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ORIGINAL PAPER

Application of a Portable Infrared Instrument for Simultaneous Analysis of Sugars, Asparagine and Glutamine Levels in Raw Potato Tubers

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Abstract The level of reducing sugars and asparagine in raw potatoes is critical for potato breeders and the food industry for production of commonly consumed food products including potato chips and French fries. Our objective was to evaluate the use of a portable infrared instrument for the rapid quantitation of major sugars and amino acids in raw potato tubers using single-bounce attenuated total reflectance (ATR) and dial path accessories as an alternative to time-consuming chromatographic techniques. Samples representing a total of 84 experimental and commercial potato varieties harvested in two consecutive growing seasons (2012 and 2013) were used in this study. Samples had wide ranges of sugars determined by HPLC-RID (non-detectable (ND)-7.7 mg glucose, ND-9.4 mg fructose and 0.4–5.4 mg sucrose per 1 g fresh weight), and asparagine and glutamine levels determined by GC-FID (0.7–2.9 mg and 0.3–1.7 mg per 1 g fresh weight). Infrared spectra collected from 64 varieties were used to create partial least squares regression (PLSR) calibration models that predicted the sugar and amino acid levels in an independent set of 16 validation potato varieties. Excellent linear correlations between infrared predicted and reference values were obtained. PLSR models had a high correlation coefficient of prediction (rPred >0.95) and residual predictive deviation (RPD) values ranging between 3.1 and 5.5. Overall, the results indicated that the models could be used to simultaneously predict sugars, free asparagine and glutamine levels in the raw tubers, significantly benefiting potato breeding, certain aspects of crop management, crop production and research.

Keywords Infrared spectroscopy · Potatoes · Acrylamide · Sugars · Asparagine · Glutamine

Abbreviations

ATR	Attenuated total reflectance
GC-FID	Gas chromatography-flame ionization detector
FTIR	Fourier transform infrared spectroscopy
HPLC-RID	High-performance liquid chromatography-refractive index detector
PLSR	Partial least squares regression
rCV	Correlation coefficient of cross-validation
RPD	Residual predictive deviation
rPred	Correlation coefficient of prediction
SECV	Standard error of cross-validation
SEP	Standard error of prediction

Introduction

Potato is the fifth most produced crop worldwide after sugar cane, maize, wheat and rice with a production surpasing 368 million tons in 2012 [1]. Among the many potato products

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available, potato chips and French fries are the most popular. The quality of these products is highly dependent on the composition of the raw potatoes, which makes the monitoring of tuber composition a critical step for effectively planning breeding lines to produce tubers suitable for adequate processing in the food industry [2].

Factors such as variety, storage temperature and time, as well as the level of nitrogen and phosphorous in the soil can alter the level of tubers' reducing sugars and free amino acids [3], the key components that cause browning reactions that occur during cooking. Previous labelling studies have shown that asparagine provides the backbone of the acrylamide molecule (2-propenamide, CAS Registry No. 79-06-1) [4], a known human neurotoxin, rodent carcinogen and "probable carcinogen to humans" [5]. Even though there are several pathways proposed for acrylamide formation [6], it is generally accepted that acrylamide is predominantly formed through the Maillard reaction pathway, with free asparagine and reducing sugars (*e.g.*, glucose and fructose) as the major reactants present in foods [7]. Gerendás *et al.* [3] reported that these major reactants in potatoes were found at their highest levels when grown with high N and low K supply. Additionally, storing potato tubers at temperatures lower than 8 °C can cause rapid accumulation of sugars (cold sweetening) [8] in a genotype-specific manner [9]. Among the amino acids in potato tubers, asparagine and glutamine are found at the highest concentrations, with asparagine being the most abundant and accounting for about one-third of the total free amino acids [10, 11]. Compared to the typical level of sugars in potatoes, asparagine is usually present at higher concentrations; therefore, reducing sugars are the most important elements needed for Maillard reactions [12].

The most popular methods used to determine the levels of sugars and amino acids in raw potatoes require intensive sample preparations and chromotographic separations with high-performance liquid chromatography (HPLC) or gas chromatography (GC). Unlike many traditional methods used in food quality testing, infrared spectroscopy provides valuable information about the biochemical composition of the samples, quickly and with minimal or no sample preparation needed [13]. Along with improvements in optical technology and modern computing technology for chemometric analysis of infrared spectra, portable and handheld spectrophotometers are now available as practical and economical alternatives to their benchtop counterparts.

The objective of this study was to develop simple and robust methods for simultaneous quantification of sugars (glucose, fructose and sucrose), free asparagine and glutamine levels in raw potatoes using a portable FTIR system equipped with dial path and ATR accessories. The methods would be developed based on highly specific mid-infrared (MIR) spectroscopic signature profiles and supervised pattern recognition techniques.

Materials and Methods

Potato tubers from 2012 (47 varieties) and 2013 harvests (37 varieties) representing a total of 84 experimental clones or commercial varieties (some used or in development for chip production) were obtained from the Ohio Agricultural Research and Development Center in Wooster, Ohio, USA. Five potato tubers of each clone were washed under running tap water and dried using paper towels. Tubers were then cut into quarters and frozen immediately at −40 °F until used. Potato quarters were blended with liquid nitrogen and the fine powder obtained was used for all further experiments. Additionally, sugar, asparagine and glutamine levels in potatoes were determined using the reference methods as described in electronic supplementary material 1.

Infrared Spectroscopy

Approximately 1 g of potato powder was weighed into a 2 ml capacity microcentrifuge tube and centrifuged at 3000 *g* for 15 min. The top liquid (supernatant) after centrifugation, obtained from the tuber water content in potato powders (74–81 % fw) (electronic supplementary material 2, Fig. 1a), was used for infrared spectra collection. Two replicates of 1 g powder were centrifuged per each potato. A Cary 630 FTIR spectrometer (Agilent Technologies Inc., Danbury, CT, USA) equipped with ZnSe beam splitter and deuterated triglycine sulfate (DTGS) detector was used to collect the MIR spectra of the potato tubers. Two different accessories of the Cary 630 FTIR spectrometers were used for infrared spectra collection: a 30 μm dial path (electronic supplementary material 2, Fig. 1b) and ATR accessories (electronic supplementary material 2, Fig. 1c).

For the application with dial path accessory, 10 μL of the supernatant was directly placed onto the transmission cell of the instrument with 30 μm path length as shown in electronic supplementary material 2, Fig. 1b. One spectrum for each of the centrifuged potato powders (total of two spectra per each potato clone) was collected. For the ATR accessory, 1 μL of the supernatant was placed onto the ATR crystal of the instrument and vacuum dried for 1 min as displayed in electronic supplementary material 2, Fig. 1c. Then, one spectrum from each centrifuged potato powder was collected (total of two spectra per each potato clone). The spectral resolution was 4 cm^{-1} and 64 spectra were co-added to improve the signal to noise ratio over the frequency range 4000–700 cm^{-1}. Spectral backgrounds were collected before each sample. The absorbance spectrum was obtained by ratioing the sample spectrum against that of a blank optical path (background spectrum). The collected spectra were recorded using Agilent MicroLab PC software (Agilent Technologies Inc., Danbury, CT, USA) on a personal laptop.

Partial Least Squares Regression (PLSR)

The spectra collected using both dial path and ATR accessories of the Cary 630 system were imported into Pirouette software (Infometrix, Bothell, WA, USA). The data was normalized, second derivative transformed (Savitzky-Golay second order polynomial filter with a 25-point window) and smoothed (Savitzky-Golay second order polynomial filter with a 25-point window) prior to PLSR analysis. PLSR models were developed using the infrared spectra and reference values obtained for glucose, fructose, reducing sugars (sum of the glucose and fructose), sucrose (from HPLC-RID) and free asparagine and glutamine (from GC-FID). Separate PLSR models were developed for the dial path and ATR accessories of the system for each compound of interest. Full cross-validation (leave-one-out approach) was used to internally validate the calibration models, and an independent sample set consisting of 16 potato clones (out of the 84 potato clones used in the study) was used for their external validation. Samples were randomly assigned into either calibration or independent validation sets ensuring that both replicates belonging to the same clone were allocated into the same category. PLSR with the features adapted from both principal component analysis (PCA) and multi linear regression (MLR), uses not the thousands of wavenumbers collected in the spectra, but the extracted important latent variables (PLS-factors) to explain the variation in the samples [14]. PLS regression takes into consideration that measured values obtained from the reference analyses such as sugar levels by HPLC-RID and free amino acid levels by GC-FID may contain errors associated with sample preparation [15]. Using the measured values from the reference method and the corresponding spectra collected, the program predicts a value for the compound being analyzed in the model. To evaluate the performance of a model, loading vectors, standard error of cross validation, prediction correlation coefficient (r) and outlier diagnostics (Standard Residual of Sample *vs.* Leverage) were used. The SEP shows the magnitude of error expected when independent samples are introduced into the calibration models and the compound concentrations in the unknown samples are predicted. During the model development, samples with large residuals, unusual pattern and high leverage are considered outliers and removed from the models. To further evaluate the strength of a model and/or compare the models to each other, the residual predictive deviation (RPD) values were calculated by dividing the standard deviation of the reference (measured) values for the samples in the independent set, to the standard error of the prediction obtained. RPD classification previously reported [16] was used to analyze the strength of the PLSR models. According to the authors, models with RPD values above 2.5 and 3 are considered as "good" and "excellent", respectively. However, models with RPD values under 1.5 indicate a very poor model that would not be suitable for use. Models with RPD values between 1.5 and 2.0 are only valid to distinguish among high and low constituent concentration levels, while models with RPD of 2–2.5 can be used to make approximate predictions.

T-test

In order to analyze means differences between the clones from the year of 2012 and 2013 for each reference analysis, unequal variances and unbalance *T*-test were used. *P*-values were calculated for each comparison, and significant levels were assigned to probabilities lower than 0.05 ($\alpha=0.05$) (Microsoft Excel software, Redmond, WA, USA).

Result and Discussion

Characterization of the Potato Tubers

Representative chromatograms obtained from the reference methods are displayed in electronic supplementary material 2, Fig. 2. Figure 2a and b illustrate chromatograms for amino acids using GC-FID and for sugars using HPLC-RID, respectively. A summary of the reference values obtained for free asparagine, glutamine, glucose, fructose, reducing sugars (sum of glucose and fructose) and sucrose levels in the potato tubers analyzed in this study is presented in electronic supplementary material 3, Table 1 based on their harvest year.

The range and the mean value for asparagine levels were higher for the tubers harvested in 2012 compared to 2013 ($p<0.05$). In 2012, the level of free asparagine in potato tubers ranged between 0.7 and 2.9 mg/g fresh weight, averaging at 1.9 mg/g fresh weight; while in 2013 the range was between 0.8 and 2.0 mg/g fresh weight with the mean value of 1.3 mg/g fresh weight. A similar trend was seen for free glutamine levels. The level of free glutamine in the tubers was between 0.4 and 1.7 mg/g fresh weight (mean value was 0.8 mg/g fresh weight) in 2012, which was higher than the values obtained in 2013 (0.3 to 1.1 mg/g fresh weight with a mean value of 0.7 mg/g fresh weight). Although variety, preharvest and postharvest conditions can affect the levels of free asparagine and glutamine in tubers, our data showed reasonably similar levels to those previously reported, as shown in electronic supplementary material 3, Table 1.

The higher analyte concentrations observed in 2012 compared to 2013 ($p<0.05$) were more pronounced for the potato tuber sugars, with levels for reducing sugars and sucrose being 52 and 3 times higher, respectively, in 2012 compared to 2013. Among the other factors, this could be primarily due to the difference in postharvest storage temperature. The pronounced cold sweetening was expected to occur in tubers from 2012 which were stored at lower temperatures and analyzed in December in our laboratories. After harvesting and

prior to analysis, the tubers in 2012 were kept in a humidified refrigerated storage at 3 °C whereas the tubers from 2013 were kept in a humidified refrigerator at 9 °C [17]. Similar findings were reported, Biedermann *et al.* [18] stored potatoes of cultivar *Erntestolz* at 4 °C for 15 days and observed an increase in reducing sugars from 80 to 2250 mg per kg fresh weight. Fortunately, the resulting variation provided wider range of sugar levels, which we considered an advantage for this infrared study.

Regression Analysis

Average transmission and single bounce ATR spectra obtained from potato powder supernatants showed strong water absorption bands as shown in electronic supplementary material 2, Fig. 3. In transmission spectra collected by the dial path accessory, the strong infrared absorptivity of the water saturated the signal between the region of 3750 cm^{-1} and 2800 cm^{-1}. An additional effect of water absorption due to the OH stretching vibrations was seen in the region of 1800 cm^{-1}–1500 cm^{-1}. Therefore, these regions were excluded during the development of the PLSR models and only the 1500 cm^{-1}–900 cm^{-1} fingerprint region was used. The application of 1 min quick vacuum drying on the ATR accessory of the Cary 630 system helped reduce the strong effect of water in the spectra upon drying and allowed the use of the spectral region from 1800 cm^{-1} to 1500 cm^{-1} in the free asparagine and glutamine models. The most important bands in the regression vectors of the PLSR models for the main soluble potato components (asparagine and reducing sugars) are shown in electronic supplementary material 2, Fig. 4. Even though the regression vectors of the PLSR models for other compounds (glucose, fructose, sucrose and glutamine) are not illustrated, they are discussed as well.

The most important bands in the regression vectors for asparagine (electronic supplementary material 2, Fig. 4a) and glutamine models using the ATR accessory were related to 1677 cm^{-1}, 1627 cm^{-1}, 1401 cm^{-1} and 1345 cm^{-1}, which were assigned as C=O stretch vibration, NH_2 deformation, C-N stretches and C-H deformation, respectively [19]. Vacuum drying the potato supernatant revealed the amide vibration bands of Asn and Gln side chains that were masked by the strong water stretching vibration in the 1800 cm^{-1}–1600 cm^{-1} for measurements using the dial-path accessory. Nevertheless, models for asparagine and glutamine using the dial path showed important bands centered at 1429 cm^{-1}, 1400 cm^{-1} and 1357 cm^{-1} (electronic supplementary material 2, Fig. 4a) corresponding to C-N stretches and C-H deformation, respectively [19].

The regression vectors of the PLSR models developed for sugars were dominated by the region of 1200 cm^{-1}–1000 cm^{-1} which is associated with C-C ring vibrations, overlapped with the stretching vibrations of C-OH side groups and the C-O-C glycosidic band vibrations of carbohydrates. Loading vectors for glucose were associated with bands at 1015 cm^{-1}, 1034 cm^{-1} and 1060 cm^{-1} associated with C-O-H deformation and C-O stretch vibration, respectively [19]. Fructose models were dominated by bands related to C-O-H deformation (1428 and 1358 cm^{-1}) and C-O stretching vibrations (1051 cm^{-1}) [20]. Major bands in the regression models of the reducing sugars (combined glucose and fructose) (electronic supplementary material 2, Fig. 4b) were in the 1030 cm^{-1}–1070 cm^{-1} region corresponding to C-O stretch vibrations [21]. Sucrose models showed a predominant band centered at 997 cm^{-1} which is associated with the disaccharide linkage between α-D-glucopyranosyl and β-D-fructofuranosyl groups [21]. However, there was an additional band at 1062 cm^{-1} in the regression vector of the sucrose model with dial path accessory and characteristic of the C-O stretch vibration [22].

The sample statistics for calibration and external validation sets used in the development of PLSR models for each parameter measured in this study are presented in electronic supplementary material 3, Table 2. For all the PLSR models, the same 16 potato tuber genotypes randomly chosen from both 2012 and 2013 harvests were used as an independent validation set. Even though there were 68 tuber genotypes in the calibration set, the numbers in electronic supplementary material 3, Table 2 are different due to a few outliers taken out while developing the model.

Performance statistics obtained for each of the PLSR models are shown in electronic supplementary material 3, Table 3. Similar number of factors ranging between 4 and 6 were used in the models avoiding the potential overfitting problem, which could weaken the ability of the models to predict the concentrations in the unknown samples. In general, the dial path and ATR accessories of the Cary 630 showed similar performances in terms of SECV, SEP, rCV, rPred and RPD values.

High correlations between reference values obtained from GC-FID and the infrared predicted levels for the two major free amino acids (asparagine and glutamine) in the calibration and independent validation sets are shown in electronic supplementary material 2, Fig. 5. The amino acid models with dial path and ATR accessories both used five factors. SEP for asparagine was about 0.15 mg/g fresh weight yielding to an RPD value of 3.4 for both of the accessories in the asparagine models. SEP values for glutamine were about 0.08 mg/g fresh weight for both accessories and the model with dial path yielded a slightly higher RPD value than the model with the ATR (3.4 *versus* 3.1).

The optimum number of factors used for the glucose, fructose and reducing sugar (sum of glucose and fructose) models was 6. Glucose models gave SEP of 0.46 and 0.38 mg/g fresh weight for ATR and dial path accessories respectively, and RPred of 0.98 in both cases. RPD value for glucose using dial

path was slightly higher than the ATR (5.5 *versus* 4.6). For fructose, SEP was about 0.7 mg/g fresh weight and RPD values were 3.9 for ATR and 4.1 for dial path. PLS regression plots for reducing sugars and sucrose content between reference values and infrared predicted levels are shown in electronic supplementary material 2, Fig. 6. The SEP obtained for reducing sugars was 1.15 mg/g fresh weight for both applications, and RPD values were again slightly higher for the dial path with values quite similar to those from fructose models (4.2 *versus* 3.9). Lastly, sucrose models using 4 and 5 factors with ATR and dial path, respectively resulted in SEP of about 0.32 mg/g fresh weight and RPD of 3.5 for ATR and 3.2 for dial path applications. Overall, good correlations (rPred 0.95–0.98) were obtained for all the models. Based on the scale reported [16], all models gave RPD values above 3 (between 3.1 and 5.5) indicating that they are excellent models and can be used for predicting concentration levels in unknown samples. Even though the dial path accessory was generally yielding higher RPD values in comparison to those of ATR models, both accessories gave excellent performances for these applications since the SEP and RPD values obtained for the independent validation sets were quite similar between the models.

Similar PLSR model performances were obtained by analyzing the supernatant after centrifuging potato powders at 3000 and 12,000 *g* indicating that simple portable fixed speed centrifuge units can be used, increasing the practical applicability of the proposed techniques. To our knowledge, this is the first study done with raw potatoes to predict their level of sugars and amino acids by using an MIR spectrophotometer and particularly a portable MIR device. Previous related research in the literature used near infrared (NIR) spectroscopy for online measurement of reducing sugars in potatoes and reported very low accuracy of predictions compared to the acceptable standards [23]. For instance, Haase [2] used NIR spectroscopy to predict the quality of ground raw potatoes. The author developed calibration models for reducing sugar and sucrose and obtained (r^2) of 0.43 for reducing sugar and 0.71 for sucrose. The RPD values for the models were unacceptably low (1.7) and low (2.4) for reducing sugar and sucrose, respectively. On the other hand, Chen *et al.* [24] evaluated the performance of a NIR fiber optic probe as a non-destructive method for determination of carbohydrate content in potatoes with model performances of SEP of 0.98 %, rVal of 0.86 and RPD of 2.8 using eight factors with dominant bands associated with potato starch. Hartman & Büning-Pfaue [25] used NIR to predict the level of dry matter, starch, crude protein and sugars (glucose, fructose, sucrose and reducing sugar) content in 120 peeled and homogenized potatoes. Their sugar models gave the best performance for fructose but showed high SEP for glucose and sucrose because of the structural symmetry of glucose to dominant starch content of potatoes. All our sugar models (electronic supplementary material 3, Table 3) showed superior performances to reported NIR values. Hartmann & Büning-Pfaue [25] also emphasized the field practicality of developing a reducing sugar model as opposed to individual glucose and fructose models and the technological importance of mobile spectrometers providing transportation flexibility.

Conclusions

Based on the data obtained from the PLSR models developed, it can be said that the spectra obtained by using both ATR and dial path accessories of the modern Cary 630 portable FT-IR system paired with multivariate analysis, yielded very strong models, providing low SEP and high RPD values. Using the same spectra, separate free asparagine, free glutamine, glucose, fructose, reducing sugars and sucrose PLSR models were successfully developed. Using the portable systems is simple, cost-effective and requires low sample volume; once the instrument is purchased, there are minimal operational costs involved to perform the tests. Additionally, portable systems provide increased flexibility and great potential for in-field applications compared to bench-top IR systems or chromatographic systems such as HPLC and GC, which can only be used in a laboratory setting. Therefore, PIRT can significantly benefit potato breeding and certain aspects of crop management, crop production and research.

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Conflict of Interest The authors declare that they have no conflict of interest.

Human and Animal Rights and Informed Consent This article does not contain any studies with human or animal subjects.

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