031               | 0.00                         | 13.28                           |
| 62032     | 62032               | 0.00                         | 12.64                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Wu Jia Pi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60149-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Wu Jia Pi; Acanthopanax cortex; Acanthopanax cortex radiceis

### Special notes

When selecting the *Wu Jia Pi* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Wu Jia Pi*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Wu Jia Pi | G002H0402621 | 62047     | 40      | from supplier |
| PhytoComm | Wu Jia Pi | G002H0402621 | 62048     | 40      | from supplier |

## Validation samples

A total of 37 600 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 Jia Pi*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Wu Jia Pi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Wu Jia Pi | G002H0402621 | 62047 <sup>†</sup> | 20      |
| PhytoComm | Wu Jia Pi | G002H0402621 | 62048 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Wu Jia Pi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Wu Jia Pi | G002H0402321 | 2       |
| PhytoComm | Wu Jia Pi | G002H0402321 | 2       |
| Phytocomm | Wu Jia Pi | g002h0402321 | 1       |
| PhytoComm | Wu Jia Pi | H0402021     | 1       |
| Phytocomm | Wu Jia Pi | H042021      | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1974 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Wu Jia Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wu Jia Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 7              | 1974          |

The substance/substance group *Wu Jia Pi* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4415 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 62047     | 62047               | 0.00                         | 8.18                            |
| 62048     | 62048               | 0.00                         | 7.99                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Wu Mei**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60021-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G167H1026421 | 61673     | 40      | from supplier |
| PhytoComm | Wu Mei    | G167H1026521 | 61785     | 40      | from supplier |
| PhytoComm | Wu Mei    | G167H1026521 | 61830     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Wu Mei*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Wu Mei*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Wu Mei    | G167H1026421 | 61673 <sup>†</sup> | 20      |
| PhytoComm | Wu Mei    | G167H1026521 | 61785 <sup>†</sup> | 20      |
| PhytoComm | Wu Mei    | G167H1026521 | 61830 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Wu Mei*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Wu Mei    | G167H1026421 | 1       |
| PhytoComm | Wu Mei    | G167H1026121 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Wu Mei    | G167H1026121 | 1       |
| Phytocomm | Wu Mei    | G167H1026221 | 1       |
| phytocomm | Wu Mei    | H1026021     | 2       |
| PhytoComm | Wu Mei    | H1026021     | 2       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Wu 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 3              | 2             | 6              | 1970          |

The substance/substance group *Wu Mei* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.8756 % (> 99.5963 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61673     | 61673               | 0.00                         | 19.56                           |
| 61785     | 61785               | 0.00                         | 18.18                           |
| 61830     | 61830               | 0.00                         | 17.99                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Wu Wei Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60001-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G220H0401421 | 61444     | 40      | from supplier |
| PhytoComm | Wu Wei Zi | G220H0401621 | 61925     | 40      | from supplier |
| PhytoComm | Wu Wei Zi | G220H0401621 | 61926     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Wu Wei Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 115 spectra of 3 reference samples from the substance/substance group *Wu Wei Zi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Wu Wei Zi | G220H0401421 | 61152              | 75      |
| PhytoComm | Wu Wei Zi | G220H0401621 | 61925 <sup>†</sup> | 20      |
| PhytoComm | Wu Wei Zi | G220H0401621 | 61926 <sup>†</sup> | 20      |

- 13 938 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Wu Wei Zi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| phytoComm | Wu Wei Zi | H0401021     | 1       |
| Phytocomm | Wu Wei Zi | G220H0401421 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Wu Wei Zi | G220H0401122 | 1       |
| PhytoComm | Wu Wei Zi | H0401021     | 2       |
| Phytocomm | Wu Wei Zi | H0401021     | 2       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Wu Wei Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wu Wei Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 113           | 2              | 13 938        |
| <b>Type C</b> | 0              | 2             | 6              | 1973          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 98.2609 % (> 95.6522 %)  |
| <b>Type C</b> | 100.0000 % (> 99.4414 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61444     | 61444               | 0.00                         | 29.44                           |
| 61925     | 61925               | 0.00                         | 45.23                           |
| 61926     | 61926               | 0.00                         | 44.95                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Wu Yao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60040-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G140H1025521 | 61734     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Wu Yao*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Wu Yao*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Wu Yao    | G140H1025521 | 61734 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Wu Yao*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Wu Yao    | G140H1025521 | 2       |
| PhytoComm | Wu Yao    | G140H1025521 | 1       |
| PhytoComm | Wu Yao    | G140H1025221 | 2       |
| Phytocomm | Wu Yao    | g140h1025221 | 1       |
| phytocomm | Wu Yao    | H1025021     | 1       |
| PhytoComm | Wu Yao    | H1025021     | 3       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1971 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Wu Yao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wu Yao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 1              | 2             | 8              | 1970          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9781 % (> 99.6986 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61734     | 61734               | 0.00                         | 8.71                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Wu Zhu Yu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50356-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Wu Zhu Yu; Evodiae rutecarpae fructus

### Special notes

When selecting the *Wu Zhu Yu* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Zhu Yu*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Wu Zhu Yu | G103H0766522 | 61773     | 40      | from supplier |
| PhytoComm | Wu Zhu Yu | G103H0766522 | 61831     | 40      | from supplier |

## Validation samples

A total of 37 600 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 Zhu Yu*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Wu Zhu Yu*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Wu Zhu Yu | G103H0766522 | 61773 <sup>†</sup> | 20      |
| PhytoComm | Wu Zhu Yu | G103H0766522 | 61831 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 5 batches from the substance/substance group *Wu Zhu Yu*.

| Supplier  | Substance | Batch          | Spectra |
|-----------|-----------|----------------|---------|
| PhytoComm | Wu Zhu Yu | G103H0766321   | 2       |
| PhytoComm | Wu Zhu Yu | (G103)H0766321 | 1       |
| PhytoComm | Wu Zhu Yu | G103H0766021   | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Wu Zhu Yu | G103H0766021 | 1       |
| PhytoComm | Wu Zhu Yu | G103H0766022 | 1       |
| Phytocomm | Wu Zhu Yu | G103H0766022 | 3       |
| Phytocomm | Wu Zhu Yu | G103H0766321 | 1       |
| Phytocomm | Wu Zhu Yu | G13H0766021  | 1       |

- 1970 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Wu Zhu Yu* can be 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 Zhu Yu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 9              | 40            | 0              | 14 004        |
| <b>Type C</b> | 7              | 0             | 11             | 1963          |

The substance/substance group *Wu Zhu Yu* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 99.9620 % (> 99.9276 %)  | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.5300 % (> 99.2506 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61773     | 61773               | 0.00                         | 7.93                            |
| 61831     | 61831               | 0.00                         | 7.30                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Xi Xian Cao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60103-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G229H1431521 | 61903     | 40      | from supplier |
| PhytoComm | Xi Xian Cao | G229H1431521 | 61904     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Xi Xian Cao*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Xi Xian Cao | G229H1431521 | 61903 <sup>†</sup> | 20      |
| PhytoComm | Xi Xian Cao | G229H1431521 | 61904 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 6 *Apo-Ident* customers from 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 | G229H1431121 | 1       |
| PhytoComm | Xi Xian Cao | G229H1431121 | 2       |
| Phytocomm | Xi Xian Cao | G229H1431121 | 4       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1972 spectra from 16 *Apo-Ident* customers from a total of 962 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Xi 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 9              | 1972          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4413 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61903     | 61903               | 0.00                         | 11.43                           |
| 61904     | 61904               | 0.00                         | 11.47                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Xi Yang Shen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60422-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G324HS4070L1 | 61726     | 40      | from supplier |
| PhytoComm | Xi Yang Shen | G324HS407PP1 | 61863     | 40      | from supplier |
| PhytoComm | Xi Yang Shen | G324HS407PP1 | 61864     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Xi Yang Shen*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Xi Yang Shen*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Xi Yang Shen | G324HS4070L1 | 61726 <sup>†</sup> | 20      |
| PhytoComm | Xi Yang Shen | G324HS407PP1 | 61863 <sup>†</sup> | 20      |
| PhytoComm | Xi Yang Shen | G324HS407PP1 | 61864 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Xi Yang Shen*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| PhytoComm | Xi Yang Shen | G324HS4070L1 | 1       |
| PhytoComm | Xi Yang Shen | G324H0647321 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Xi Yang Shen | G324H0647021 | 2       |
| Phytocomm | Xi Yang Shen | g324h0647321 | 1       |
| Phytocomm | Xi Yang Shen | G324H0647321 | 1       |

- 1975 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Xi Yang Shen* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xi Yang Shen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 0              | 1             | 5              | 1975          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4417 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61726     | 61726               | 0.00                         | 7.67                            |
| 61863     | 61863               | 0.00                         | 13.19                           |
| 61864     | 61864               | 0.00                         | 13.21                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Xia Ku Cao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60080-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G202H1064421 | 61006     | 20      | from supplier |
| PhytoComm | Xia Ku Cao | G202H1064421 | 61464     | 40      | from supplier |
| PhytoComm | Xia Ku Cao | G202H1064421 | 61760     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 100 spectra of 3 reference samples from the substance/substance group *Xia Ku Cao*. These samples are listed above in the [calibration samples](#) section.
- 21 466 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 95 spectra of 2 reference samples from the substance/substance group *Xia Ku Cao*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Xia Ku Cao | G202H1064421 | 61172              | 75      |
| PhytoComm | Xia Ku Cao | G202H1064421 | 61760 <sup>†</sup> | 20      |

- 13 958 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Xia Ku Cao*.

| Supplier  | Substance  | Batch        | Spectra |
|-----------|------------|--------------|---------|
| Phytocomm | Xia Ku Cao | g202h1064121 | 1       |
| Phytocomm | Xia Ku Cao | G202H1064022 | 1       |
| PhytoComm | Xia Ku Cao | G202H1064121 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Xia Ku Cao | G202H1064221 | 3       |
| PhytoComm | Xia Ku Cao | G202H1064221 | 2       |
| Phytocomm | Xia Ku Cao | G202H1064421 | 1       |
| Phytocomm | Xia Ku Cao | H1064922     | 1       |

- 1971 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Xia Ku Cao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xia Ku Cao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 100           | 0              | 21 466        |
| <b>Type B</b> | 0              | 93            | 2              | 13 958        |
| <b>Type C</b> | 0              | 0             | 10             | 1971          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 94.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 97.8947 % (> 94.7368 %)  |
| <b>Type C</b> | 100.0000 % (> 99.4412 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61006     | 61006               | 0.00                         | 74.76                           |
| 61464     | 61464               | 0.00                         | 78.96                           |
| 61760     | 61760               | 0.00                         | 87.32                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Xian Mao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60316-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Xian Mao; Curculiginis orchoidis rhizoma

### Special notes

When selecting the *Xian Mao* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Mao*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Xian Mao  | G304H0549621 | 61887     | 40      | from supplier |
| PhytoComm | Xian Mao  | G304H0549621 | 61888     | 40      | from supplier |
| PhytoComm | Xian Mao  | G304H0549621 | 62049     | 40      | from supplier |
| PhytoComm | Xian Mao  | G304H0549621 | 62050     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Xian Mao*. These samples are listed above in the [calibration samples](#) section.
- 21 406 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 80 spectra of 4 reference samples from the substance/substance group *Xian Mao*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Xian Mao  | G304H0549621 | 61887 <sup>†</sup> | 20      |
| PhytoComm | Xian Mao  | G304H0549621 | 61888 <sup>†</sup> | 20      |
| PhytoComm | Xian Mao  | G304H0549621 | 62049 <sup>†</sup> | 20      |
| PhytoComm | Xian Mao  | G304H0549621 | 62050 <sup>†</sup> | 20      |

- 13 973 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 3 batches from the substance/substance group *Xian Mao*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Xian Mao  | G304H0549521 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Xian Mao  | G304H0549021 | 3       |
| Phytocomm | Xian Mao  | G304H0549321 | 2       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Xian Mao* can be 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 Mao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 80            | 0              | 13 973        |
| <b>Type C</b> | 3              | 2             | 5              | 1971          |

The substance/substance group *Xian Mao* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.5000 %) |
| <b>Type C</b> | 99.9411 % (> 99.6619 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61887     | 61887               | 0.00                         | 8.96                            |
| 61888     | 61888               | 0.00                         | 9.37                            |
| 62049     | 62049               | 0.00                         | 8.39                            |
| 62050     | 62050               | 0.00                         | 8.94                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

IdentModul 1.3-2017-03

Validated substance/substance group **Xiang Fu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60185-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

## Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

## Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G088H0930521 | 61711     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Xiang Fu*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Xiang Fu*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Xiang Fu  | G088H0930521 | 61711 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 17 spectra from 9 *Apo-Ident* customers from 6 batches from the substance/substance group *Xiang Fu*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Xiang Fu  | G088H0930521 | 5       |
| PhytoComm | Xiang Fu  | G088H0930521 | 1       |
| Phytocomm | Xiang Fu  | G088H0930123 | 4       |
| Phytocomm | Xiang Fu  | g088h0930123 | 1       |
| PhytoComm | Xiang Fu  | G088H0930123 | 1       |
| Phytocomm | Xiang Fu  | g088h09      | 1       |
| PhytoComm | Xiang Fu  | H0930021     | 1       |
| Phytocomm | Xiang Fu  | H0930021     | 1       |
| PhytoComm | Xiang Fu  | G088H0930321 | 2       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1964 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 7             | 10             | 1964          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4408 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61711     | 61711               | 0.00                         | 7.12                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Xiao Hui Xiang**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60209-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Xiao Hui Xiang; Foeniculi vulgaris fructus

### Special notes

When selecting the *Xiao Hui Xiang* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Xiao Hui Xiang*:

| Supplier  | Substance      | Batch        | Sample ID | Spectra | Certificate   |
|-----------|----------------|--------------|-----------|---------|---------------|
| PhytoComm | Xiao Hui Xiang | G104H0339522 | 61717     | 40      | from supplier |
| PhytoComm | Xiao Hui Xiang | G104H0339622 | 61987     | 40      | from supplier |
| PhytoComm | Xiao Hui Xiang | G104H0339622 | 61988     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Xiao Hui Xiang*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Xiao Hui Xiang*.

| Supplier  | Substance      | Batch        | Sample ID          | Spectra |
|-----------|----------------|--------------|--------------------|---------|
| PhytoComm | Xiao Hui Xiang | G104H0339522 | 61717 <sup>†</sup> | 20      |
| PhytoComm | Xiao Hui Xiang | G104H0339622 | 61987 <sup>†</sup> | 20      |
| PhytoComm | Xiao Hui Xiang | G104H0339622 | 61988 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Xiao Hui Xiang*.

| Supplier  | Substance      | Batch        | Spectra |
|-----------|----------------|--------------|---------|
| Phytocomm | Xiao Hui Xiang | g104h0339321 | 1       |
| Phytocomm | Xiao Hui Xiang | G104H0339522 | 3       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Xiao Hui Xiang | G104H0339321 | 1       |
| PhytoComm | Xiao Hui Xiang | H0339021     | 2       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Xiao Hui Xiang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xiao Hui Xiang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 3              | 3             | 4              | 1971          |

The substance/substance group *Xiao Hui Xiang* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.9300 % (> 99.6508 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61717     | 61717               | 0.00                         | 11.08                           |
| 61987     | 61987               | 0.00                         | 8.98                            |
| 61988     | 61988               | 0.00                         | 9.50                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Xie Bai**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60362-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Xie Bai; Allii bulbus; Allii macrostemonis bulbus

### Special notes

When selecting the *Xie Bai* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G504H1830422 | 61674     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Xie Bai*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Xie Bai*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Xie Bai   | G504H1830422 | 61674 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Xie Bai*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Xie Bai   | G504H1830422 | 1       |
| Phytocomm | Xie Bai   | G504H1830421 | 1       |
| PhytoComm | Xie Bai   | G504H1830121 | 1       |
| PhytoComm | Xie Bai   | G504H1830321 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1977 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Xie Bai* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xie Bai* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 1              | 2             | 2              | 1976          |

The substance/substance group *Xie Bai* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9751 % (> 99.6963 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61674     | 61674               | 0.00                         | 9.80                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Xin Yi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60231-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G153H0758521 | 61659     | 40      | from supplier |
| PhytoComm | Xin Yi    | G153H0758523 | 61981     | 40      | from supplier |
| PhytoComm | Xin Yi    | G153H0758523 | 61982     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Xin Yi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Xin Yi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Xin Yi    | G153H0758521 | 61659 <sup>†</sup> | 20      |
| PhytoComm | Xin Yi    | G153H0758523 | 61981 <sup>†</sup> | 20      |
| PhytoComm | Xin Yi    | G153H0758523 | 61982 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 10 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Xin Yi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Xin Yi    | 161213xy     | 1       |
| Phytocomm | Xin Yi    | G153H0758521 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Xin Yi    | G153H0758121 | 3       |
| Phytocomm | Xin Yi    | G153H0758121 | 3       |
| PhytoComm | Xin Yi    | G153H0758321 | 2       |

- 1971 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Xin Yi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xin Yi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 0              | 3             | 7              | 1971          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4412 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61659     | 61659               | 0.00                         | 14.39                           |
| 61981     | 61981               | 0.00                         | 16.44                           |
| 61982     | 61982               | 0.00                         | 16.67                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Xu Duan**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60245-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Xu Duan*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Xu Duan   | G092H2106621 | 62007     | 40      | from supplier |
| PhytoComm | Xu Duan   | G092H2106621 | 62008     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Xu Duan*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Xu Duan*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Xu Duan   | G092H2106621 | 62007 <sup>†</sup> | 20      |
| PhytoComm | Xu Duan   | G092H2106621 | 62008 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Xu Duan*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Xu Duan   | G092H2106422 | 1       |
| PhytoComm | Xu Duan   | G092H2106023 | 2       |
| PhytoComm | Xu Duan   | G092H2106321 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1977 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Xu Duan* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xu Duan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 1              | 0             | 4              | 1976          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.9254 % (> 99.6466 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 62007     | 62007               | 0.00                         | 12.20                           |
| 62008     | 62008               | 0.00                         | 12.06                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Xuan Fu Hua**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60223-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Xuan Fu Hua; Inulae flos

### Special notes

When selecting the *Xuan Fu Hua* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Xuan Fu Hua*:

| Supplier  | Substance   | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-------------|--------------|-----------|---------|---------------|
| PhytoComm | Xuan Fu Hua | G126H1168521 | 61664     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Xuan Fu Hua*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Xuan Fu Hua*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Xuan Fu Hua | G126H1168521 | 61664 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Xuan Fu Hua*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| PhytoComm | Xuan Fu Hua | G126H1168521 | 1       |
| PhytoComm | Xuan Fu Hua | G126H1168121 | 1       |
| PhytoComm | Xuan Fu Hua | G126H1168121 | 1       |
| PhytoComm | Xuan Fu Hua | H1168921     | 2       |
| PhytoComm | Xuan Fu Hua | H1168921     | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1975 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Xuan Fu Hua* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xuan Fu Hua* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 2              | 1             | 5              | 1973          |

The substance/substance group *Xuan Fu 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.8934 % (> 99.6143 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61664     | 61664               | 0.00                         | 9.26                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Xuan Shen**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60095-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G223H0537421 | 61442     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

**Type A** All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Xuan Shen*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 75 spectra of 1 reference samples from the substance/substance group *Xuan Shen*.

| Supplier  | Substance | Batch        | Sample ID | Spectra |
|-----------|-----------|--------------|-----------|---------|
| PhytoComm | Xuan Shen | G223H0537421 | 61150     | 75      |

- 13 978 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Xuan Shen*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Xuan Shen | G223H0537421 | 1       |
| PhytoComm | Xuan Shen | G223H0537221 | 3       |
| Phytocomm | Xuan Shen | G223H0537221 | 1       |
| PhytoComm | Xuan Shen | G223H0537322 | 1       |
| Phytocomm | Xuan Shen | g22h0537322  | 1       |
| Phytocomm | Xuan Shen | H0537021     | 2       |
| Euro OTC  | Xuan Shen | H0537021     | 1       |
| PhytoComm | Xuan Shen | H0537021     | 2       |

- 1969 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Xuan Shen* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xuan Shen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 75            | 0              | 13 978        |
| <b>Type C</b> | 1              | 5             | 7              | 1968          |

The substance/substance group *Xuan Shen* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.0000 %) |
| <b>Type C</b> | 99.9804 % (> 99.7009 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61442     | 61442               | 0.00                         | 9.98                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Yan Hu Suo**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60439-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G081H0805521 | 61733     | 40      | from supplier |
| PhytoComm | Yan Hu Suo | G081H0805622 | 62039     | 40      | from supplier |
| PhytoComm | Yan Hu Suo | G081H0805622 | 62040     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Yan Hu Suo*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Yan Hu Suo*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Yan Hu Suo | G081H0805521 | 61733 <sup>†</sup> | 20      |
| PhytoComm | Yan Hu Suo | G081H0805622 | 62039 <sup>†</sup> | 20      |
| PhytoComm | Yan Hu Suo | G081H0805622 | 62040 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 12 spectra from 9 *Apo-Ident* customers from 6 batches from the substance/substance group *Yan Hu Suo*.

| Supplier  | Substance  | Batch        | Spectra |
|-----------|------------|--------------|---------|
| PhytoComm | Yan Hu Suo | G081F1000301 | 3       |
| Phytocomm | Yan Hu Suo | G081F1000301 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Yan Hu Suo | g081f1000301 | 1       |
| Phytocomm | Yan Hu Suo | G081H0805221 | 1       |
| PhytoComm | Yan Hu Suo | G081H0805221 | 1       |
| PhytoComm | Yan Hu Suo | G081H0805223 | 1       |
| Phytocomm | Yan Hu Suo | G081H0805521 | 1       |
| PhytoComm | Yan Hu Suo | G081H0805521 | 1       |
| PhytoComm | Yan Hu Suo | G081H0805223 | 1       |
| PhytoComm | Yan Hu Suo | G081H0805223 | 1       |

- 1969 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Yan Hu Suo* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yan Hu Suo* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 1              | 2             | 10             | 1968          |

The substance/substance group *Yan Hu Suo* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.9585 % (> 99.6791 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61733     | 61733               | 0.00                         | 7.62                            |
| 62039     | 62039               | 0.00                         | 7.59                            |
| 62040     | 62040               | 0.00                         | 7.59                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ye Jiao Teng**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60068-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Ye Jiao Teng*:

| Supplier  | Substance    | Batch        | Sample ID | Spectra | Certificate   |
|-----------|--------------|--------------|-----------|---------|---------------|
| PhytoComm | Ye Jiao Teng | G288H0885522 | 61750     | 40      | from supplier |
| PhytoComm | Ye Jiao Teng | G288H0885522 | 62051     | 40      | from supplier |
| PhytoComm | Ye Jiao Teng | G288H0885522 | 62052     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Ye Jiao Teng*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Ye Jiao Teng*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Ye Jiao Teng | G288H0885522 | 61750 <sup>†</sup> | 20      |
| PhytoComm | Ye Jiao Teng | G288H0885522 | 62051 <sup>†</sup> | 20      |
| PhytoComm | Ye Jiao Teng | G288H0885522 | 62052 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Ye Jiao Teng*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| Phytocomm | Ye Jiao Teng | G288H0885223 | 2       |
| Phytocomm | Ye Jiao Teng | G288H0885522 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Ye Jiao Teng | G288H0885522 | 2       |
| Phytocomm | Ye Jiao Teng | g228h0085223 | 1       |
| PhytoComm | Ye Jiao Teng | H0885021     | 1       |
| Phytocomm | Ye Jiao Teng | H0885922     | 1       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Ye Jiao Teng* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ye Jiao Teng* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 0              | 4             | 5              | 1972          |

The substance/substance group *Ye Jiao Teng* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4413 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61750     | 61750               | 0.00                         | 23.00                           |
| 62051     | 62051               | 0.00                         | 23.29                           |
| 62052     | 62052               | 0.00                         | 23.18                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Yi Mu Cao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60105-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G134H1050421 | 61519     | 40      | from supplier |
| PhytoComm | Yi Mu Cao | G134H1050521 | 61671     | 40      | from supplier |
| PhytoComm | Yi Mu Cao | G134H1050621 | 61983     | 40      | from supplier |
| PhytoComm | Yi Mu Cao | G134H1050621 | 61984     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Yi Mu Cao*. These samples are listed above in the [calibration samples](#) section.
- 21 406 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 135 spectra of 4 reference samples from the substance/substance group *Yi Mu Cao*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Yi Mu Cao | G134H1050421 | 61228              | 75      |
| PhytoComm | Yi Mu Cao | G134H1050521 | 61671 <sup>†</sup> | 20      |
| PhytoComm | Yi Mu Cao | G134H1050621 | 61983 <sup>†</sup> | 20      |
| PhytoComm | Yi Mu Cao | G134H1050621 | 61984 <sup>†</sup> | 20      |

- 13 918 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 9 *Apo-Ident* customers from 5 batches from the substance/substance group *Yi Mu Cao*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| PhytoComm | Yi Mu Cao | G134H1050521 | 3       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | G134H1050521 | 1       |
| PhytoComm | Yi Mu Cao | G134H1050023 | 3       |
| Phytocomm | Yi Mu Cao | G134H1050023 | 1       |
| Phytocomm | Yi Mu Cao | G134H1050024 | 3       |
| PhytoComm | Yi Mu Cao | G134H1050024 | 1       |
| Phytocomm | Yi Mu Cao | g134h1050024 | 1       |
| PhytoComm | Yi Mu Cao | G134H1050321 | 2       |

- 1966 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Yi Mu Cao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yi Mu Cao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 135           | 0              | 13 918        |
| <b>Type C</b> | 0              | 3             | 12             | 1966          |

The substance/substance group *Yi Mu Cao* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.5556 %) |
| <b>Type C</b> | 100.0000 % (> 99.4409 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61519     | 61519               | 0.00                         | 12.44                           |
| 61671     | 61671               | 0.00                         | 17.80                           |
| 61983     | 61983               | 0.00                         | 10.90                           |
| 61984     | 61984               | 0.00                         | 10.90                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Yi Yi Ren**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60174-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G078H1701323 | 60925     | 40      | from supplier |
| PhytoComm | Yi Yi Ren | G078H1701421 | 61095     | 40      | from supplier |
| PhytoComm | Yi Yi Ren | G078H1701323 | 61559     | 40      | from supplier |
| PhytoComm | Yi Yi Ren | G078H1701522 | 61791     | 40      | from supplier |
| PhytoComm | Yi Yi Ren | G078H1701522 | 61817     | 40      | from supplier |
| PhytoComm | Yi Yi Ren | G078H1701522 | 62067     | 40      | from supplier |
| PhytoComm | Yi Yi Ren | G078H1701522 | 62068     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

**Type A** All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Yi Yi Ren*. These samples are listed above in the [calibration samples](#) section.
- 21 286 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 175 spectra of 6 reference samples from the substance/substance group *Yi Yi Ren*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Yi Yi Ren | G078H1701421 | 61095 <sup>†</sup> | 20      |
| PhytoComm | Yi Yi Ren | G078H1701323 | 61268              | 75      |
| PhytoComm | Yi Yi Ren | G078H1701522 | 61791 <sup>†</sup> | 20      |
| PhytoComm | Yi Yi Ren | G078H1701522 | 61817 <sup>†</sup> | 20      |
| PhytoComm | Yi Yi Ren | G078H1701522 | 62067 <sup>†</sup> | 20      |
| PhytoComm | Yi Yi Ren | G078H1701522 | 62068 <sup>†</sup> | 20      |

- 13 878 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 19 spectra from 6 *Apo-Ident* customers from 6 batches from the substance/substance group *Yi Yi Ren*.

<sup>†</sup>These spectra were recorded from 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 | Yi Yi Ren | G078H1701522 | 3       |
| Phytocomm | Yi Yi Ren | G078H1701222 | 3       |
| PhytoComm | Yi Yi Ren | G078H1701323 | 1       |
| Phytocomm | Yi Yi Ren | G078H1701323 | 1       |
| Phytocomm | Yi Yi Ren | g078h1701323 | 1       |
| Phytocomm | Yi Yi Ren | H1701021     | 8       |
| PhytoComm | Yi Yi Ren | H1701021     | 1       |
| PhytoComm | Yi Yi Ren | H1701923     | 1       |

- 1962 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

### Validation results

The validation runs checked whether the substance/substance group *Yi Yi Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yi Yi Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 280           | 0              | 21 286        |
| <b>Type B</b> | 0              | 175           | 0              | 13 878        |
| <b>Type C</b> | 0              | 10            | 9              | 1962          |

The substance/substance group *Yi Yi Ren* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.8571 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 100.0000 % (> 96.5714 %) |
| <b>Type C</b> | 100.0000 % (> 99.4408 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

### Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 60925     | 60925               | 0.00                         | 34.37                           |
| 61095     | 61095               | 0.00                         | 40.22                           |
| 61559     | 61559               | 0.00                         | 37.73                           |
| 61791     | 61791               | 0.00                         | 44.88                           |
| 61817     | 61817               | 0.00                         | 43.52                           |
| 62067     | 62067               | 0.00                         | 43.03                           |
| 62068     | 62068               | 0.00                         | 44.64                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Yi Zhi Ren**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60172-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Yi Zhi Ren; Alpiniae fructus; Alpiniae oxyphyllae fructus

### Special notes

When selecting the *Yi Zhi Ren* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G015H1051521 | 61740     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Yi Zhi Ren*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Yi Zhi Ren*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Yi Zhi Ren | G015H1051521 | 61740 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Yi Zhi Ren*.

| Supplier    | Substance  | Batch        | Spectra |
|-------------|------------|--------------|---------|
| PhytoComm   | Yi Zhi Ren | G015H1051022 | 2       |
| Herbasinica | Yi Zhi Ren | G015H1051321 | 1       |
| Phytocomm   | Yi Zhi Ren | G015H1051321 | 1       |
| Phytocomm   | Yi Zhi Ren | G015H1051521 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1976 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Yi Zhi Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yi Zhi Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 1              | 20            | 0              | 14 032        |
| <b>Type C</b> | 1              | 0             | 5              | 1975          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 99.9919 % (> 99.9576 %)  | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9534 % (> 99.6744 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61740     | 61740               | 0.00                         | 7.34                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Yin Chen Hao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60163-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G034H1030421 | 61688     | 40      | from supplier |
| PhytoComm | Yin Chen Hao | G034H1030621 | 61832     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Yin Chen Hao*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Yin Chen Hao*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Yin Chen Hao | G034H1030421 | 61688 <sup>†</sup> | 20      |
| PhytoComm | Yin Chen Hao | G034H1030621 | 61832 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Yin Chen Hao*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| Fagron    | Yin Chen Hao | G034H1030421 | 2       |
| PhytoComm | Yin Chen Hao | G034H1030022 | 1       |
| Phytocomm | Yin Chen Hao | G034H1030022 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Yin Chen Hao | G034H1030121 | 3       |
| PhytoComm | Yin Chen Hao | G034H1030121 | 1       |
| PhytoComm | Yin Chen Hao | H1030021     | 1       |
| Phytocomm | Yin Chen Hao | H1030021     | 1       |

- 1971 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Yin Chen Hao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yin Chen Hao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 1              | 40            | 0              | 14 012        |
| <b>Type C</b> | 6              | 2             | 8              | 1965          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 99.9879 % (> 99.9534 %)  | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.7104 % (> 99.4310 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61688     | 61688               | 0.00                         | 6.85                            |
| 61832     | 61832               | 0.00                         | 8.10                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Yin Yang Huo**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60228-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G098H1114422 | 61388     | 40      | from supplier |
| PhytoComm | Yin Yang Huo | G098H1114621 | 61774     | 40      | from supplier |
| PhytoComm | Yin Yang Huo | G098H1114621 | 61827     | 40      | from supplier |

## Validation samples

A total of 37 600 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 Yang Huo*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Yin Yang Huo*.

| Supplier  | Substance    | Batch        | Sample ID          | Spectra |
|-----------|--------------|--------------|--------------------|---------|
| PhytoComm | Yin Yang Huo | G098H1114422 | 61388 <sup>†</sup> | 20      |
| PhytoComm | Yin Yang Huo | G098H1114621 | 61774 <sup>†</sup> | 20      |
| PhytoComm | Yin Yang Huo | G098H1114621 | 61827 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 10 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Yin Yang Huo*.

| Supplier  | Substance    | Batch        | Spectra |
|-----------|--------------|--------------|---------|
| phythocom | Yin Yang Huo | G098H1114222 | 1       |
| Phytocomm | Yin Yang Huo | G098H1114422 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Yin Yang Huo | G098H1114121 | 2       |
| phytocomm | Yin Yang Huo | FA1114702    | 1       |
| Phytocomm | Yin Yang Huo | G098H1114121 | 1       |
| PhytoComm | Yin Yang Huo | G098H1114222 | 1       |
| Phytocomm | Yin Yang Huo | G098H1114222 | 1       |
| PhytoComm | Yin Yang Huo | H1114923     | 1       |

- 1971 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Yin Yang Huo* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yin Yang Huo* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 3              | 2             | 8              | 1968          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.8259 % (> 99.5465 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61388     | 61388               | 0.00                         | 10.76                           |
| 61774     | 61774               | 0.00                         | 7.56                            |
| 61827     | 61827               | 0.00                         | 7.08                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Yu Jin**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60171-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G084H2201521 | 61792     | 40      | from supplier |
| PhytoComm | Yu Jin    | G084H2201521 | 61823     | 40      | from supplier |
| PhytoComm | Yu Jin    | G084H2201621 | 62019     | 40      | from supplier |
| PhytoComm | Yu Jin    | G084H2201621 | 62020     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 406 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 80 spectra of 4 reference samples from the substance/substance group *Yu Jin*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Yu Jin    | G084H2201521 | 61792 <sup>†</sup> | 20      |
| PhytoComm | Yu Jin    | G084H2201521 | 61823 <sup>†</sup> | 20      |
| PhytoComm | Yu Jin    | G084H2201621 | 62019 <sup>†</sup> | 20      |
| PhytoComm | Yu Jin    | G084H2201621 | 62020 <sup>†</sup> | 20      |

- 13 973 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Yu Jin*.

| Supplier  | Substance | Batch     | Spectra |
|-----------|-----------|-----------|---------|
| Phytocomm | Yu Jin    | 422901803 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Yu Jin    | G084H2201221 | 1       |
| PhytoComm | Yu Jin    | G084H2201322 | 1       |
| PhytoComm | Yu Jin    | H2201021     | 1       |
| Phytocomm | Yu Jin    | H2201021     | 1       |

- 1976 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Yu 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 160           | 0              | 21 406        |
| <b>Type B</b> | 0              | 80            | 0              | 13 973        |
| <b>Type C</b> | 0              | 1             | 4              | 1976          |

The substance/substance group *Yu Jin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 96.2500 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 92.5000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4420 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61792     | 61792               | 0.00                         | 9.04                            |
| 61823     | 61823               | 0.00                         | 9.08                            |
| 62019     | 62019               | 0.00                         | 8.13                            |
| 62020     | 62020               | 0.00                         | 7.89                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Yu Xing Cao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60606-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Yu Xing Cao*:

| Supplier  | Substance   | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-------------|--------------|-----------|---------|---------------|
| PhytoComm | Yu Xing Cao | G124H1149423 | 61662     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

**Type A** All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Yu Xing Cao*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Yu Xing Cao*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Yu Xing Cao | G124H1149423 | 61662 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 7 batches from the substance/substance group *Yu Xing Cao*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| Phytocomm | Yu Xing Cao | G124H1149423 | 2       |
| Phytocomm | Yu Xing Cao | g124h1149222 | 1       |
| Phytocomm | Yu Xing Cao | 612yxc       | 1       |
| Phytocomm | Yu Xing Cao | G124H1149122 | 5       |
| Phytocomm | Yu Xing Cao | G124H1149222 | 1       |
| PhytoComm | Yu Xing Cao | H1149821     | 1       |
| Phytocomm | Yu Xing Cao | g124h1149122 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1969 spectra from 16 *Apo-Ident* customers from a total of 957 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Yu Xing Cao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yu Xing Cao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 12             | 1969          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4410 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61662     | 61662               | 0.00                         | 10.48                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Yu Zhu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60056-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G195H0517421 | 61374     | 40      | from supplier |
| PhytoComm | Yu Zhu    | G195H0517521 | 61941     | 40      | from supplier |
| PhytoComm | Yu Zhu    | G195H0517521 | 61942     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Yu Zhu*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Yu Zhu*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Yu Zhu    | G195H0517421 | 61374 <sup>†</sup> | 20      |
| PhytoComm | Yu Zhu    | G195H0517521 | 61941 <sup>†</sup> | 20      |
| PhytoComm | Yu Zhu    | G195H0517521 | 61942 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 4 batches from the substance/substance group *Yu Zhu*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Yu Zhu    | G195H0517421 | 2       |
| PhytoComm | Yu Zhu    | G195H0517121 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Yu Zhu    | G195H0517321 | 1       |
| PhytoComm | Yu Zhu    | H0517022     | 2       |
| Phytocomm | Yu Zhu    | H0517022     | 1       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Yu 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 57            | 3              | 13 993        |
| <b>Type C</b> | 6              | 2             | 5              | 1968          |

The substance/substance group *Yu 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 95.0000 % (> 90.0000 %)  |
| <b>Type C</b> | 99.7313 % (> 99.4520 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61374     | 61374               | 0.00                         | 12.22                           |
| 61941     | 61941               | 0.00                         | 5.31                            |
| 61942     | 61942               | 0.00                         | 5.67                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Yuan Zhi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60100-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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  | G194H1406522 | 61742     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Yuan Zhi*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Yuan Zhi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Yuan Zhi  | G194H1406522 | 61742 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Yuan Zhi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| phythocom | Yuan Zhi  | g194h1406222 | 1       |
| Phytocomm | Yuan Zhi  | G194H1406522 | 2       |
| Phytocomm | Yuan Zhi  | g194h140622  | 1       |
| Phytocomm | Yuan Zhi  | 421401802    | 1       |
| Phytocomm | Yuan Zhi  | G194H1406222 | 2       |
| PhytoComm | Yuan Zhi  | H1406924     | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1973 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Yuan Zhi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yuan Zhi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 1              | 2             | 6              | 1972          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9534 % (> 99.6741 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61742     | 61742               | 0.00                         | 8.19                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ze Lan**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60322-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Ze Lan; Lycopi lucidi herba

### Special notes

When selecting the *Ze 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Lan*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Ze Lan    | G268H1606421 | 61634     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

**Type A** All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Ze Lan*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Ze Lan*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Ze Lan    | G268H1606421 | 61634 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Ze Lan*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Ze Lan    | G268H1606421 | 1       |
| PhytoComm | Ze Lan    | G268H1606021 | 2       |
| Phytocomm | Ze Lan    | G268H1606022 | 1       |
| PhytoComm | Ze Lan    | G268H1606022 | 2       |
| PhytoComm | Ze Lan    | G268H1606221 | 1       |
| Phytocomm | Ze Lan    | g268h1606221 | 1       |
| Phytocomm | Ze Lan    | G268H1606221 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1972 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Ze 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 *Ze 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 5              | 1             | 8              | 1967          |

The substance/substance group *Ze Lan* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.7761 % (> 99.4968 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61634     | 61634               | 0.00                         | 9.85                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Ze Xie**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60165-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G011H1605422 | 61611     | 40      | from supplier |
| PhytoComm | Ze Xie    | G011H1605422 | 61695     | 40      | from supplier |
| PhytoComm | Ze Xie    | G011H1605521 | 61736     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Ze Xie*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 115 spectra of 3 reference samples from the substance/substance group *Ze Xie*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Ze Xie    | G011H1605422 | 61320              | 75      |
| PhytoComm | Ze Xie    | G011H1605422 | 61695 <sup>†</sup> | 20      |
| PhytoComm | Ze Xie    | G011H1605521 | 61736 <sup>†</sup> | 20      |

- 13 938 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 13 spectra from 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Ze Xie*.

| Supplier  | Substance | Batch          | Spectra |
|-----------|-----------|----------------|---------|
| PhytoComm | Ze Xie    | (G011)H1605122 | 1       |
| Phytocomm | Ze Xie    | G011H1605422   | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Ze Xie    | G011H1605521 | 5       |
| PhytoComm | Ze Xie    | G011H1605122 | 1       |
| Phytocomm | Ze Xie    | g011h1605122 | 1       |
| PhytoComm | Ze Xie    | H1605022     | 3       |
| Phytocomm | Ze Xie    | H1605022     | 1       |

- 1968 spectra from 16 *Apo-Ident* customers from a total of 958 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Ze Xie* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ze Xie* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 115           | 0              | 13 938        |
| <b>Type C</b> | 13             | 9             | 4              | 1955          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 94.7826 %) |
| <b>Type C</b> | 99.0214 % (> 98.7419 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61611     | 61611               | 0.00                         | 6.48                            |
| 61695     | 61695               | 0.00                         | 8.65                            |
| 61736     | 61736               | 0.00                         | 5.47                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Zhe Bei Mu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50388-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G108H0712422 | 61353     | 40      | from supplier |
| PhytoComm | Zhe Bei Mu | G108H0712521 | 61715     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Zhe Bei Mu*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Zhe Bei Mu*.

| Supplier  | Substance  | Batch        | Sample ID          | Spectra |
|-----------|------------|--------------|--------------------|---------|
| PhytoComm | Zhe Bei Mu | G108H0712422 | 61353 <sup>†</sup> | 20      |
| PhytoComm | Zhe Bei Mu | G108H0712521 | 61715 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 3 batches from the substance/substance group *Zhe Bei Mu*.

| Supplier  | Substance  | Batch        | Spectra |
|-----------|------------|--------------|---------|
| Phytocomm | Zhe Bei Mu | G108H0712121 | 7       |
| PhytoComm | Zhe Bei Mu | G108H0712121 | 2       |
| PhytoComm | Zhe Bei Mu | G108H0712321 | 2       |
| Phytocomm | Zhe Bei Mu | G108H0712422 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1969 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Zhe Bei Mu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zhe Bei Mu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 3              | 3             | 9              | 1966          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.7201 % (> 99.4407 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61353     | 61353               | 0.00                         | 8.41                            |
| 61715     | 61715               | 0.00                         | 11.09                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Zhi Gan Cao**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60016-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Zhi Gan Cao; Glycyrrhizae radix et rhizoma praeparata cum melle

### Special notes

When selecting the *Zhi 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Gan Cao*:

| Supplier  | Substance   | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-------------|--------------|-----------|---------|---------------|
| PhytoComm | Zhi Gan Cao | G118H0881522 | 61655     | 40      | from supplier |
| PhytoComm | Zhi Gan Cao | G118H0881622 | 61985     | 40      | from supplier |
| PhytoComm | Zhi Gan Cao | G118H0881622 | 61986     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Zhi Gan Cao*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Zhi Gan Cao*.

| Supplier  | Substance   | Batch        | Sample ID          | Spectra |
|-----------|-------------|--------------|--------------------|---------|
| PhytoComm | Zhi Gan Cao | G118H0881522 | 61655 <sup>†</sup> | 20      |
| PhytoComm | Zhi Gan Cao | G118H0881622 | 61985 <sup>†</sup> | 20      |
| PhytoComm | Zhi Gan Cao | G118H0881622 | 61986 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Zhi Gan Cao*.

| Supplier  | Substance   | Batch        | Spectra |
|-----------|-------------|--------------|---------|
| Phytocomm | Zhi Gan Cao | G118H0881522 | 4       |
| PhytoComm | Zhi Gan Cao | G118H0881322 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Zhi Gan Cao | G118H0881122 | 3       |
| Phytocomm | Zhi Gan Cao | G118H0881221 | 1       |
| PhytoComm | Zhi Gan Cao | G118H0881221 | 1       |
| Phytocomm | Zhi Gan Cao | g118h0881322 | 1       |

- 1969 spectra from 16 *Apo-Ident* customers from a total of 959 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Zhi 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 *Zhi 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 17             | 5             | 7              | 1952          |

The substance/substance group *Zhi Gan 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.6117 % (> 99.3322 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61655     | 61655               | 0.00                         | 11.66                           |
| 61985     | 61985               | 0.00                         | 8.34                            |
| 61986     | 61986               | 0.00                         | 8.37                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Zhi Ke**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60158-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G043H0921422 | 61347     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

**Type A** All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Zhi Ke*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Zhi Ke*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Zhi Ke    | G043H0921422 | 61347 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Zhi Ke*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Zhi Ke    | G043H0921422 | 2       |
| PhytoComm | Zhi Ke    | G043H0921221 | 2       |
| Phytocomm | Zhi Ke    | G043H0921221 | 1       |
| PhytoComm | Zhi Ke    | H0921021     | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1975 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Zhi 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 1              | 2             | 4              | 1974          |

The substance/substance group *Zhi Ke* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.8756 % (> 99.5965 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61347     | 61347               | 0.00                         | 13.34                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Zhi Mu**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60196-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Zhi Mu; Anemarrhenae radix; Anemarrhenae rhizoma

### Special notes

When selecting the *Zhi Mu* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G019HS1530N1 | 61687     | 40      | from supplier |
| PhytoComm | Zhi Mu    | G019H0824521 | 62027     | 40      | from supplier |
| PhytoComm | Zhi Mu    | G019H0824521 | 62028     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Zhi Mu*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Zhi Mu*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Zhi Mu    | G019HS1530N1 | 61687 <sup>†</sup> | 20      |
| PhytoComm | Zhi Mu    | G019H0824521 | 62027 <sup>†</sup> | 20      |
| PhytoComm | Zhi Mu    | G019H0824521 | 62028 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Zhi Mu*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| PhytoComm | Zhi Mu    | G019H0824221 | 1       |
| PhytoComm | Zhi Mu    | G019H0824321 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Zhi Mu    | H0824922 | 2       |
| Phytocomm | Zhi Mu    | H0824922 | 2       |

- 1974 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Zhi Mu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zhi Mu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 0              | 0             | 7              | 1974          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4415 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61687     | 61687               | 0.00                         | 9.84                            |
| 62027     | 62027               | 0.00                         | 11.32                           |
| 62028     | 62028               | 0.00                         | 10.08                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Zhi Shi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60145-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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   | G044H0922521 | 61720     | 40      | from supplier |
| PhytoComm | Zhi Shi   | G044H0922522 | 62035     | 40      | from supplier |
| PhytoComm | Zhi Shi   | G044H0922522 | 62036     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Zhi Shi*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 60 spectra of 3 reference samples from the substance/substance group *Zhi Shi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Zhi Shi   | G044H0922521 | 61720 <sup>†</sup> | 20      |
| PhytoComm | Zhi Shi   | G044H0922522 | 62035 <sup>†</sup> | 20      |
| PhytoComm | Zhi Shi   | G044H0922522 | 62036 <sup>†</sup> | 20      |

- 13 993 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 18 spectra from 9 *Apo-Ident* customers from 8 batches from the substance/substance group *Zhi Shi*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Zhi Shi   | G044H0922521 | 3       |
| PhytoComm | Zhi Shi   | G044H0922021 | 2       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Zhi Shi   | G044H0922021 | 1       |
| PhytoComm | Zhi Shi   | G044H0922121 | 1       |
| Phytocomm | Zhi Shi   | G044H0922121 | 1       |
| PhytoComm | Zhi Shi   | G044H0922221 | 1       |
| Phytocomm | Zhi Shi   | G044H0922221 | 2       |
| Phytocomm | Zhi Shi   | g044h0922221 | 1       |
| PhytoComm | Zhi Shi   | G044H0922321 | 2       |
| Phytocomm | Zhi Shi   | G044H0922321 | 2       |
| phytocomm | Zhi Shi   | g044h0922321 | 1       |
| PhytoComm | Zhi Shi   | H0922921     | 1       |

- 1963 spectra from 16 *Apo-Ident* customers from a total of 956 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Zhi 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 60            | 0              | 13 993        |
| <b>Type C</b> | 5              | 3             | 15             | 1958          |

The substance/substance group *Zhi Shi* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9310 %) | 100.0000 % (> 90.0000 %) |
| <b>Type C</b> | 99.8781 % (> 99.5985 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61720     | 61720               | 0.00                         | 25.54                           |
| 62035     | 62035               | 0.00                         | 18.83                           |
| 62036     | 62036               | 0.00                         | 19.48                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Zhi Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60367-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G110H1137321 | 61027     | 40      | from supplier |
| PhytoComm | Zhi Zi    | G110H1137321 | 61628     | 40      | from supplier |
| PhytoComm | Zhi Zi    | G110H1137521 | 61686     | 40      | from supplier |
| PhytoComm | Zhi Zi    | G110H1137321 | 61752     | 40      | from supplier |
| PhytoComm | Zhi Zi    | G110H1137523 | 61995     | 40      | from supplier |
| PhytoComm | Zhi Zi    | G110H1137523 | 61996     | 40      | from supplier |

## Validation samples

A total of 37 600 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 Zi*. These samples are listed above in the [calibration samples](#) section.
- 21 326 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 140 spectra of 5 reference samples from the substance/substance group *Zhi Zi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Zhi Zi    | G110H1137321 | 61337              | 60      |
| PhytoComm | Zhi Zi    | G110H1137521 | 61686 <sup>†</sup> | 20      |
| PhytoComm | Zhi Zi    | G110H1137321 | 61752 <sup>†</sup> | 20      |
| PhytoComm | Zhi Zi    | G110H1137523 | 61995 <sup>†</sup> | 20      |
| PhytoComm | Zhi Zi    | G110H1137523 | 61996 <sup>†</sup> | 20      |

- 13 913 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 10 spectra from 10 *Apo-Ident* customers from 3 batches from the substance/substance group *Zhi Zi*.

<sup>†</sup>These spectra were recorded from 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 |
|-----------|-----------|--------------|---------|
| phythocom | Zhi Zi    | g110h1137121 | 1       |
| Phytocomm | Zhi Zi    | G110H1137521 | 3       |
| PhytoComm | Zhi Zi    | G110H1137521 | 1       |
| phytocomm | Zhi Zi    | G110H1137121 | 1       |
| Phytocomm | Zhi Zi    | G110H1137121 | 1       |
| PhytoComm | Zhi Zi    | G110H1137121 | 2       |
| Phytocomm | Zhi Zi    | g110h1137121 | 1       |

- 1971 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Zhi Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zhi Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 240           | 0              | 21 326        |
| <b>Type B</b> | 0              | 140           | 0              | 13 913        |
| <b>Type C</b> | 2              | 4             | 6              | 1969          |

The substance/substance group *Zhi Zi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.7143 %) |
| <b>Type C</b> | 99.9129 % (> 99.6335 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61027     | 61027               | 0.00                         | 13.31                           |
| 61628     | 61628               | 0.00                         | 15.91                           |
| 61686     | 61686               | 0.00                         | 15.46                           |
| 61752     | 61752               | 0.00                         | 16.47                           |
| 61995     | 61995               | 0.00                         | 14.28                           |
| 61996     | 61996               | 0.00                         | 14.54                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Zhu Ling**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60136-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Zhu Ling; Polypori umbellati sclerotium

### Special notes

When selecting the *Zhu 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Ling*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Zhu Ling  | G199H1509421 | 61466     | 40      | from supplier |
| PhytoComm | Zhu Ling  | G199H1509521 | 61790     | 40      | from supplier |
| PhytoComm | Zhu Ling  | G199H1509521 | 61806     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Zhu Ling*. These samples are listed above in the [calibration samples](#) section.
- 21 446 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 115 spectra of 3 reference samples from the substance/substance group *Zhu Ling*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Zhu Ling  | G199H1509421 | 61174              | 75      |
| PhytoComm | Zhu Ling  | G199H1509521 | 61790 <sup>†</sup> | 20      |
| PhytoComm | Zhu Ling  | G199H1509521 | 61806 <sup>†</sup> | 20      |

- 13 938 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Zhu Ling*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Zhu Ling  | G199H1509421 | 2       |
| PhytoComm | Zhu Ling  | G199H1509521 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 |
|-----------|-----------|--------------|---------|
| Mediherb  | Zhu Ling  |              | 1       |
| phytocomm | Zhu Ling  | G199H1509022 | 1       |
| PhytoComm | Zhu Ling  | G199H1509022 | 2       |

- 1974 spectra from 15 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Zhu 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 *Zhu 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 120           | 0              | 21 446        |
| <b>Type B</b> | 0              | 115           | 0              | 13 938        |
| <b>Type C</b> | 0              | 3             | 4              | 1974          |

The substance/substance group *Zhu 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 95.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 94.7826 %) |
| <b>Type C</b> | 100.0000 % (> 99.4415 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61466     | 61466               | 0.00                         | 12.68                           |
| 61790     | 61790               | 0.00                         | 10.95                           |
| 61806     | 61806               | 0.00                         | 10.96                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Zhu Ru**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60241-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Zhu Ru*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Zhu Ru    | G047H0625621 | 62025     | 40      | from supplier |
| PhytoComm | Zhu Ru    | G047H0625621 | 62026     | 40      | from supplier |

## Validation samples

A total of 37 600 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 *Zhu Ru*. These samples are listed above in the [calibration samples](#) section.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Zhu Ru*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Zhu Ru    | G047H0625621 | 62025 <sup>†</sup> | 20      |
| PhytoComm | Zhu Ru    | G047H0625621 | 62026 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 8 *Apo-Ident* customers from 7 batches from the substance/substance group *Zhu Ru*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Zhu Ru    | G047H0625422 | 3       |
| Phytocomm | Zhu Ru    |              | 1       |
| PhytoComm | Zhu Ru    | G047H0625121 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Zhu Ru    | G047H0625122 | 1       |
| PhytoComm | Zhu Ru    | G047H0625122 | 1       |
| PhytoComm | Zhu Ru    | G047H0625321 | 2       |
| Phytocomm | Zhu Ru    | G047H0625321 | 3       |
| Phytocomm | Zhu Ru    | g047h0625321 | 1       |
| Phytocomm | Zhu Ru    | G047h625321  | 1       |
| phytocomm | Zhu Ru    | g047h0625321 | 1       |

- 1966 spectra from 16 *Apo-Ident* customers from a total of 957 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Zhu Ru* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zhu Ru* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 3              | 1             | 14             | 1963          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.8713 % (> 99.5918 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 62025     | 62025               | 0.00                         | 7.31                            |
| 62026     | 62026               | 0.00                         | 7.36                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Zi Hua Di Ding**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50376-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Zi Hua Di Ding*:

| Supplier  | Substance      | Batch        | Sample ID | Spectra | Certificate   |
|-----------|----------------|--------------|-----------|---------|---------------|
| PhytoComm | Zi Hua Di Ding | G249H1216621 | 61901     | 40      | from supplier |
| PhytoComm | Zi Hua Di Ding | G249H1216621 | 61902     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 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 | G249H1216621 | 61901 <sup>†</sup> | 20      |
| PhytoComm | Zi Hua Di Ding | G249H1216621 | 61902 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 Hua Di Ding*.

| Supplier  | Substance      | Batch        | Spectra |
|-----------|----------------|--------------|---------|
| PhytoComm | Zi Hua Di Ding | G249H1216121 | 2       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1979 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Zi Hua Di Ding* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zi Hua Di Ding* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 2              | 0             | 2              | 1977          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 99.9322 % (> 99.6544 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61901     | 61901               | 0.00                         | 5.79                            |
| 61902     | 61902               | 0.00                         | 5.49                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Zi Su Ye**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60134-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

Zi Su Ye; Perillae frutescentis folium

### Special notes

When selecting the *Zi Su 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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 Ye*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Zi Su Ye  | G182HS2680P1 | 61658     | 40      | from supplier |

### Validation samples

A total of 37 600 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 *Zi Su Ye*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group *Zi Su Ye*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Zi Su Ye  | G182HS2680P1 | 61658 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Zi Su Ye*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| Phytocomm | Zi Su Ye  | G182H1214321 | 2       |
| PhytoComm | Zi Su Ye  | G182HS2680P1 | 1       |
| PhytoComm | Zi Su Ye  | G182H1214021 | 3       |
| PhytoComm | Zi Su Ye  | G182H1214321 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1974 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Zi Su 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 *Zi Su 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 |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 1             | 6              | 1974          |

The substance/substance group *Zi Su Ye* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4415 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61658     | 61658               | 0.00                         | 18.99                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Zi Su Zi**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60133-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Zi Su Zi*:

| Supplier  | Substance | Batch        | Sample ID | Spectra | Certificate   |
|-----------|-----------|--------------|-----------|---------|---------------|
| PhytoComm | Zi Su Zi  | G183H1213621 | 61933     | 40      | from supplier |
| PhytoComm | Zi Su Zi  | G183H1213621 | 61934     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 486 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

### Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 40 spectra of 2 reference samples from the substance/substance group *Zi Su Zi*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Zi Su Zi  | G183H1213621 | 61933 <sup>†</sup> | 20      |
| PhytoComm | Zi Su Zi  | G183H1213621 | 61934 <sup>†</sup> | 20      |

- 14 013 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

### Type C Spectra of independent samples not included in the database structure. *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 *Zi Su Zi*.

| Supplier  | Substance | Batch    | Spectra |
|-----------|-----------|----------|---------|
| PhytoComm | Zi Su Zi  | H1213921 | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 1980 spectra from 16 *Apo-Ident* customers from a total of 963 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Zi Su Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zi Su Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 80            | 0              | 21 486        |
| <b>Type B</b> | 0              | 40            | 0              | 14 013        |
| <b>Type C</b> | 0              | 0             | 1              | 1980          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9612 %) | 100.0000 % (> 92.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9311 %) | 100.0000 % (> 85.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4487 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61933     | 61933               | 0.00                         | 14.22                           |
| 61934     | 61934               | 0.00                         | 14.84                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **Zi Wan**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60155-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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    | G038H1215321 | 61001     | 40      | from supplier |
| PhytoComm | Zi Wan    | G038H1215321 | 61601     | 40      | from supplier |
| PhytoComm | Zi Wan    | G038H1215321 | 61693     | 40      | from supplier |
| PhytoComm | Zi Wan    | G038H1215621 | 62045     | 40      | from supplier |
| PhytoComm | Zi Wan    | G038H1215621 | 62046     | 40      | from supplier |

## Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Zi Wan*. These samples are listed above in the [calibration samples](#) section.
- 21 366 spectra from a total of 327 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 135 spectra of 4 reference samples from the substance/substance group *Zi Wan*.

| Supplier  | Substance | Batch        | Sample ID          | Spectra |
|-----------|-----------|--------------|--------------------|---------|
| PhytoComm | Zi Wan    | G038H1215321 | 61310              | 75      |
| PhytoComm | Zi Wan    | G038H1215321 | 61693 <sup>†</sup> | 20      |
| PhytoComm | Zi Wan    | G038H1215621 | 62045 <sup>†</sup> | 20      |
| PhytoComm | Zi Wan    | G038H1215621 | 62046 <sup>†</sup> | 20      |

- 13 918 spectra from a total of 329 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 *Zi Wan*.

| Supplier  | Substance | Batch        | Spectra |
|-----------|-----------|--------------|---------|
| phytocomm | Zi Wan    | g038h1215022 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | Zi Wan    | G038H1215321 | 2       |
| PhytoComm | Zi Wan    | G038H1215022 | 2       |
| Phytocomm | Zi Wan    | G038H1215022 | 1       |
| Phytocomm | Zi Wan    | H1215021     | 2       |

- 1973 spectra from 16 *Apo-Ident* customers from a total of 960 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *Zi Wan* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zi Wan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 200           | 0              | 21 366        |
| <b>Type B</b> | 0              | 135           | 0              | 13 918        |
| <b>Type C</b> | 1              | 2             | 6              | 1972          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9309 %) | 100.0000 % (> 95.5556 %) |
| <b>Type C</b> | 99.9689 % (> 99.6896 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61001     | 61001               | 0.00                         | 11.99                           |
| 61601     | 61601               | 0.00                         | 12.44                           |
| 61693     | 61693               | 0.00                         | 12.60                           |
| 62045     | 62045               | 0.00                         | 10.55                           |
| 62046     | 62046               | 0.00                         | 10.85                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group **(Bai) Dou Kou**  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60177-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

(Bai) Dou Kou; Amomi cardamomi fructus; Amomi rotundi fructus

### Special notes

When selecting the *(Bai) Dou Kou* substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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) Dou Kou*:

| Supplier  | Substance     | Batch        | Sample ID | Spectra | Certificate   |
|-----------|---------------|--------------|-----------|---------|---------------|
| PhytoComm | (Bai) Dou Kou | G016H0508521 | 61700     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

## Type A All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group (*Bai*) *Dou Kou*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group (*Bai*) *Dou Kou*.

| Supplier  | Substance     | Batch        | Sample ID          | Spectra |
|-----------|---------------|--------------|--------------------|---------|
| PhytoComm | (Bai) Dou Kou | G016H0508521 | 61700 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 (*Bai*) *Dou Kou*.

| Supplier  | Substance     | Batch        | Spectra |
|-----------|---------------|--------------|---------|
| Phytocomm | (Bai) Dou Kou | G016H0508021 | 1       |
| Phytocomm | (Bai) Dou Kou | G016H0508521 | 1       |
| Phytocomm | (Bai) Dou Kou | G016H0508521 | 1       |

- 1978 spectra from 16 *Apo-Ident* customers from a total of 961 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

<sup>†</sup>These spectra were recorded from 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*) *Dou Kou* can be 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*) *Dou Kou* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 1              | 2             | 1              | 1977          |

The substance/substance group (*Bai*) *Dou Kou* 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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.9534 % (> 99.6749 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61700     | 61700               | 0.00                         | 10.43                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group (Huai) Niu Xi  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60148-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

(Huai) Niu Xi; Achyranthis bidentatae radix

### Special notes

When selecting the (Huai) Niu Xi substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]  
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group (Huai) Niu Xi:

| Supplier  | Substance     | Batch        | Sample ID | Spectra | Certificate   |
|-----------|---------------|--------------|-----------|---------|---------------|
| PhytoComm | (Huai) Niu Xi | G003H1905422 | 61637     | 40      | from supplier |

### Validation samples

A total of 37 600 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 (*Huai*) *Niu Xi*. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group (*Huai*) *Niu Xi*.

| Supplier  | Substance            | Batch        | Sample ID          | Spectra |
|-----------|----------------------|--------------|--------------------|---------|
| PhytoComm | (Huai) <i>Niu Xi</i> | G003H1905422 | 61637 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 8 *Apo-Ident* customers from 7 batches from the substance/substance group (*Huai*) *Niu Xi*.

| Supplier  | Substance            | Batch        | Spectra |
|-----------|----------------------|--------------|---------|
| Phytocomm | (Huai) <i>Niu Xi</i> | G003H1905422 | 1       |
| Phytocomm | (Huai) <i>Niu Xi</i> | G003H1905222 | 1       |
| Phytocomm | (Huai) <i>Niu Xi</i> | G003H1905222 | 1       |
| Phytocomm | (Huai) <i>Niu Xi</i> | G003H1905122 | 1       |
| PhytoComm | (Huai) <i>Niu Xi</i> | G003H1905122 | 1       |
| PhytoComm | (Huai) <i>Niu Xi</i> | H1905021     | 3       |
| Phytocomm | (Huai) <i>Niu Xi</i> | G003H1905321 | 2       |
| PhytoComm | (Huai) <i>Niu Xi</i> | G003H1905422 | 1       |
| PhytoComm | (Huai) <i>Niu Xi</i> | G003H1905222 | 3       |
| PhytoComm | (Huai) <i>Niu Xi</i> | G003H190522  | 1       |

<sup>†</sup>These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.



- 1966 spectra from 16 *Apo-Ident* customers from a total of 957 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group (*Huai*) *Niu Xi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with (*Huai*) *Niu Xi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 3              | 4             | 11             | 1963          |

The substance/substance group (*Huai*) *Niu Xi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

|               | Specificity              | Recognition rate         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 99.8401 % (> 99.5605 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61637     | 61637               | 0.00                         | 9.24                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.



# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group (Ku) Xing Ren  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 50290-2017-06-01  
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 2.2.40 Ph. Eur. durch Apo-Ident* [4]  
AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group (Ku) Xing Ren:

| Supplier  | Substance     | Batch        | Sample ID | Spectra | Certificate   |
|-----------|---------------|--------------|-----------|---------|---------------|
| PhytoComm | (Ku) Xing Ren | G029H0708622 | 61838     | 40      | from supplier |

### Validation samples

A total of 37 600 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

### Type A All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group (Ku) Xing Ren. These samples are listed above in the [calibration samples](#) section.
- 21 526 spectra from a total of 328 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 20 spectra of 1 reference samples from the substance/substance group (Ku) Xing Ren.

| Supplier  | Substance     | Batch        | Sample ID          | Spectra |
|-----------|---------------|--------------|--------------------|---------|
| PhytoComm | (Ku) Xing Ren | G029H0708622 | 61838 <sup>†</sup> | 20      |

- 14 033 spectra from a total of 330 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 18 spectra from 8 *Apo-Ident* customers from 8 batches from the substance/substance group (Ku) Xing Ren.

| Supplier  | Substance     | Batch        | Spectra |
|-----------|---------------|--------------|---------|
| PhytoComm | (Ku) Xing Ren | G029H0708322 | 1       |
| PhytoComm | (Ku) Xing Ren | G029H0708125 | 1       |
| Phytocomm | (Ku) Xing Ren | 161213xr     | 1       |
| PhytoComm | (Ku) Xing Ren | G029H0708024 | 1       |
| Phytocomm | (Ku) Xing Ren | G029H0708024 | 2       |
| Phytocomm | (Ku) Xing Ren | G029H0708122 | 4       |
| PhytoComm | (Ku) Xing Ren | G029H0708122 | 1       |
| Phytocomm | (Ku) Xing Ren | G029H0708125 | 3       |
| Phytocomm | (Ku) Xing Ren | g029h0708122 | 1       |

*continued on the next page*

<sup>†</sup>These spectra were recorded from 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 | (Ku) Xing Ren | g029h0708322 | 2       |
| PhytoComm | (Ku) Xing Ren | G029H708125  | 1       |

- 1963 spectra from 16 *Apo-Ident* customers from a total of 956 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *(Ku) Xing Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *(Ku) Xing Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 40            | 0              | 21 526        |
| <b>Type B</b> | 0              | 20            | 0              | 14 033        |
| <b>Type C</b> | 0              | 0             | 18             | 1963          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9614 %) | 100.0000 % (> 85.0000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9315 %) | 100.0000 % (> 70.0000 %) |
| <b>Type C</b> | 100.0000 % (> 99.4408 %) | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61838     | 61838               | 0.00                         | 26.54                           |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group (Sheng) Di Huang  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60005-2017-06-01  
Executing company HiperScan GmbH  
Weiskeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

(Sheng) Di Huang; Rehmanniae radix; Rehmanniae viridae radix

### Special notes

When selecting the (Sheng) Di Huang substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G211H0532422 | 61452     | 40      | from supplier |
| PhytoComm | (Sheng) Di Huang | G211H0532521 | 61651     | 40      | from supplier |
| PhytoComm | (Sheng) Di Huang | G211H0532621 | 61797     | 40      | from supplier |
| PhytoComm | (Sheng) Di Huang | G211H0532621 | 61804     | 40      | from supplier |
| PhytoComm | (Sheng) Di Huang | G211H0532621 | 61881     | 40      | from supplier |
| PhytoComm | (Sheng) Di Huang | G211H0532621 | 61882     | 40      | from supplier |

## Validation samples

A total of 37 600 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.
- 21 326 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 175 spectra of 6 reference samples from the substance/substance group (Sheng) Di Huang.

| Supplier  | Substance        | Batch        | Sample ID          | Spectra |
|-----------|------------------|--------------|--------------------|---------|
| PhytoComm | (Sheng) Di Huang | G211H0532422 | 61160              | 75      |
| PhytoComm | (Sheng) Di Huang | G211H0532521 | 61651 <sup>†</sup> | 20      |
| PhytoComm | (Sheng) Di Huang | G211H0532621 | 61797 <sup>†</sup> | 20      |
| PhytoComm | (Sheng) Di Huang | G211H0532621 | 61804 <sup>†</sup> | 20      |
| PhytoComm | (Sheng) Di Huang | G211H0532621 | 61881 <sup>†</sup> | 20      |
| PhytoComm | (Sheng) Di Huang | G211H0532621 | 61882 <sup>†</sup> | 20      |

- 13 878 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 19 spectra from 8 *Apo-Ident* customers from 7 batches from the substance/substance group (Sheng) Di Huang.

<sup>†</sup>These spectra were recorded from 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 | (Sheng) Di Huang | G211H0532521 | 4       |
|           | (Sheng) Di Huang | g211h0532323 | 1       |
| PhytoComm | (Sheng) Di Huang | G211H0532121 | 2       |
| PhytoComm | (Sheng) Di Huang | G211H0532323 | 1       |
| Phytocomm | (Sheng) Di Huang | G211H0532121 | 3       |
| phytocomm | (Sheng) Di Huang | G211H0532121 | 1       |
| Phytocomm | (Sheng) Di Huang | g211h053221  | 1       |
| Phytocomm | (Sheng) Di Huang | G211H0532221 | 4       |
| Phytocomm | (Sheng) Di Huang | g211h0532121 | 1       |
| PhytoComm | (Sheng) Di Huang | G211H0532221 | 1       |

- 1962 spectra from 16 *Apo-Ident* customers from a total of 957 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

### Validation results

The validation runs checked whether the substance/substance group (*Sheng*) *Di Huang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with (*Sheng*) *Di Huang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 0              | 240           | 0              | 21 326        |
| <b>Type B</b> | 0              | 175           | 0              | 13 878        |
| <b>Type C</b> | 7              | 8             | 11             | 1955          |

The substance/substance group (*Sheng*) *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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 100.0000 % (> 99.9611 %) | 100.0000 % (> 97.5000 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 100.0000 % (> 96.5714 %) |
| <b>Type C</b> | 99.8200 % (> 99.5404 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

### Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61452     | 61452               | 0.00                         | 8.28                            |
| 61651     | 61651               | 0.00                         | 7.51                            |
| 61797     | 61797               | 0.00                         | 8.95                            |
| 61804     | 61804               | 0.00                         | 9.55                            |
| 61881     | 61881               | 0.00                         | 10.12                           |
| 61882     | 61882               | 0.00                         | 9.60                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

# VALIDATION REPORT

## IdentModul 1.3-2017-03

Validated substance/substance group (Shi) Chang Pu  
Substance class TCM - Granulated herbal extracts (PhytoComm)  
Report date 01/06/2017  
Report number 60426-2017-06-01  
Executing company HiperScan GmbH  
Weißeritzstraße 3  
01067 Dresden  
Germany

### Relevant substance names

(Shi) Chang Pu; Acori graminei rhizoma; Acori rhizoma

### Special notes

When selecting the (Shi) Chang Pu substance/substance group, the following information is displayed to the user:

*no information*

### Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]

AA004 *Erstellung und Validierung eines IdentModul-Updates*

### Validation method

Validation occurs after every change to the chemometric model (also “database”) and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.
2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

### Calibration samples

Only spectra which have been recorded by *HiperScan 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 | G006H0544421 | 61012     | 40      | from supplier |
| PhytoComm | (Shi) Chang Pu | G006H0544421 | 61620     | 40      | from supplier |
| PhytoComm | (Shi) Chang Pu | G006HS2700N1 | 61721     | 40      | from supplier |
| PhytoComm | (Shi) Chang Pu | G006HS270PH1 | 61851     | 40      | from supplier |
| PhytoComm | (Shi) Chang Pu | G006HS270PH1 | 61852     | 40      | from supplier |
| PhytoComm | (Shi) Chang Pu | G006HS2700N1 | 62073     | 40      | from supplier |
| PhytoComm | (Shi) Chang Pu | G006HS2700N1 | 62074     | 40      | from supplier |

## Validation samples

A total of 37 600 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 (*Shi*) *Chang Pu*. These samples are listed above in the [calibration samples](#) section.
- 21 286 spectra from a total of 326 batches from further 203 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

**Type B** Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by <sup>†</sup>.

- 175 spectra of 6 reference samples from the substance/substance group (*Shi*) *Chang Pu*.

| Supplier  | Substance      | Batch        | Sample ID          | Spectra |
|-----------|----------------|--------------|--------------------|---------|
| PhytoComm | (Shi) Chang Pu | G006H0544421 | 61329              | 75      |
| PhytoComm | (Shi) Chang Pu | G006HS2700N1 | 61721 <sup>†</sup> | 20      |
| PhytoComm | (Shi) Chang Pu | G006HS270PH1 | 61851 <sup>†</sup> | 20      |
| PhytoComm | (Shi) Chang Pu | G006HS270PH1 | 61852 <sup>†</sup> | 20      |
| PhytoComm | (Shi) Chang Pu | G006HS2700N1 | 62073 <sup>†</sup> | 20      |
| PhytoComm | (Shi) Chang Pu | G006HS2700N1 | 62074 <sup>†</sup> | 20      |

- 13 878 spectra from a total of 328 batches from further 205 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

**Type C** Spectra of independent samples not included in the database structure. *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 7 batches from the substance/substance group (*Shi*) *Chang Pu*.

<sup>†</sup>These spectra were recorded from 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   | (Shi) Chang Pu | G006HS2700N1 | 1       |
| Phytocomm   | (Shi) Chang Pu | g006h0544023 | 1       |
| PhytoComm   | (Shi) Chang Pu | G006H0544023 | 1       |
| Phytocomm   | (Shi) Chang Pu | G006H0544122 | 3       |
| Phytocomm   | (Shi) Chang Pu | G006H0544321 | 1       |
| Phytocomm   | (Shi) Chang Pu | G006H0544322 | 1       |
| Herbasinica | (Shi) Chang Pu | g006h0544321 | 1       |

- 1972 spectra from 16 *Apo-Ident* customers from a total of 957 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

## Validation results

The validation runs checked whether the substance/substance group *(Shi) Chang Pu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *(Shi) Chang Pu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

|               | False positive | True positive | False negative | True negative |
|---------------|----------------|---------------|----------------|---------------|
| <b>Type A</b> | 1              | 280           | 0              | 21 285        |
| <b>Type B</b> | 0              | 169           | 6              | 13 878        |
| <b>Type C</b> | 4              | 1             | 8              | 1968          |

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         |
|---------------|--------------------------|--------------------------|
| <b>Type A</b> | 99.9959 % (> 99.9765 %)  | 100.0000 % (> 97.8571 %) |
| <b>Type B</b> | 100.0000 % (> 99.9308 %) | 96.5714 % (> 94.8571 %)  |
| <b>Type C</b> | 99.8161 % (> 99.5367 %)  | n/a (n/a)                |

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

## Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

| Sample ID | Reference sample ID | Distance to reference sample | Distance to next foreign sample |
|-----------|---------------------|------------------------------|---------------------------------|
| 61012     | 61012               | 0.00                         | 11.74                           |
| 61620     | 61620               | 0.00                         | 7.36                            |
| 61721     | 61721               | 0.00                         | 4.34                            |
| 61851     | 61851               | 0.00                         | 5.87                            |
| 61852     | 61852               | 0.00                         | 5.60                            |
| 62073     | 62073               | 0.00                         | 5.86                            |
| 62074     | 62074               | 0.00                         | 5.47                            |

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

## *Appendix A: Additional calibration samples (Type A)*

Not required.





## ***Appendix B: Additional validation samples (Type B)***

It is necessary that spectra also enter the validation which cannot be identified with this model. In this manner, it is verified that the model also rejects unknown substances. The spectra for these samples were recorded by *HiperScan GmbH*. They are allocated to the *Type B*. They also include the calibration spectra for other models.

The samples originate from 6 batches. From these 216 spectra were recorded. The spectra recorded on independent samples of substances which can be identified with the model are listed respectively in the section *Type B* for the individual substances and do not appear again elsewhere in this list.

| Supplier  | Substance     | Batch        | Spectra | Certificate   |
|-----------|---------------|--------------|---------|---------------|
| PhytoComm | Hua Shi       | G238H1332521 | 56      | from supplier |
| PhytoComm | Hua Shi       | G238H1332621 | 27      | from supplier |
| PhytoComm | Hua Shi       | G238H1332621 | 30      | from supplier |
| PhytoComm | Mu Li (Sheng) | G178H0740621 | 43      | from supplier |
| PhytoComm | Mu Li (Sheng) | G178HS128PN1 | 30      | from supplier |
| PhytoComm | Mu Li (Sheng) | G178HS128PN1 | 30      | from supplier |



## Appendix C: Additional validation samples (*Type C*)

Spectra for substances from the field which cannot be identified with this model also enter the validation. In this manner, it is verified that the model also rejects unknown substances. The spectra for these samples were recorded by *Apo-Ident* customers. They belong to *Type C*. The information provided by the customer regarding the manufacturer and batch number is taken over by *HiperScan GmbH* to a large extent unchecked.

The samples originate from 152 batches. From these, 251 spectra were recorded. The spectra recorded on independent samples of substances from the field which can be identified with the model are listed respectively in the section *Type C* for the individual substances and do not appear again elsewhere in this list.

| Supplier     | Substance       | Batch         | Spectra |
|--------------|-----------------|---------------|---------|
| Bios         | Lu Hui          | 424263        | 3       |
| Herba Natura | Qu Mai          | 8950          | 1       |
| Herbasin     | Fang Ji         | G236H0727123  | 2       |
| Herbasin     | Hua Shi         | G238H332121   | 1       |
| phythocom    | She Chuang Zi   | G076H1154122  | 3       |
| phytocomm    | Bai Bu          | G235H0608021  | 1       |
| phytocomm    | E Bu Shi Cao    | G061H1801022  | 3       |
| phytocomm    | E Jiao          | G036H0861022  | 2       |
| phytocomm    | Fang Ji         | FA0727901     | 2       |
| phytocomm    | Gu Ya           | G177H1513021  | 2       |
| phytocomm    | Hai Piao Xiao   | G305BP051026  | 1       |
| phytocomm    | Hu Zhang        | G197H0851021  | 2       |
| phytocomm    | Huo Xiang       | H2005021      | 5       |
| phytocomm    | Lu Jiao Jiao    | g323h1158121  | 1       |
| phytocomm    | Lu Rong         | G296BP031136  | 1       |
| phytocomm    | Mang Xiao       | G160H0627121  | 1       |
| phytocomm    | Mi Meng Hua     | G054BP021404  | 2       |
| phytocomm    | Wu Gong         | G311H1411021  | 3       |
| phytocomm    | Xian He Cao     | g008h0547321  | 1       |
| phytocomm    | Ye Ju Hua       | G514H1187021  | 3       |
| Phytocomm    | (Bai) Jiang Can | G269H0513222  | 3       |
| Phytocomm    | (Bai) Jiang Can | G269H0513321  | 2       |
| Phytocomm    | (Bai) Jiang Can | g144h1708221  | 1       |
| Phytocomm    | (Bai) Jiang Can | g269h0513222  | 1       |
| Phytocomm    | (Fen) Bi Xie    | G290BP021212  | 1       |
| Phytocomm    | (Fen) Bi Xie    | G290H1251121  | 3       |
| Phytocomm    | (Fen) Bi Xie    | G29H1251121   | 1       |
| Phytocomm    | Bai Bian Dou    | G093H0510221  | 1       |
| Phytocomm    | Bai Bian Dou    | g093h0510221  | 1       |
| Phytocomm    | Bai Bu          | G235H0608321  | 1       |
| Phytocomm    | Bai Bu          | G235H0608121  | 2       |
| Phytocomm    | Bai Bu          | H0608921      | 1       |
| Phytocomm    | Bai Jie Zi      | H0518921      | 1       |
| Phytocomm    | Bing Lang       | G027H1825221  | 2       |
| Phytocomm    | Chong Wei Zi    | G317BP021046  | 1       |
| Phytocomm    | Chong Wei Zi    | g317bp021046  | 1       |
| Phytocomm    | Chuan Bei Mu    | g107f11021    | 1       |
| Phytocomm    | Chuan Bei Mu    | G107F110721   | 1       |
| Phytocomm    | Chuan Bei Mu    | G107BP020722A | 2       |
| Phytocomm    | Chuan Bei Mu    | g107f110721   | 2       |
| Phytocomm    | Da Fu Pi        | G293H0321221  | 1       |
| Phytocomm    | Da Fu Pi        | G293H0321122  | 2       |
| Phytocomm    | Da Fu Pi        | G293H0321021  | 1       |
| Phytocomm    | Da Huang        | g212h0320023  | 1       |
| Phytocomm    | Da Huang        | G212H0320521  | 3       |
| Phytocomm    | Dan Zhu Ye      | G046H1105021  | 3       |

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| <b>Supplier</b> | <b>Substance</b> | <b>Batch</b>   | <b>Spectra</b> |
|-----------------|------------------|----------------|----------------|
| Phytocomm       | Dan Zhu Ye       | G046H1105321   | 4              |
| Phytocomm       | Dan Zhu Ye       | G046H110521    | 1              |
| Phytocomm       | Deng Xin Cao     | G306F100617    | 1              |
| Phytocomm       | Deng Xin Cao     | f100707        | 1              |
| Phytocomm       | Di Yu            | G2150604121    | 1              |
| Phytocomm       | Di Yu            | G215H0604322   | 1              |
| Phytocomm       | Ding Xiang       | G058H0210021   | 1              |
| Phytocomm       | Ding Xiang       | H0210921       | 1              |
| Phytocomm       | E Bu Shi Cao     | G061H1801122   | 2              |
| Phytocomm       | E Jiao           | g036h0861121   | 1              |
| Phytocomm       | E Jiao           | G036H0861421   | 2              |
| Phytocomm       | E Jiao           | g036h0861221   | 1              |
| Phytocomm       | Fang Ji          | G236H0727321   | 1              |
| Phytocomm       | Fang Ji          | G236H0727321   | 1              |
| Phytocomm       | Hai Tong Pi      | G100H1076221   | 2              |
| Phytocomm       | Han Lian Cao     | G095H0770521   | 4              |
| Phytocomm       | Han Lian Cao     | G095H0770321   | 1              |
| Phytocomm       | Han Lian Cao     | g095h0770321   | 1              |
| Phytocomm       | He Zi            | G291H1239021   | 2              |
| Phytocomm       | He Zi            | G291H1239221   | 3              |
| Phytocomm       | Hu Zhang         | g197h0851321   | 1              |
| Phytocomm       | Hu Zhang         | G197H0851321   | 2              |
| Phytocomm       | Hua Shi          | g238h1332121   | 1              |
| Phytocomm       | Hua Shi          | G238H1332121   | 3              |
| Phytocomm       | Jie Cao          | H2111921       | 1              |
| Phytocomm       | Jin Ying Zi      | G023H0846221   | 1              |
| Phytocomm       | Jin Ying Zi      | G023H0317921   | 2              |
| Phytocomm       | Ju Hong          | G310H1623121   | 2              |
| Phytocomm       | Long Gu          | g0251706122    | 1              |
| Phytocomm       | Lu Jiao Jiao     | G323H1158022   | 1              |
| Phytocomm       | Mu Li (Sheng)    | G178H0740221   | 2              |
| Phytocomm       | Pang Da Hai      | G529H0960023   | 2              |
| Phytocomm       | Qian Shi         | G102H0836422   | 1              |
| Phytocomm       | Qing Hao         | G031H0810221   | 2              |
| Phytocomm       | Quan Xie         | G222F110314    | 1              |
| Phytocomm       | Rou Gui          | G069H0617323   | 2              |
| Phytocomm       | Rou Gui          | g069h0617123   | 1              |
| Phytocomm       | Rou Gui          | G069H0617123   | 2              |
| Phytocomm       | Sang Piao Xiao   | G282H421029201 | 1              |
| Phytocomm       | Tong Cao         | G531H114021    | 2              |
| Phytocomm       | Tong Cao         | G531H1141021   | 1              |
| Phytocomm       | Wa Leng Zi       | G508F110305    | 2              |
| Phytocomm       | Wu Gong          | G311H1411321   | 1              |
| Phytocomm       | Wu Gong          | G311H411321    | 1              |
| Phytocomm       | Xian He Cao      | G008H0547321   | 1              |
| Phytocomm       | Xian He Cao      | G008H0547121   | 2              |
| Phytocomm       | Xue Jie          | G322H0631921   | 1              |
| Phytocomm       | Yin Xing Ye      | G518H1445021   | 1              |
| Phytocomm       | Zhen Zhu Mu      | g155h0979221   | 1              |
| PhytoComm       | (Bai) Jiang Can  | H0513021       | 3              |
| PhytoComm       | (Bai) Jiang Can  | G269H0513121   | 2              |
| PhytoComm       | (Dai) Zhe Shi    | 410520701      | 1              |
| PhytoComm       | (Fen) Bi Xie     | H1251921       | 1              |
| PhytoComm       | (Fen) Bi Xie     | G0290H1251121  | 1              |
| PhytoComm       | Bai Bian Dou     | H0510921       | 1              |
| PhytoComm       | Bai Bu           | G235H0608221   | 1              |
| PhytoComm       | Bie Jia          | G507H2401121   | 3              |
| PhytoComm       | Bie Jia          | G507H2401321   | 2              |
| PhytoComm       | Bing Lang        | H1825021       | 4              |
| PhytoComm       | Cao Guo          | E241050        | 1              |

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| Supplier   | Substance     | Batch          | Spectra |
|------------|---------------|----------------|---------|
| PhytoComm  | Chong Wei Zi  | E341046        | 1       |
| PhytoComm  | Chuan Bei Mu  | H0711921       | 1       |
| PhytoComm  | Ci Shi        | F100628        | 1       |
| PhytoComm  | Da Fu Pi      | H0321922       | 1       |
| PhytoComm  | Da Huang      | G212H0320321   | 3       |
| PhytoComm  | Da Huang      | G212H0320023   | 2       |
| PhytoComm  | Dan Zhu Ye    | H1105921       | 2       |
| PhytoComm  | Deng Xin Cao  | F100707        | 1       |
| PhytoComm  | Ding Xiang    | G058h0210021   | 1       |
| PhytoComm  | Dong Kui Zi   | G001BP030505   | 1       |
| PhytoComm  | E Bu Shi Cao  | G061H180122    | 1       |
| PhytoComm  | E Jiao        | G036H0861121   | 2       |
| PhytoComm  | E Jiao        | G036H0861221   | 3       |
| PhytoComm  | Gao Ben       | H1809921       | 2       |
| PhytoComm  | Gao Ben       | G137H1809221   | 1       |
| PhytoComm  | Geng Mi       | G329H1320121   | 1       |
| PhytoComm  | Geng Mi       | 414161         | 1       |
| PhytoComm  | Gu Ya         | H1513921       | 2       |
| PhytoComm  | Gui Ban       | G530F110210    | 2       |
| PhytoComm  | Han Lian Cao  | G263H1423121   | 2       |
| PhytoComm  | Han Lian Cao  | G095H0770121   | 4       |
| PhytoComm  | Hu Zhang      | G197H081021    | 1       |
| PhytoComm  | Hua Shi       | G238H133121    | 1       |
| PhytoComm  | Lu Jiao Jiao  | G323H1158321   | 2       |
| PhytoComm  | Lu Jiao Jiao  | G323H1158121   | 2       |
| PhytoComm  | Ma Chi Xian   | G255F110310    | 3       |
| PhytoComm  | Mang Xiao     | H0627021       | 1       |
| PhytoComm  | Mao Dong Qing | G319H0411121   | 1       |
| PhytoComm  | Mu Li (Sheng) | H0740922       | 2       |
| PhytoComm  | Qian Shi      | G102H0836121   | 4       |
| PhytoComm  | Qian Shi      | H0836921       | 1       |
| PhytoComm  | Qing Hao      | G031H0810021   | 2       |
| PhytoComm  | Ren Dong Teng | H0751922       | 1       |
| PhytoComm  | Ren Dong Teng | (G297)H075122  | 1       |
| PhytoComm  | Ren Dong Teng | G297H0751222   | 1       |
| PhytoComm  | Rou Dou Kou   | G16BP020616    | 1       |
| PhytoComm  | Rou Gui       | H0617022       | 3       |
| PhytoComm  | She Chuang Zi | G076H1154021   | 2       |
| PhytoComm  | Shi Jue Ming  | H0546021       | 1       |
| PhytoComm  | Xian He Cao   | H0547021       | 3       |
| PhytoComm  | Ye Ju Hua     | (G514)H1187021 | 1       |
| PhytoComm  | Yin Chai Hu   | G368H1444221   | 1       |
| PhytoComm  | Yin Xing Ye   | H1445921       | 1       |
| PhytoComm  | Yu Li Ren     | H0967922       | 1       |
| PhytoComm  | Zhen Zhu Mu   | H0979921       | 1       |
| Sino Phyto | Long Gu       | G025H1706122   | 4       |



## Appendix D: Requirements of validation

In order to ensure adherence to the safe scientific status, the individual methods for manufacturing and testing must be validated under certain circumstances (compare § 34 para. 1 no. 3, § 35 para. 1 no. 4 and para. 4 sentence 1 no. 2 b, para. 6 sentence 3 *ApoBetrO* [Pharmacies Rules and Regulations]). The *ApoBetrO* [Pharmacies Rules and Regulations] incorporates a legal definition in § 1 a para. 16 (quotation translated):

*“Validation is the provision of documented proof which with a high degree of safety documents that, via a specific process or standard work process, a medicinal product is manufactured and tested, which is in accordance with previously determined quality features.”*

Validation documentation can be used to prove that methods or devices which are not described in the Pharmacopoeia within the meaning of § 6 para. 1 sentence 3 *ApBetrO* [Pharmacies Rules and Regulations] achieve the same results as those in the Pharmacopoeia. On the other hand, with the requirements of the demanded validation it must be observed whether the respective testing method is already incorporated in the Pharmacopoeia.

NIR spectroscopy as a general testing method need not be validated in accordance with the express ruling in the *Ph. Eur. Section 1.1* [3], as it is already described in *Section 2.2.40* of the *Ph. Eur.* as an area of application for the identification of raw materials.

However, a special validation requirement exists for the reference database. This requirement is met with the existing document. Further requirements or rules as to how this proof must be furnished do not exist. It is required that the processes guarantee the same results as the methods and devices in the Pharmacopoeia [17].

Carrying out identity tests with *Apo-Ident* is therefore also possible if the NIR spectroscopy process is not required in the Pharmacopoeia monograph of the substance for identity testing. All NIR analyses with *Apo-Ident* prove several, often all molecule groups and are therefore comparable with a series of individual, targeted chemical proofs [4]. Therefore, the identity proof with *Apo-Ident* replaces the monograph test series (with two or more test combinations).

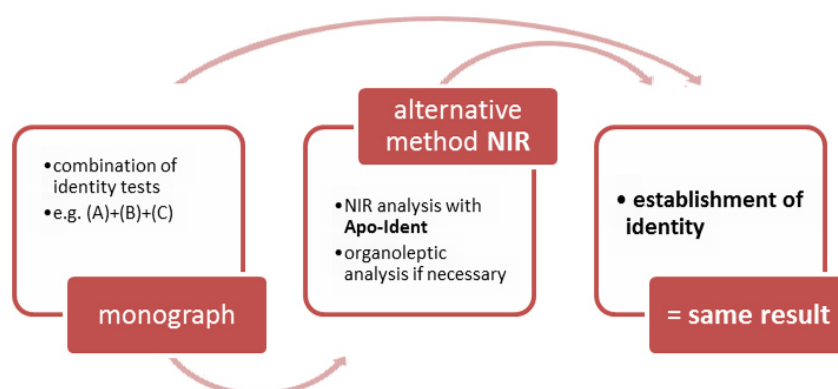


**Figure 2:** The combination of tests of the monograph is replaced by the alternative method NIR spectroscopy using *Apo-Ident*. This is permissible because both test procedures result in the establishment of the identity of the raw material.

With this validation documentation, proof is furnished that identical results are achieved with *Apo-Ident* and Pharmacopoeia methods, i.e. confirmation of the identity of the raw material [2].

## ***Appendix E: Conformity of Apo-Ident with the European pharmacopeia***

According to *Ph. Eur. Section 2.2.40*, NIR spectroscopy is basically suitable for: “Identification of agents, excipients, dosage forms, intermediate manufacturing products, chemical raw materials and packaging materials” ([3], quotation translated).

The fact that *Apo-Ident* meets the further criteria of the European Pharmacopoeia under the headings in *Section 2.2.40*

- Apparatus
- Measurement methods
- Sample preparation and presentation
- Testing the functionality of the instrument
- Identification and characterisation (qualitative analysis)
- Quantitative analysis
- Ongoing model evaluation
- Transfer of databases
- Data storage

can be proven based on the *HiperScan GmbH* documentation of “Meeting 2.2.40 *Ph. Eur.* by *Apo-Ident*” [4].



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## Index

- (Bai) Dou Kou, [819](#)  
 (Huai) Niu Xi, [823](#)  
 (Ku) Xing Ren, [827](#)  
 (Sheng) Di Huang, [831](#)  
 (Shi) Chang Pu, [835](#)
- Acanthopanax (senticosi) radix, *see* [Ci Wu Jia](#)  
 Acanthopanax cortex, *see* [Wu Jia Pi](#)  
 Acanthopanax cortex radices, *see* [Wu Jia Pi](#)  
 Achyranthis bidentatae radix, *see* [\(Huai\) Niu Xi](#)  
 Aconiti lateralis radix praeparata, *see* [Fu Zi](#)  
 Aconiti radix lateralis praep., *see* [Fu Zi](#)  
 Acori graminei rhizoma, *see* [\(Shi\) Chang Pu](#)  
 Acori rhizoma, *see* [\(Shi\) Chang Pu](#)  
 Ai Ye, [23](#)  
 Albiziae cortex, *see* [He Huan Pi](#)  
 Albiziae julibrissini cortex, *see* [He Huan Pi](#)  
 Alismatis rhizoma, *see* [Ze Xie](#)  
 Allii bulbosus, *see* [Xie Bai](#)  
 Allii fistulosi bulbosus, *see* [Cong Bai](#)  
 Allii macrostemonis bulbosus, *see* [Xie Bai](#)  
 Alpiniae fructus, *see* [Yi Zhi Ren](#)  
 Alpiniae oxyphyllae fructus, *see* [Yi Zhi Ren](#)  
 Amomi cardamomi fructus, *see* [\(Bai\) Dou Kou](#)  
 Amomi rotundi fructus, *see* [\(Bai\) Dou Kou](#)  
 Amomi villosi fructus, *see* [Sha Ren](#)  
 Andrographitis herba, *see* [Chuan Xin Lian](#)  
 Anemarrhenae radix, *see* [Zhi Mu](#)  
 Anemarrhenae rhizoma, *see* [Zhi Mu](#)  
 Angelicae dahuricae radix, *see* [Bai Zhi](#)  
 Angelicae pubescentis radix, *see* [Du Huo](#)  
 Angelicae sinensis radix, *see* [Dang Gui](#)  
 Angelicae sinensis radix extremitas, *see* [Dang Gui Wei](#)  
 Arctii fructus, *see* [Niu Bang Zi](#)  
 Arctii lappae fructus, *see* [Niu Bang Zi](#)  
 Arisaematis rhizoma, *see* [Tian Nan Xing](#)  
 Arisaematis rhizoma praep., *see* [Tian Nan Xing](#)  
 Armeniacae amarum semen, *see* [\(Ku\) Xing Ren](#)  
 Armillariella mellea rhizoma, *see* [Mi Huan Jun](#)  
 Artemisiae argyi folium, *see* [Ai Ye](#)  
 Artemisiae scopariae herba, *see* [Yin Chen Hao](#)  
 Asparagi cochinchinensis radix, *see* [Tian Men Dong](#)  
 Asteris tatarici radix, *see* [Zi Wan](#)  
 Astragali membranacei radix, *see* [Huang Qi](#)  
 Atractylodis macrocephalae rhizoma, *see* [Bai Zhu](#)  
 Atractylodis rhizoma, *see* [Cang Zhu](#)  
 Aurantii fructus immaturus, *see* [Zhi Shi](#)
- Ba Ji Tian, [27](#)  
 Bai Guo, [31](#)  
 Bai He, [35](#)  
 Bai Hua She She Cao, [39](#)  
 Bai Jiang Cao, [43](#)  
 Bai Mao Gen, [47](#)  
 Bai Qian, [51](#)  
 Bai Shao Yao, [55](#)  
 Bai Tou Weng, [59](#)  
 Bai Xian Pi, [63](#)  
 Bai Zhi, [67](#)  
 Bai Zhu, [71](#)  
 Bai Zi Ren, [75](#)  
 Bambusae in taeniae caulis, *see* [Zhu Ru](#)  
 Ban Lan Gen, [79](#)  
 Ban Xia (Jiang), [83](#)  
 Ban Zhi Lian, [87](#)  
 Belamcandae rhizoma, *see* [She Gan](#)  
 Benincasae hispidae semen, *see* [Dong Gua Zi](#)  
 Biotae orientalis cacumen, *see* [Ce Bai Ye](#)  
 Biotae orientalis semen, *see* [Bai Zi Ren](#)  
 Bo He, [91](#)  
 Bu Gu Zhi, [95](#)  
 Bupleuri radix, *see* [Chai Hu](#)
- Cang Er Zi, [99](#)  
 Cang Zhu, [103](#)  
 Cannabis semen, *see* [Huo Ma Ren](#)  
 Carthami flos, *see* [Hong Hua](#)  
 Cassiae torae semen, *see* [Jue Ming Zi](#)  
 Ce Bai Ye, [107](#)  
 Cervi corni degelatinatum, *see* [Lu Jiao Shuang](#)  
 Chaenomelis lagenariae fructus, *see* [Mu Gua](#)  
 Chai Hu, [111](#)  
 Chan Tui, [115](#)  
 Che Qian Zi, [119](#)  
 Chen Pi, [123](#)  
 Chi Shao (Yao), [127](#)  
 Chrysanthemi flos, *see* [Ju Hua](#)  
 Chuan Lian Zi, [131](#)  
 Chuan Mu Tong, [135](#)  
 Chuan Niu Xi, [139](#)  
 Chuan Xin Lian, [143](#)  
 Chuan Xiong, [147](#)  
 Chuang Mu Xiang, [151](#)  
 Ci Wu Jia, [155](#)  
 Cicadae periostracum, *see* [Chan Tui](#)  
 Cimicifugae rhizoma, *see* [Sheng Ma](#)  
 Cinnamomi cassiae ramulus, *see* [Gui Zhi](#)

- Cistanchis herba, *see* [Rou Cong Rong](#)  
 Citri aurantii fructus, *see* [Zhi Ke](#)  
 Citri reticulatae pericarpium, *see* [Chen Pi](#)  
 Citri reticulatae viride pericarpium, *see* [Qing Pi](#)  
 Citri sarcodactylis fructus, *see* [Fo Shou](#)  
 Clematidis armandii caulis, *see* [Chuan Mu Tong](#)  
 Clematidis radix, *see* [Wei Ling Xian](#)  
 Codonopsis pilosulae radix, *see* [Dang Shen](#)  
 Coicis semen, *see* [Yi Yi Ren](#)  
 Colla carapax et plastrum chrysemys, *see* [Gui Ban Jiao](#)  
 Cong Bai, [159](#)  
 Coptidis rhizoma, *see* [Huang Lian](#)  
 Corni officinalis fructus, *see* [Shan Yu Rou](#)  
 Corydalis rhizoma, *see* [Yan Hu Suo](#)  
 Crataegi fructus, *see* [Shan Zha](#)  
 Curculiginis orchioideis rhizoma, *see* [Xian Mao](#)  
 Curcumae longae rhizoma, *see* [Jiang Huang](#)  
 Curcumae tuber, *see* [Yu Jin](#)  
 Curcumae zedoariae rhizoma, *see* [E Zhu](#)  
 Cuscutae semen, *see* [Tu Si Zi](#)  
 Cyathulae radix, *see* [Chuan Niu Xi](#)  
 Cynanchi stauntonii rhizoma et radix, *see* [Bai Qian](#)  
 Cynomorii songarici herba, *see* [Suo Yang](#)  
 Cyperi rotundi rhizoma, *see* [Xiang Fu](#)
- Da Qing Ye, [163](#)  
 Da Zao, [167](#)  
 Dan Dou Chi, [171](#)  
 Dan Shen, [175](#)  
 Dang Gui, [179](#)  
 Dang Gui Wei, [183](#)  
 Dang Shen, [187](#)  
 Di Fu Zi, [191](#)  
 Di Gu Pi, [195](#)  
 Di Long, [199](#)  
 Dictamni cortex, *see* [Bai Xian Pi](#)  
 Dictamni dasycarpi cortex radices, *see* [Bai Xian Pi](#)  
 Dioscoreae oppositae rhizoma, *see* [Shan Yao](#)  
 Dipsaci radix, *see* [Xu Duan](#)  
 Dong Gua Zi, [203](#)  
 Drynariae rhizoma, *see* [Gu Sui Bu](#)  
 Du Huo, [207](#)  
 Du Zhong, [211](#)
- E Zhu, [215](#)  
 Eleutherococci radix, *see* [Ci Wu Jia](#)  
 Endothelium corneum gigeriae galli, *see* [Ji Nei Jin](#)  
 Ephedrae herba, *see* [Ma Huang](#)  
 Ephedrae radix, *see* [Ma Huang Gen](#)  
 Epimedii herba, *see* [Yin Yang Huo](#)  
 Equiseti hiemalis herba, *see* [Mu Zei](#)  
 Eriobotryae japonicae folium, *see* [Pi Pa Ye](#)
- Eucommiae ulmoidis cortex, *see* [Du Zhong](#)  
 Euphorbiae longanae arillus, *see* [Long Yan Rou](#)  
 Evodiae rutecarpae fructus, *see* [Wu Zhu Yu](#)
- Fang Feng, [219](#)  
 Farfarae flos, *see* [Kuan Dong Hua](#)  
 Fo Shou, [223](#)  
 Foeniculi vulgaris fructus, *see* [Xiao Hui Xiang](#)  
 Forsythiae fructus, *see* [Lian Qiao](#)  
 Forsythiae suspensae fructus, *see* [Lian Qiao](#)  
 Fritillariae thunbergii bulbis, *see* [Zhe Bei Mu](#)  
 Fu Ling, [227](#)  
 Fu Pen Zi, [231](#)  
 Fu Shen, [235](#)  
 Fu Xiao Mai, [239](#)  
 Fu Zi, [243](#)
- Gan Cao, [247](#)  
 Gan Jiang, [251](#)  
 Ganoderma, *see* [Ling Zhi](#)  
 Gardeniae fructus, *see* [Zhi Zi](#)  
 Ge Gen, [255](#)  
 Gentianae longdancao radix, *see* [Long Dan \(Cao\)](#)  
 Gentianae macrophyllae radix, *see* [Qin Jiao](#)  
 Gentianae scabrae radix, *see* [Long Dan \(Cao\)](#)  
 Ginkgonis bilobae semen, *see* [Bai Guo](#)  
 Ginseng radix et rhizoma, *see* [Ren Shen](#)  
 Glehniae radix, *see* [Sha Shen \(Bei\)](#)  
 Glycyrrhizae radix, *see* [Gan Cao](#)  
 Glycyrrhizae radix et rhizoma praeparata cum melle, *see* [Zhi Gan Cao](#)  
 Gou Qi Zi, [259](#)  
 Gou Teng, [263](#)  
 Gu Sui Bu, [267](#)  
 Gua Lou, [271](#)  
 Gua Lou Ren, [275](#)  
 Guang Huo Xiang, [279](#)  
 Gui Ban Jiao, [283](#)  
 Gui Zhi, [287](#)  
 Gynostemma herba, *see* [Jiao Gu Lan](#)  
 Gypsum fibrosum, *see* [Shi Gao](#)
- He Huan Pi, [291](#)  
 He Shou Wu, [295](#)  
 He Ye, [299](#)  
 Hei Zhi Ma, [303](#)  
 Hong Hua, [307](#)  
 Hong Jing Tian, [311](#)  
 Hordei vulgaris fructus germinatus, *see* [Mai Ya](#)  
 Hou Po, [315](#)  
 Houttuyniae herba, *see* [Yu Xing Cao](#)  
 Huai Hua, [319](#)  
 Huang Bo, [323](#)  
 Huang Jing, [327](#)  
 Huang Lian, [331](#)  
 Huang Qi, [335](#)

- Huang Qin, [339](#)  
Huo Ma Ren, [343](#)
- Imperatae cylindrica rhizoma, *see* [Bai Mao Gen](#)
- Inulae flos, *see* [Xuan Fu Hua](#)  
Isatidis folium, *see* [Da Qing Ye](#)  
Isatidis radix, *see* [Ban Lan Gen](#)
- Ji Li, [347](#)  
Ji Nei Jin, [351](#)  
Ji Xue Teng, [355](#)  
Jiang Huang, [359](#)  
Jiao Gu Lan, [363](#)  
Jie Geng, [367](#)  
Jin Qian Cao, [371](#)  
Jin Yin Hua, [375](#)  
Jing Jie, [379](#)  
Ju Hua, [383](#)  
Jue Ming Zi, [387](#)
- Kochiae scopariae fructus, *see* [Di Fu Zi](#)  
Ku Shen, [391](#)  
Kuan Dong Hua, [395](#)
- Lai Fu Zi, [399](#)  
Leonuri heterophylli herba, *see* [Yi Mu Cao](#)  
Lepidii semen, *see* [Ting Li Zi](#)  
Lian Qiao, [403](#)  
Lian Zi, [407](#)  
Ligustici chuanxiong rhizoma, *see* [Chuan Xiong](#)  
Ligustici wallichii radix, *see* [Chuan Xiong](#)  
Ligustri lucidi fructus, *see* [Nü Zhen Zi](#)  
Lilii bulbosus, *see* [Bai He](#)  
Linderae radix, *see* [Wu Yao](#)  
Ling Zhi, [411](#)  
Lini semen, *see* [Huo Ma Ren](#)  
Liquidambaris fructus, *see* [Lu Lu Tong](#)  
Long Dan (Cao), [415](#)  
Long Yan Rou, [419](#)  
Lonicerae japonicae flos, *see* [Jin Yin Hua](#)  
Lu Gen, [423](#)  
Lu Jiao Shuang, [427](#)  
Lu Lu Tong, [431](#)  
Lumbricus, *see* [Di Long](#)  
Lycii chinensis fructus, *see* [Gou Qi Zi](#)  
Lycii chinensis radices cortex, *see* [Di Gu Pi](#)  
Lycopi lucidi herba, *see* [Ze Lan](#)  
Lysimachiae herba, *see* [Jin Qian Cao](#)
- Ma Bian Cao, [435](#)  
Ma Huang, [439](#)  
Ma Huang Gen, [443](#)  
Magnoliae flos, *see* [Xin Yi](#)  
Magnoliae officinalis cortex, *see* [Hou Po](#)  
Mai Men Dong, [447](#)  
Mai Ya, [451](#)
- Man Jing Zi, [455](#)  
Massa fermentata medicinalis, *see* [Shen Qu](#)  
Meliae toosendan fructus, *see* [Chuan Lian Zi](#)  
Menthae haplocalysis herba, *see* [Bo He](#)  
Mi Huan Jun, [459](#)  
Mo Yao, [463](#)  
Mori albae ramulus, *see* [Sang Zhi](#)  
Mori albi folium, *see* [Sang Ye](#)  
Mori cortex, *see* [Sang Bai Pi](#)  
Mori fructus, *see* [Sang Shen](#)  
Morindae officinalis radix, *see* [Ba Ji Tian](#)  
Moutan cortex radices, *see* [Mu Dan Pi](#)  
Mu Dan Pi, [467](#)  
Mu Gua, [471](#)  
Mu Zei, [475](#)  
Myrrha resina, *see* [Mo Yao](#)
- Nü Zhen Zi, [483](#)  
Nelumbinis nuciferae folium, *see* [He Ye](#)  
Nelumbinis semen, *see* [Lian Zi](#)  
Niu Bang Zi, [479](#)  
Notoginseng radix, *see* [San Qi](#)  
Notopterygii rhizoma et radix, *see* [Qiang Huo](#)
- Oldenlandiae diffusae herba, *see* [Bai Hua She She Cao](#)
- Olibanum, *see* [Ru Xiang](#)  
Ophiopogonis radix, *see* [Mai Men Dong](#)
- Paeoniae lactiflorae albus radix, *see* [Bai Shao Yao](#)  
Paeoniae radix rubra, *see* [Chi Shao \(Yao\)](#)  
Panacis quinquefolii radix, *see* [Xi Yang Shen](#)  
Patriniae herba, *see* [Bai Jiang Cao](#)  
Perillae fructus, *see* [Zi Su Zi](#)  
Perillae frutescentis folium, *see* [Zi Su Ye](#)  
Persicae semen, *see* [Tao Ren](#)  
Peucedani radix, *see* [Qian Hu](#)  
Phellodendri cortex chinensis, *see* [Huang Bo](#)  
Phragmitis communis rhizoma, *see* [Lu Gen](#)  
Pi Pa Ye, [487](#)  
Pinelliae rhizoma praeparatum cum zingibere, *see* [Ban Xia \(Jiang\)](#)  
Plantaginis semen, *see* [Che Qian Zi](#)  
Platycladi semen, *see* [Bai Zi Ren](#)  
Platycodi grandiflori radix, *see* [Jie Geng](#)  
Pogostemonis herba, *see* [Guang Huo Xiang](#)  
Polygalae radix, *see* [Yuan Zhi](#)  
Polygonati odorati rhizoma, *see* [Yu Zhu](#)  
Polygonati rhizoma, *see* [Huang Jing](#)  
Polygoni multiflori caulis, *see* [Ye Jiao Teng](#)  
Polygoni multiflori radix, *see* [He Shou Wu](#)  
Polypori umbellati sclerotium, *see* [Zhu Ling](#)  
Poriae cocos sclerotium, *see* [Fu Ling](#)  
Poriae cocos sclerotium paradicis, *see* [Fu Shen](#)  
Prunellae vulgaris spica, *see* [Xia Ku Cao](#)  
Pruni mume fructus, *see* [Wu Mei](#)

- Pseudoginseng radix, *see* [San Qi](#)  
Pseudostellariae heterophyllae radix, *see* [Tai Zi Shen](#)  
Psoraleae corylifoliae fructus, *see* [Bu Gu Zhi](#)  
Pu Gong Ying, [491](#)  
Pu Huang, [495](#)  
Puerariae radix, *see* [Ge Gen](#)  
Pulsatillae radix, *see* [Bai Tou Weng](#)  
Pyrososiae folium, *see* [Shi Wei](#)
- Qian Hu, [499](#)  
Qiang Huo, [503](#)  
Qin Jiao, [507](#)  
Qing Pi, [511](#)  
Quisqualis fructus, *see* [Shi Jun Zi](#)
- Raphani sativi semen, *see* [Lai Fu Zi](#)  
Rehmanniae praeparata radix, *see* [Shu Di \(Huang\)](#)  
Rehmanniae radix, *see* [\(Sheng\) Di Huang](#)  
Rehmanniae radix praep., *see* [Shu Di \(Huang\)](#)  
Rehmanniae viridae radix, *see* [\(Sheng\) Di Huang](#)  
Ren Shen, [515](#)  
Rhodiola crenulata radix, *see* [Hong Jing Tian](#)  
Rou Cong Rong, [519](#)  
Ru Xiang, [523](#)  
Rubi chingii fructus, *see* [Fu Pen Zi](#)
- Salviae miltiorrhizae radix, *see* [Dan Shen](#)  
San Leng, [527](#)  
San Qi, [531](#)  
Sang Bai Pi, [535](#)  
Sang Ji Shend, [539](#)  
Sang Shen, [543](#)  
Sang Ye, [547](#)  
Sang Zhi, [551](#)  
Saposhnikoviae radix, *see* [Fang Feng](#)  
Schisandrae chinensis fructus, *see* [Wu Wei Zi](#)  
Schizonepetae tenuifoliae herba, *see* [Jing Jie](#)  
Scrophulariae ningpoensis radix, *see* [Xuan Shen](#)  
Scutellariae baicalensis radix, *see* [Huang Qin](#)  
Scutellariae barbatae herba, *see* [Ban Zhi Lian](#)  
Sesami indici semen, *see* [Hei Zhi Ma](#)  
Sesami semen nigrum, *see* [Hei Zhi Ma](#)  
Sha Ren, [555](#)  
Sha Shen (Bei), [559](#)  
Shan Yao, [563](#)  
Shan Yu Rou, [567](#)  
Shan Zha, [571](#)  
She Gan, [575](#)  
Shen Qu, [579](#)  
Sheng Jiang, [583](#)  
Sheng Ma, [587](#)  
Shi Gao, [591](#)  
Shi Jun Zi, [595](#)
- Shi Wei, [599](#)  
Shu Di (Huang), [603](#)  
Siegesbeckiae herba, *see* [Xi Xian Cao](#)  
Smilacis glabrae rhizoma, *see* [Tu Fu Ling](#)  
Sojae semen praeparatum, *see* [Dan Dou Chi](#)  
Sophorae flavescentis radix, *see* [Ku Shen](#)  
Sophorae japonicae flos, *see* [Huai Hua](#)  
Sparganii rhizoma, *see* [San Leng](#)  
Spatholobi caulis, *see* [Ji Xue Teng](#)  
Suan Zao Ren, [607](#)  
Suo Yang, [611](#)
- Tai Zi Shen, [615](#)  
Tao Ren, [619](#)  
Taraxaci mongolici herba cum radice, *see* [Pu Gong Ying](#)  
Taxilli herba, *see* [Sang Ji Shend](#)  
Tian Hua Fen, [623](#)  
Tian Men Dong, [627](#)  
Tian Nan Xing, [631](#)  
Ting Li Zi, [635](#)  
Tribuli terrestris fructus, *see* [Ji Li](#)  
Trichosanthis fructus, *see* [Gua Lou](#)  
Trichosanthis radix, *see* [Tian Hua Fen](#)  
Trichosanthis semen, *see* [Gua Lou Ren](#)  
Tritici aestivi semen levis, *see* [Fu Xiao Mai](#)  
Tu Fu Ling, [639](#)  
Tu Si Zi, [643](#)  
Tussilaginis farfarae flos, *see* [Kuan Dong Hua](#)  
Typhae pollen, *see* [Pu Huang](#)
- Uncariae ramulus cum uncis, *see* [Gou Teng](#)
- Vaccariae semen, *see* [Wang Bu Liu Xing](#)  
Verbenae officinalis herba, *see* [Ma Bian Cao](#)  
Violae herba, *see* [Zi Hua Di Ding](#)  
Viticis fructus, *see* [Man Jing Zi](#)  
Vladimirae radix, *see* [Chuang Mu Xiang](#)
- Wang Bu Liu Xing, [647](#)  
Wei Ling Xian, [651](#)  
Wu Jia Pi, [655](#)  
Wu Mei, [659](#)  
Wu Wei Zi, [663](#)  
Wu Yao, [667](#)  
Wu Zhu Yu, [671](#)
- Xanthii fructus, *see* [Cang Er Zi](#)  
Xi Xian Cao, [675](#)  
Xi Yang Shen, [679](#)  
Xia Ku Cao, [683](#)  
Xian Mao, [687](#)  
Xiang Fu, [691](#)  
Xiao Hui Xiang, [695](#)  
Xie Bai, [699](#)  
Xin Yi, [703](#)  
Xu Duan, [707](#)  
Xuan Fu Hua, [711](#)

Xuan Shen, [715](#)

Yan Hu Suo, [719](#)

Ye Jiao Teng, [723](#)

Yi Mu Cao, [727](#)

Yi Yi Ren, [731](#)

Yi Zhi Ren, [735](#)

Yin Chen Hao, [739](#)

Yin Yang Huo, [743](#)

Yu Jin, [747](#)

Yu Xing Cao, [751](#)

Yu Zhu, [755](#)

Yuan Zhi, [759](#)

Ze Lan, [763](#)

Ze Xie, [767](#)

Zhe Bei Mu, [771](#)

Zhi Gan Cao, [775](#)

Zhi Ke, [779](#)

Zhi Mu, [783](#)

Zhi Shi, [787](#)

Zhi Zi, [791](#)

Zhu Ling, [795](#)

Zhu Ru, [799](#)

Zi Hua Di Ding, [803](#)

Zi Su Ye, [807](#)

Zi Su Zi, [811](#)

Zi Wan, [815](#)

Zingiberis rhizoma, *see* [Gan Jiang](#)

Zingiberis rhizoma recens, *see* [Sheng Jiang](#)

Zizyphi jujubae fructus, *see* [Da Zao](#)

Zizyphi spinosae semen, *see* [Suan Zao Ren](#)