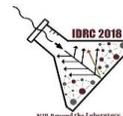




**19<sup>th</sup> International Diffuse Reflectance Conference**  
**July 29 – August 2, 2018**  
**Chambersburg, PA**



**IDRC 2018 Poster Abstracts**

**E-01 Sae Tanaka**

Dušan Kojić, Roumiana Tsenkova and Masato Yasui  
Keio University, Japan  
Experienced

Glucose is the most widely used monosaccharide in living organisms. The stereochemical isomers that have different position of OH group on the C1 carbon ( $\alpha$ -D-glucose: axial,  $\beta$ -D-glucose: equatorial), are termed anomers. In aqueous solution,  $\beta$ -D-glucose is major (~62%) and  $\alpha$ -D-glucose is minor (~38%) (Figure 1), and the stability is thought to depend on the hydrogen bonding with the surrounding water molecules. In this study, our aim is to elucidate the influence of the hydrogen bond between saccharides and water on the covalent OH bond of water using NIRS. We obtained spectra of each anomers solution (200 mM) at 5, 30, 60, 120, and 180 min after dissolving to observe the spectral change during equilibrating. At the same time, the optical rotations of these solutions were measured by polarimeter in order to determine the ratio of anomers. The significant spectral difference in the C-H region was observed, and we found it corresponding well to the optical rotation. It suggests that near-infrared spectra can predict ratio of anomers in solution quantitatively.

**E-02 Konni Biegert**

Roy McCormick  
Kompetenzzentrum Obstbau-Bodensee, Germany  
Experienced

After harvest, many types of fresh fruit and vegetables are sorted and graded into quality classes using modern state of the art computer-controlled machines equipped with a range of measurement technologies that also include vis/NIR spectroscopy. However, in contrast apple growers have been slow to apply non-destructive vis/NIR spectroscopy in the pre-harvest period, to determine possible changes in quality parameters while fruit grow and develop on the tree in the orchard. We present some initial results from a 3-year research project using a handheld spectrometer (F750, Felix Instruments, Camas, USA) to repeatedly scan the same apples during fruit growth on the tree and obtain time-series data to track the changes in plant pigments (e.g. chlorophyll and anthocyanins) in the visible spectrum and to follow the increases in the fruit dry matter content and carbohydrates (total solid solids) using information from the near infrared spectrum (729-975 nm). Results from field experiments involving different temperature treatments applied to whole trees during early fruit development (cell division period) and three different levels of crop-loading (number of fruit per tree), will be presented. The influence of spring temperatures and crop-loading can be clearly observed in the spectral data. Possible approaches to use these field data in 'BigData' prediction modelling and improved fruit quality classification will be discussed.

**E-03 Roy McCormick**

Konni Biegert  
Kompetenzzentrum Obstbau-Bodensee, Germany  
Experienced

When light passes through fruit tissue, the spectrum observed is a result of both absorption and scattering processes. It is possible to separate these effects with laboratory methods. The reducing scattering coefficient can potentially provide information about tissue structure. As apples ripen on the tree, the tissues change dynamically on a daily basis, as cells grow and the intercellular volume increases. In addition, the spaces between the cells, and the cell membranes and cell walls can either be filled with fluid or air. A vis/NIR spectrometer (F750, Felix Instruments, Camas, USA) was fitted with a movable external light source, in an attempt to build a very basic hand-held mobile spatial resolved spectrometer. Repeated scans of ripening apples attached to the tree were conducted with the sensor placed at the same location on the fruit surface and the external light source able to be moved between two external positions. Scans were taken during darkness (morning and/or night) and data from the calibration scan (shutter open, internal lamp off) used for analysis. The area under the wavelength versus spectral intensity curves for scans from the two external light positions were compared. The following trends were observed: As fruit ripen, the amount of light recorded from the external light source decreases dramatically, most likely because of increased internal scattering. Variation between individual fruit is very large. Differences between morning and evening scans on the same day could be observed. The influence of rainfall on light movement through fruit tissues needs further investigation.

**E-04 Dongsheng Bu**

Jim Pratt and Gary McGeorge  
BMS, US  
Experienced

We have developed and implemented a Real Time Release testing method for Assay determination (drug content within a tablet) of a pharmaceutical product. Quantitative multivariate models incorporating near infrared (NIR) spectroscopy with partial least squares (PLS) modeling were applied and model validation was carried out as an essential part of model development and implementation. This presentation will discuss a few selected elements we think are important in general for multivariate quantitative method deployment. The presentation will focus on the method validation procedures/acceptance criteria and after deployment the continuous monitoring to ensure that the models are still fit for purpose and don't drift over time. Current analytical method validation guidelines, e.g. ICH Q2(R1), are usually applied to univariate models, and it is necessary to modify testing procedures, such as linearity and specificity, in order to be applicable to multivariate model validation. In addition to general rules and a statistical basis, we have considered model performance design when setting acceptance criteria. Then we will discuss the concept of continuous model verification over time throughout the lifecycle of the product that is somewhat specific to spectroscopic multivariate methods since their calibration set is not "re-built" at the time of use as in traditional HPLC Assay methods.

#### **E-05 Perrine Hebert**

Jean Guilment (Arkema), Safia Montagnier (Arkema), Sylvie roussel (Ondalys), Jordane Lallemand (Ondalys)  
ARKEMA, France  
Experienced

ARKEMA produces various polyamides in its Serquigny (27) plant. For quality reasons, it can be interesting to differentiate the polymer bases' type between polyamide 11 (plasticized or not plasticized) and polyamide 12. This can be easily done using a conventional FT-NIR instrument with an integrating sphere but the cost is high compared to the industrial interest. We decided to test the performances of a mini NIR spectrometer (Spectral Engine NIRONE Sensor, IDIL Sensor) whose cost is more compatible with the expected gains. Thanks to a chemometric discrimination method like PLS DA[1] (Partial Least Square Discriminant Analysis), we can separate the various classes of polymeric bases (PA 11 not plasticized, PA 12 not plasticized, PA 11 plasticized level 1, PA 11 plasticized level 2 and others). We also tested the quantitative ability of the system in order to predict the plasticizer content.

#### **E-06 Nicola Caporaso**

Martin B. Whitworth, Ian D. Fisk  
University of Nottingham, UK  
Post-Doc

Hyperspectral imaging (HSI) adds spatial information to the spectral data. When using HSI in the NIR range, it is capable of analyzing the chemical distribution of materials. Its application in food science allows investigating the composition and natural variability of food commodities in a rapid and non-destructive way, without the need of sample preparation or extraction. The aim of the current work was to use HSI in the reflectance mode under the "push-broom" approach using the NIR spectral range 1000–2500 nm to analyze the composition of whole cocoa beans. The fermentation index (FI), total polyphenols (TP) and antioxidant activity (AA) were predicted on individual dry fermented beans scanned on a single seed basis. From each of the seventeen batches, 10 cocoa beans were randomly selected. PLS regression models were built on 170 samples. The developed HSI predictive models were able to quantify three quality-related parameters with sufficient performance for screening purposes, with external validation  $R^2$  of 0.50 (RMSEP = 0.27, RPD = 1.40), 0.70 (RMSEP = 34.1 mg ferulic acid  $g^{-1}$ , RPD = 1.77) and 0.74 (60.0 mmol Trolox  $kg^{-1}$ , RPD = 1.91) for FI, TP and AA, respectively. Calibrations were subsequently applied at a single bean and pixel level, so that the distribution was visualized within and between single seeds (chemical images). HSI is thus suggested as a promising approach to estimate cocoa bean composition rapidly and non-destructively, thus offering a valid tool for food inspection and quality control. This research is the first one applying HSI on cocoa, and it gives a potential benefit to the industry and to breeders/researchers to analyse the quality of this commodity.

#### **E-07 Jordi Cruz**

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Salesian University, Spain  
Post-Doc

Diseases in plants cause major production and economic losses in the agricultural industry worldwide. Near Infrared spectroscopy (NIR) is a well-established technique for food characterization. For this reason, a new strategy for detecting pathologies of bean seeds and NIR spectroscopy is proposed in this work. A representative collection of bean seeds with their different geographical origin has been selected and NIR & Visible spectra have been registered. The seeds have been planted later, and the appearance of pathologies in the plants has been observed. A relationship between spectra of bean seeds and the geographical origin has been investigated by using Principal Component Analysis (PCA). Effectively there exist relationships between the seed's geographical precedence and the NIR spectra as the scores plots of the PCA show. A relationship between pathologies of bean seeds has been investigated by using Partial Least Squares Regression (PLSR). The prediction of future pathologies has been tested by using Partial Least Squares Regression (PLSR), concretely for two different white mold Sclerotinia fungus types with good results.

#### **S-01 Natasha L. Velez**

Shikhar Mohan; Carl A. Anderson; James K. Drennen, III

Duquesne University, US  
Student

Blending of pharmaceutical powders is a fundamental unit operation in the manufacturing of solid dosage forms. The main objective of blending is to reduce inhomogeneities in composition to acceptable levels. Different approaches exist to monitor the progression of the blending process and confirm that the blend has reached an adequate level of homogeneity (i.e. blending end-point). Near-infrared (NIR) spectroscopy is a fast, non-destructive and non-invasive analytical technique that has been widely recognized as a powerful tool for the evaluation of blend quality. Numerous NIR qualitative and quantitative methods have been developed and implemented for the on-line monitoring of powder blending. While quantitative models provide substantial information about the blend composition, they often require wet chemistry analysis of a large number of blend samples, which is often impractical. Qualitative models, on the other hand, are typically simpler and more feasible to use for blend monitoring. The statistical determination of blending end-point by Mean Square Successive Difference Test (MSSDT) is a recently developed NIR qualitative method. This study focuses on demonstrating the capability of NIR-MSSDT approach to detect accurately blending end-point when compared to multiple widely used NIR qualitative and quantitative methods.

#### **S-02 Natasha L. Velez**

Shikhar Mohan; Carl A. Anderson; James K. Drennen, III  
Duquesne University, US  
Student

The success of continuous pharmaceutical manufacturing depends on the effective implementation of process analytical technology (PAT) for real-time quality monitoring of the process stream. Near Infrared (NIR) spectroscopy is the most widely applied PAT method to monitor continuous processes involving powdered materials. The physical variation of continuous flowing materials such as powder flow rate, powder stream thickness and density causes differences in NIR spectral response, which thus can affect the performance of the analytical models. Different flow rates of the powder stream are often necessary to match the production requirements of a continuous tableting process. This study focuses on the development of a NIR method for monitoring the relative density of a continuous flowing powder stream at different flow rates. Diffuse reflectance spectra were collected from powder streams flowing from a loss-in-weight feeder at multiple flow rate conditions. Simultaneously, live images of the powder streams were collected using a CANTY® camera-light source imaging system. Image analysis was performed to determine powder streams solid to air ratio. A diffuse reflectance NIR method was developed and evaluated for its ability to monitor continuous powder stream relative density.

#### **S-03 Adam Rish**

Shikhar Mohan; Carl A. Anderson; James K. Drennen, III  
Duquesne University, US  
Student

Blending of pharmaceutical powders is a fundamental unit operation in the manufacturing of solid dosage forms. The main objective of blending is to reduce inhomogeneities in composition to acceptable levels. Different approaches exist to monitor the progression of the blending process and confirm that the blend has reached an adequate level of homogeneity (i.e. blending end-point). Near-infrared (NIR) spectroscopy is a fast, non-destructive and non-invasive analytical technique that has been widely recognized as a powerful tool for the evaluation of blend quality. Numerous NIR qualitative and quantitative methods have been developed and implemented for the on-line monitoring of powder blending. While quantitative models provide substantial information about the blend composition, they often require wet chemistry analysis of a large number of blend samples, which is often impractical. Qualitative models, on the other hand, are typically simpler and more feasible to use for blend monitoring. The statistical determination of blending end-point by Mean Square Successive Difference Test (MSSDT) is a recently developed NIR qualitative method. This study focuses on demonstrating the capability of NIR-MSSDT approach to detect accurately blending end-point when compared to multiple widely used NIR qualitative and quantitative methods.

#### **S-04 Shikhar Mohan**

Noritaka Odani, Hanzhou Feng, James K. Drennen III, Carl A. Anderson  
Duquesne University, US  
Student

Tablet coating is an important unit operation in the manufacturing of solid oral dosage forms. Coating thickness and uniformity are often considered critical quality attributes (CQA) for the coating process. For enteric and sustained-release coating, polymer thickness determines the location of drug release in the gastro-intestinal tract and drug release kinetics respectively. Also for drugs that are sensitive to light, humidity, and oxygen, coating thickness dictates the chemical stability of the final product. Near-Infrared (NIR) spectroscopy has been demonstrated as a Process Analytical Technology (PAT) tool for monitoring coating thickness in a pan coating unit operation. A major disadvantage of NIR is that it is not a primary technique and requires a reference method. Typical reference methods for coating quality purposes include weight gain based values as a surrogate for coating thickness. This study investigated Terahertz pulsed imaging (TPI) as a reference method to improve the accuracy of NIR coating thickness estimates in a non-destructive manner. The relative error for the NIR model with TPI based reference values was significantly lower than with the more traditional reference method based on tablet weight.

**S-05 Pholisa Dumalisile**

Marena Manley, Louw Hoffman, Paul Williams  
University of Stellenbosch, South Africa  
Student

Meat and meat products are often targets for species substitution and adulteration (fraud) due to their high market value. Game meat offers a healthy alternative to South African red meat eaters as it is known to have low fat and high protein levels. In addition, South African game meat can be considered as an organic product since the animals are wild and free roaming. Portable near infrared (NIR) spectroscopy was used to explore its potential to differentiate meat samples from six different game species. Game meat species, included middle sized antelopes (Impala (22), Blesbok (17) and Springbok (10)) and big sized species (Eland (15), Black wildebeest (9) and Zebra (22)) meat, that were harvested from different South African farms. *Longissimus thoracis et lumborum* (LTL) muscle cuts were scanned with a portable NIR spectrophotometer (900-1700 nm). Spectra were treated with smoothing, standard normal variate (SNV) + detrend pre-processing; explored by principal component analysis (PCA) and further classified by partial least squares discriminant analysis (PLS-DA).

**S-06 Carlos Ortega-Zuniga**

Ricardo Navarro, Rodolfo Romanach  
University of Puerto Rico at Mayaguez, US  
Student

*Purpose*: Understanding of the sources of error in calibration models developed with a low heterogeneity system analyzed by NIR. Representative layer theory (RLT) states that samples can be thought of as a matrix composed of multiple layers, each representative of the sample as a whole. *Method*: Polyethylene mixed with polypropylene films were used to develop calibration models that predicted either the percent composition or number of polyethylene films on each sample. Polymers used constitute a system with reduced heterogeneity which can be confirmed by the correlation coefficients of the spectra (0.9182) and thickness similarities. The number of polyethylene films was varied from 1-10 to evaluate the linearity of NIR predictions. Spectra were acquired using two FT-NIR spectrometers from two laboratories. Calibration models were prepared using PLS regressions. The validations performed were done with the same films used on a slave instrument and the procedures were exactly the same as validations done with the master instrument. *Results*: Calibration models on 9500-6500 $\text{cm}^{-1}$  spectral region using first derivative pretreatment with 3 PLS factors. Moreover, using the percent composition of polypropylene as a y-variable yielded better results than using the number of films as a y-variable. SNV-1<sup>st</sup> derivative yielded better results when is compared the validations with a slave instrument. *Conclusion*: Models analyzed in this study showed lack of systematic error and were more representative of the errors obtained due to the physics of the NIR methodology.

**S-07 Adriluz Sanchez-Paternina**

Nobel O. Sierra Vega, Vanesa Cardenas, Rafael Méndez, Kim H. Esbensen, Rodolfo J. Romañach.  
University of Puerto Rico at Mayaguez, US  
Student

Keywords: Heterogeneity, Pharmaceutical high purity blends, Theory of sampling (TOS), Near infrared spectroscopy (NIRS), Multivariate analysis, Partial least square regression (PLSr), Variographic analysis. *Purpose*: Development of variographic analysis for the elucidation of sampling errors in pharmaceutical samples using Near Infrared Spectroscopy (NIRS). Variographic analysis is a tool used to determine the total process variance and to evaluate the behavior of a continuous variable in a pharmaceutical 1-D sampling. *Method*: A new sampling procedure was designed based on Theory of Sampling principles and Pharmaceutical powder blends of low heterogeneity were analyzed. Three PLS models were developed using different concentration range (90-100; 85-100 and 65-100% w/w API). The calibration models developed include SNV as spectral pretreatment. Four validations set with different heterogeneity levels (90,95,97,100 % w/w API) were evaluated in the three models. *Results*: The results shown that RMSEP values decrease as a function of sample heterogeneity (direct proportionality). 2. The lowest standard deviation values for the validation sample of pure analyte (0.036 - 0.057 % w/w t). Additionally, low bias values were obtained (0.005- 0.193 % w/w). *Conclusion*: Variographic analysis showed that variograms are a function of the heterogeneity of validation blends. The highest variability  $V(j)$  is observed in the validation blend of 90% w/w Met in all models developed. The lowest variability  $V(j)$  was obtained in the validation of the pure analyte.

**S-08 Barbara Alvarado-Hernandez**

Rodolfo Romanach  
University of Puerto Rico at Mayaguez, US  
Student

Keywords: NIR, Heterogeneity, Theory of Sampling, Method Transfer, Chemometrics Purpose: Development of NIR calibration models for the determination of blending adequacy for two excipients in a continuous manufacturing process while considering the theory of sampling guidelines. This study will help provide faster, more efficient and representative sampling and transfer methodologies. Methods: Two NIR calibration models were developed to monitor the concentration for an excipient blend. Initial model application and transfer will be done with data collected from development plant at Rutgers University. Also, the determination of sampling adequacy will be done by evaluating the sampling method in terms of accuracy and precision. Results: Differences between equipment lead to a significant increase in bias and standard deviation. A global evaluation of the bias when comparing data obtained in UPRM and Rutgers show this difference, -1.62 (%w/w) and 8.70 (%w/w) respectively. Also, poor flow behavior from the excipients lead to a high number of outliers. Spectra with different baselines can be indicative of possible flow interruptions as the material passes through the NIR equipment interface. Conclusion: The differences found between equipment in this study have a significant impact on model predictability. The model predictability will also be affected by the powder flow behavior and other sources of variation not reproducible at a laboratory scale.

#### **S-09 Pedro A. Martinez Cartagena**

Rodolfo Romañach, Rafel Mendez  
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Student

Keywords: NIR, Mixing Process, NIR Interface Purpose: A near-infrared (NIR) spectroscopic method was developed for the real time analysis of flowing pharmaceutical powder mixtures in a continuous manufacturing process using an innovative NIR interface. The design of the NIR interface used in this study is based on theory of sampling (TOS) strategies that have been successful in reducing sampling errors in mining and metallurgical applications for more than six decades. Methods: Five calibration blends were prepared with laboratory scale equipment with a concentration range between 10.5-19.5% of active pharmaceutical ingredient (API) target concentration. The NIR calibration model was validated using three independent validation blends which were also prepared with laboratory scale equipment. Real-time NIR spectra were obtained with an interface in which the pharmaceutical powders flowed at an angle of 60 degrees with respect to the normal and with a controlled flowrate. Physical properties of the pharmaceutical powder mixtures such as: compressibility, cohesion and density were analyzed before and after the continuous process to determine if the interface was altering such powder properties. Results: A total of 800 NIR spectra were obtained throughout the continuous manufacturing runs. The physical properties of the pharmaceutical powder mixtures showed minimum variation when comparing them before and after the continuous process. The best calibration model yielded a low Bias and RMSEP demonstrating excellent accuracy. Conclusion: The NIR interface used in this study provided spectra with minimum variation in their baseline. The developed calibration model was able to effectively predict the API concentration within the established flowrate.

#### **S-10 Maritza Reyna-Liriano**

Vanessa Cardenas, Rodolfo Romanach,  
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Student

Keywords: NIR, PLS factor, Mixing process, Chemometrics Purpose: Develop an approach for the selection of PLS factors in methods to evaluate degree of mixing using NIR spectroscopy. The evaluation of a mixing process requires both accuracy and precision in PLS predictions. A tradeoff between accuracy and precision has been discussed in the literature (Kalivas and Palmer 2014). Methods: Four calibration models were developed. Bias and variance were plotted versus number of PLS factors for the calibration models. Variance was determined through repeatability studies. Two calibration models were developed with calibration samples that showed significant correlation among the components of the blends. The other calibration models were obtained with samples prepared following a design to reduce the correlation between the components. Results: The initial predictions for the calibration models showed lowest bias and standard deviation with the design to reduce correlation between components. Principal component showed a bias of 0.188 and a standard deviation of 1.054 for 3 PLS factors. Figure 1 provides an example of the results obtained. Conclusion: The bias-variance plot is useful for understanding the sources of error in NIR measurements. This approach could be valuable in the validation of NIR methods to evaluate mixing in industrial processes.

#### **S-11 Judi Psarrakis**

PJ Williams, GO Sigge and C Lamprecht  
Stellenbosch University, South Africa  
Student

Water is one of the most abundant components in biological systems and has been the focus of many studies over the years. Water, as a medium, changes its absorbance pattern when adapting to physical or chemical changes within its respective environment, and near-infrared (NIR) spectroscopy can be used to show these changes in the vibrations of water molecules. Aquaphotomics provides the possibility for the extraction of information hidden within the NIR spectrum of water, which is not possible with other methods. This study focuses on the discrimination of bottled water sourced from different geographical locations with the use of near-infrared spectroscopy and aquaphotomics. Aquagrams were constructed for each water source which is used to identify at which wavelengths differences in the water occur. The Aquagrams of the different water sources is used to differentiate between different water types.

**S-12 Verena Wiedemair MSc.**

Verena Wiedemair, Reinhold Ramoner, Christian W. Huck

University of Innsbruck, Austria

Student

Millet, buckwheat and oat are considered to be minor crops, hence chemical profiles for different cultivars are rare. The examination of a sum parameter, like the total antioxidative capacity (TAC) can thus be a first step to systematically assess the quality of different cultivars of aforementioned gluten-free grains and thereby serve as an indicator for the selection of cultivars for food processing and breeding. TAC of 20 common buckwheat, 14 proso millet and six common oat cultivars was analysed using Folin-Ciocalteu assay and four NIR spectrometer, one benchtop and three handheld devices. PLS regressions for milled and intact samples established using the benchtop instrument yielded a  $R^2(CV)$  of 0.892 and 0.929. The SEPs for milled and intact samples were approximately 1.7 and 1.6 mgGAE/g. Multivariate LOD and LOQ were also calculated. LODmax for intact and milled samples was 1.72 and 2.80 mgGAE/g. TAC varies considerably among cultivars of one species, emphasising the need for full chemical profiles. Values for LOD and LOQ show that established PLS-R models can be used to quantify TAC of buckwheat and oat cultivars. TAC of millet cultivars can be detected, however not quantified. An additional comparison with the handheld devices showed that similar and in some cases even better results can be yielded with a restricted wavenumber region and resolution. The best regression model for a handheld devices yielded a  $R^2(CV)$  of 0.9513, a RMSEP of 1.0214 and a LODmax of 1.83 mgGAE/g.

**S-13 Princess Tiffany Dantes**

Charles Hurburgh and Dirk Maier

Iowa State University, US

Student

Recent issues on quality and safety of animal-derived food products have prompted the grain and feed industry to thoroughly consider all aspects of food production and of the feed supply chain, and to ensure conformity to quality and traceability standards. To achieve these goals, testing methods for quality and safety attributes that are accurate, non-destructive, rapid and applicable for on-line monitoring are therefore needed. Near-infrared hyperspectral imaging (NIR HSI) is a promising technique that combines near-infrared spectroscopy and machine vision. It has been explored in various food and agricultural applications. In this review, the focus are on the principle of NIR HSI and the recent studies done with this technology to solve problems related to feed quality and safety. NIR HSI is not yet a standard tool due to its limitations and disadvantages. With its promising breakthrough in the feed industry, it is essential to maximize its potential and explore other research areas to transform this from being a laboratory tool to an industrial technique for on-line or at-line processing operations.

**S-14 Christian G. Kirchler**

Julia Schmelzer, Cornelia K. Pezzei, Raphael Henn, Christian W. Huck

University of Innsbruck, Austria

Student

The presented study shows the ability of handheld NIR spectrometers in direct comparison to benchtop devices for the quantification of relevant plant ingredients in black tea (*Theae nigrae folium*) and rosemary leaves (*Rosmarini folium*). The benchtop device was represented by the NIRFlex N-500 FT-NIR spectrometer (Buchi, Flawil, Switzerland) equipped with the Solids Cell N500-001. The handheld devices applied in this study were the microPHAZIR (Thermo Fisher Scientific, Waltham, USA) and MicroNIR 2200 spectrometer (Viavi Solutions (former: JDS Uniphase Corporation), Milpitas, USA). The determined relevant plant ingredients were caffeine as well as L-theanine in black tea and rosmarinic acid in rosemary leaves. The dried plant samples were milled or grounded before spectra were recorded in diffuse reflection mode. PLS regression models were established and evaluated. The results revealed that the benchtop as well as both handheld spectrometers are suited for the shown applications, whereas handheld devices had an approximately 1.5 times higher SEP in average.