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ORIGINAL PAPER

Determination of In-Shell Peanut Oil and Fatty Acid Composition Using Near-Infrared Reflectance Spectroscopy

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Abstract NIR reflectance spectroscopy was used to analyze the total oil and fatty acid concentration of Virginia and Valencia types of in-shell peanuts rapidly and nondestructively. NIR absorbance spectra were collected in the wavelength range from 400 to 2,500 nm using a NIR instrument. Average total oil concentrations of all samples were determined by a standard Soxtec extraction method. Fatty acids were converted to the corresponding methyl esters and measured using gas chromatography. Partial least squares analysis was performed on the calibration set, and models were developed for predicting total oil and fatty acids. The best model was selected based on coefficient of determination (R^2), standard error of prediction, and residual percent deviation (RPD) values. Virginia-type in-shell peanuts had RPD values of >5.0 for both absorbance and reflectance models, indicating that the method could be used for quality control and analysis. Valencia peanuts had an RPD value of 3.01, which indicates that the model is good for initial screening purposes. For both types of peanuts, fatty acid prediction gave RPD values of <5 for all the models, indicating they could be used for initial screening purposes.

Keywords Nondestructive · NIR reflectance spectroscopy · Partial least squares · In-shell peanut · Total oil · Fatty acids

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Introduction

Oil and fatty acid concentrations of peanuts (*Arachis hypogaea* L.) are important factors in peanut processing. The total oil concentration is important for peanut processing because it determines how the peanuts can be processed into different products such as roasted peanuts, peanut butter, and peanuts for candy and cereal bars. Therefore, measurement of peanut oil is a relevant factor for processing. It is also important to know the fatty acid profile of the peanut oil as a quality parameter. Methods used for total oil and fatty acid concentration measurements are laborious and time consuming and include analytical and chromatographic procedures. The samples used in these tests are discarded and cumulatively result in the loss of edible peanuts. In-shell measurement of the kernel oil and fatty acids would result in considerable savings of both time and money during grading and processing.

Single-kernel devices are used to find the moisture and oil concentrations in nuts and grains by crushing a kernel of a nut or grain from the bulk sample and measuring its conductivity [1, 2]. These types of instruments provide valuable information regarding the variability of oil and fatty acid concentrations within a sample, but these methods are destructive and time consuming when performed on large samples. Techniques using near-infrared (NIR) spectroscopy for food quality measurements are now being applied in food processing and quality inspection. NIR spectroscopy has several advantages over conventional physical and chemical analytical methods for food quality analysis. NIR is rapid, nondestructive, and provides more information about the components present in the raw materials and formulated food products.

Spectra measured using NIR contain absorbance bands that are mainly due to three chemical bonds: C–H, which is

usually from fats and oil; O–H bond, found in water; and N–H bonds, which are found in protein [3]. Other chemical bonds may appear in overtone bands in the NIR region, but they are generally too weak to consider for analysis in complex food systems like peanuts, which contain water, oil, fat, protein, etc. NIR is ideal for quantitatively determining oil, protein and moisture by deducing C–H, N–H and O–H bonds. In addition, high scatter coefficients allow for excellent diffuse reflectance spectra of solids. NIR spectroscopy may be applied with minimal sample preparation and has been used successfully for oil analysis in many other crops, including soybean [4], sunflower [5], rape seeds [6], canola [7], and flax seeds [8]. NIR has also been used to determine peanut fatty acid concentrations of individual peanut kernels [9, 10] and peanut oil [11]. NIR has also been used to predict the total oil and fatty acid concentrations of peanut pods [12, 13]. The primary objective of this research was to develop calibration models that can predict the oil and fatty acid concentration of the peanut kernels based on NIR reflectance spectroscopy of in-shell peanuts.

Materials and Methods

Materials

About 50 kg of Virginia- and Valencia-type peanut pods were obtained from crops harvested in 2008 and 2007, respectively. Petroleum ether (Fisher Chemicals, USA) was used for oil extraction to develop standard values for total oil analysis. Cyclohexane, acetone, and sodium methoxide were purchased from Sigma-Aldrich (St. Louis, MO, USA) and used to prepare and chromatographically analyze the fatty acid methyl esters obtained from oil samples.

Methods

Sample Preparation

The initial moisture concentration (MC) of whole peanuts was measured as 6% for both Virginia and Valencia market type peanuts using a standard air oven method [14]. These peanut lots were divided into 12 (Valencia) and 15 (Virginia) sub-lots and each was placed in a separate vapor sealed/air tight plastic container. Appropriate quantities of water were added to each container to raise the moisture level of the peanuts in 2% increments. The appropriate amount of water was determined based on the weight, initial moisture content, and the expected moisture percentage of the sample. The amount of water added to the samples ranged from 3 to 180 mL depending on the weights and the initial and final expected moisture contents of the samples. The amount of water added increased with increasing final expected moisture percentage. The containers were sealed and allowed to equilibrate at 4 °C for two weeks. The containers were periodically rotated during this period to allow uniform moisture distribution. It generally takes 10–15 days to reach a uniform moisture distribution. Once a uniform moisture distribution was reached, the moisture content of the samples in each container was determined using a standard air oven method. This resulted in 12 and 15 moisture levels for Valencia- and Virginia-type peanuts, respectively. The final MC ranged from 7 to 27% for Virginia- and from 6 to 22% for Valencia-type peanuts. Different moisture levels were prepared to obtain various oil percentages on a weight basis. By adding water to increase the moisture content, the moisture contents of both the shells and the kernels were increased by equilibrating the samples in airtight closed containers. By changing the moisture concentration of the seeds, the total oil percentage was varied. After the samples had reached a uniform moisture distribution, the containers were removed from cold storage and allowed to equilibrate to room temperature before the NIR spectroscopy measurements were performed.

Total Oil Determination

A Soxtec[1] 2050 semi-automated solvent extractor (Foss Tecator AB, Höganäs, Sweden) was used to measure the total oil concentration. In this method, petroleum ether was used to extract the oil from ground peanut kernel samples. Good (undamaged, nondiscolored, well matured) intact peanut kernels were selected from among the samples of both varieties with different moisture levels. Kernel samples were frozen before grinding to minimize loss of oil. About 1–1.2 g of homogeneously ground, fine peanut meal were weighed and placed in a cellulose thimble. This was covered with a thin layer of defatted cotton to avoid splashing petroleum ether during reflux. This thimble was attached to the metal ring and placed into the extractor. Tared aluminum cups were placed below the thimbles to collect the extracted oil samples. Initially, 90 mL of petroleum ether were added through the top of the device to each thimble. Heat was supplied to reflux the petroleum ether and extract the oil from the peanut meal. The temperature was maintained at 135 ± 2 °C for 45 min. The extracted oil was collected into the cups located below the thimbles and heating was continued without refluxing the solvent for another 45 min at 135 ± 2 °C to evaporate the residual petroleum ether from the oil. The samples were cooled for 15 min, and the petroleum ether was

[1] Company or trade names are mentioned for the purposes of description only, and this does not imply any endorsement by the USDA.

recovered by condensation. The collecting cups were removed and kept in an air oven at 40 °C for 30 min to evaporate any traces of petroleum ether. The total oil concentration was calculated from the weights of the empty collecting cups, the cups with oil, and the initial ground peanut kernel meal, and is expressed here in weight percent (wt%). Oil determinations were performed in triplicate for each oil (moisture) level for both peanut types.

Fatty Acid Analysis

Fatty acids present in the peanut oil samples were analyzed using an Agilent 6890 gas chromatograph (Agilent Technologies, Palo Alto, CA, USA) equipped with a flame ionization detector (FID). Oil samples obtained by the Soxtec extraction method were used for fatty acid analysis. About 10–12 mg of peanut oil were reacted with 0.2 mL of sodium methoxide to convert the oil into the corresponding fatty acid methyl esters. The mixture of oil and sodium methoxide was heated to 50 °C and mixed by sonication for 5 min to complete this transesterification reaction. The esters were recovered after the addition of 0.5 mL of cyclohexane. This mixture was sonicated for about 10–15 min and allowed to separate into two phases. A 10–20 μL sample was taken from the upper organic phase and diluted with 1 mL of acetone for analysis by GC. Separation was achieved using an SP-2380 column (30 m × 0.25 mm × 0.2 μm; Supelco, Bellefonte, PA, USA). Helium carrier gas was used at a flow rate of 0.6 mL/min with an injection volume of 1 μL. The inlet and detector temperatures were 200 and 220 °C, respectively. Baseline separation of the major fatty acids was achieved with an oven temperature of 185 °C and an analysis time of 20 min. The esters (e.g., methyl oleate, methyl linoleate, methyl linolenate, methyl stearate, and methyl palmitate) were identified by comparing their retention times to those of known standards.

NIR Spectroscopy Measurements

After conditioning, the peanut samples were separated into two groups: calibration and validation. The number of sets in the calibration group was eight for Virginia- and seven for Valencia-type peanuts. The number of sets in the validation group was seven for Virginia- and five for Valencia-type peanuts. NIR spectral measurements were performed using a scanning monochromator (model 6500, Foss NIRSystems, Silver Springs, MD, USA). Spectral data were collected using Vision software (version 1.0, Foss NIRSystems, Silver Springs, MD, USA). Peanut pods from each set were scanned 30 times to get 30 replicated spectra. In each scan, NIR light was allowed to fall on the bottom of the sample holder containing the peanuts, where it penetrated and interacted with the samples. The reflected energy was measured over the wavelength range of 400–2,500 nm. This reflected light spectrum carried absorption information. The average spectra obtained from 30 scans of the two sets of peanut samples of Virginia and Valencia type are given in Fig. 1 as representative spectral data.

Data Analysis

NIR spectral data were analyzed using multivariate data analysis software (Unscrambler, version 9.7, CAMO ASA, USA). Reflectance spectra were obtained between 400 and 2,500 nm (interval: 0.5 nm) for use as independent variables. Oil and fatty acids were the dependent variables. Using the spectral data from the calibration dataset, partial least squares (PLS) regression analysis was conducted to develop an empirical equation for predicting the total oil concentration and fatty acids (oleic, linolenic, linoleic, palmitic and stearic acids). Absorption spectral data were also converted into respective reflectance data and stored as a separate file. Both the absorption and reflectance data were used during model development. Before these data were used for model development, both the absorption and reflectance spectral data were transformed mathematically to obtain their second derivatives with respect to wavelength. The spectral data were transformed using the Norris gap function with a gap size of 5. Transformed data from the calibration groups were used for model development. This model was tested on transformed spectral data from the validation groups. The derivative transformation was used to remove any baseline shifting and avoid overlapping peaks. After applying the derivative transformation, the modified wavelength spectrum shows more detail since the low frequencies are suppressed and the high frequencies enhanced (Fig. 2). Derivative analysis was limited to second order to avoid loss of sensitivity for characteristic peaks with higher order derivatives, which would generally occur.

PLS analysis was performed on the transformed spectral data of the calibration groups to determine the best calibration model based on the standard error of calibration[2] (SEC) and the coefficient of multiple determinations (R^2). PLS models were used to predict the peanut compositions from the spectral data of the validation group peanuts. Goodness of fit was evaluated based on the standard error of prediction[3] (SEP) when comparing measured values

[2] $\mathrm{SEC} = \left(\frac{1}{n-p-1}\sum_{i=1}^{n} e_i^2\right)^{\frac{1}{2}}$, where n is the number of observations, p is the number of variables in the regression equation, and e_i is the difference between the observed and reference values for the ith observation.

[3] $\mathrm{SEP} = \left(\frac{1}{n-1}\sum_{i=1}^{n} (e_i - \bar{e})^2\right)^{\frac{1}{2}}$, where n is the number of observations, e_i is the difference between the predicted and measured moisture contents for the ith sample, and $\bar{e}$ is the mean e_i for all samples.

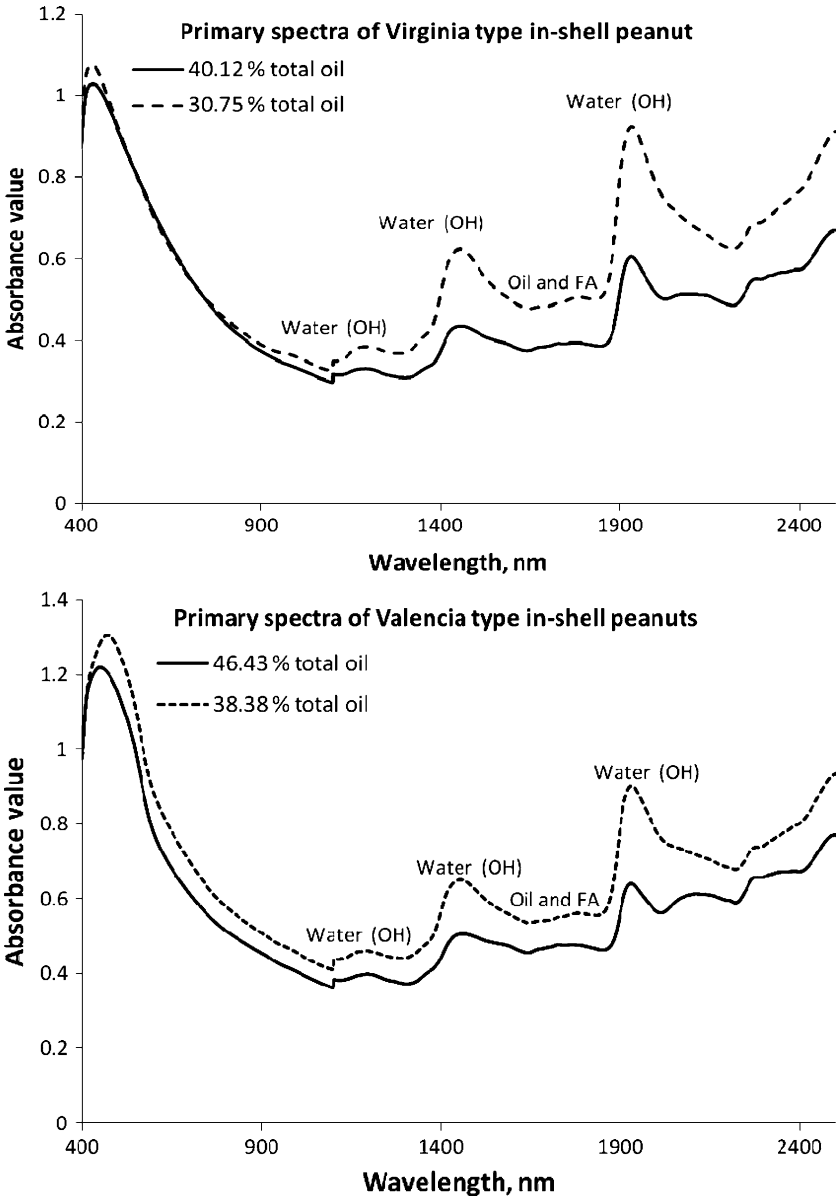

Fig. 1 Representative primary spectra of in-shell peanuts

to predicted values of oil and individual fatty acid concentration. The ratio of the standard deviation of predicted values to the SEP, called the residual percent deviation (RPD), was also used to evaluate the goodness of fit. The RPD values usually range from 1 to 10. Higher values indicate a stronger calibration model for the accurate prediction of unknown sample composition. RPD values of 1 or less are an indication of an inadequate model. RPD values in the range of 3.1–4.9 are good for initial screening purposes (where an accurate prediction is not needed when a large number of peanut batches are handled), and greater than 5 (the range 5–6.4) is good for quality control and prediction [15, 16]. *T* and *U* scores of developed PLS calibration models were also plotted against the wavelength to show the fitness of the developed calibration models. *T* scores are the new coordinates of the data points in the *X* (wavelength) variable space, and they were computed using the wavelengths that were mostly used to predict the *Y* values (peanut composition). *U* scores provide a summary of the predicted components given by the *X* values in the developed model. A plot of *T* and *U* scores shows the relationship between the *X* and *Y* variables and also shows outliers that contribute to a poor calibration model.

Results and Discussion

Figure 1 shows the primary NIR absorption spectra of both Virginia- and Valencia-type in-shell peanuts at two

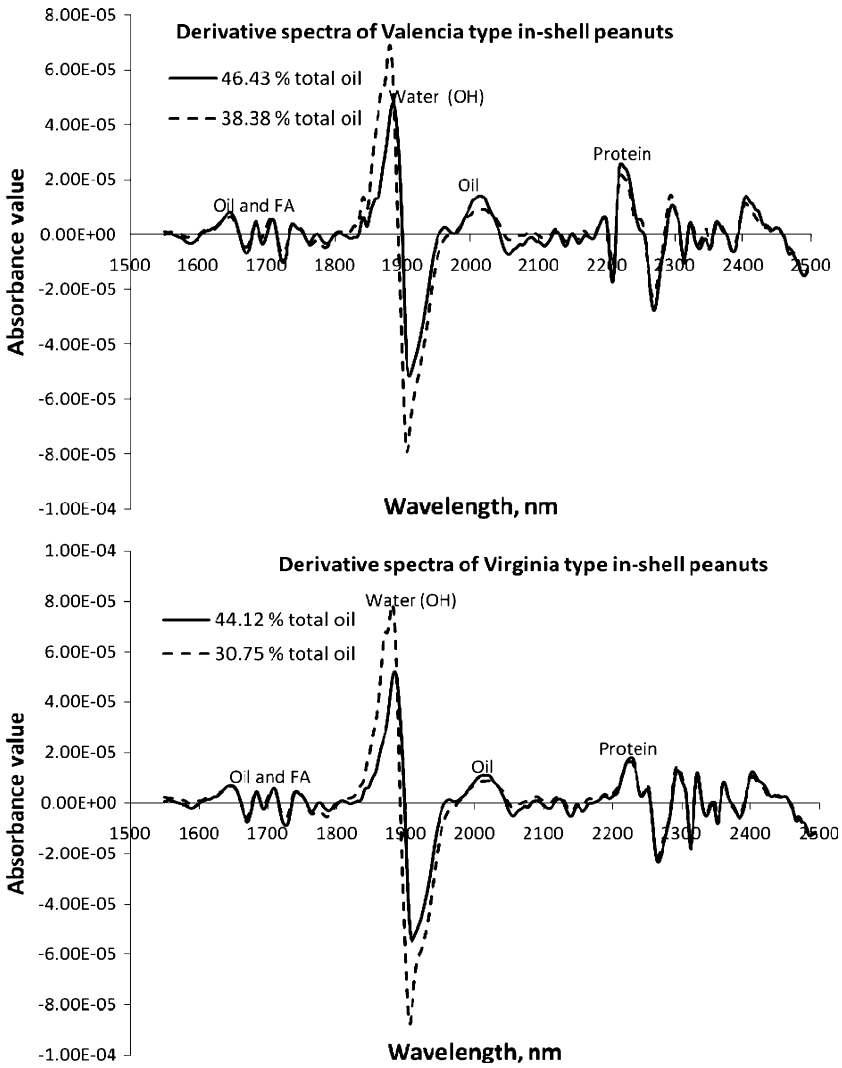

Fig. 2 Representative derivative spectra for in-shell peanuts

different total oil percentages. The peaks and valleys in the NIR region represent the absorption of electromagnetic energy. Strong NIR absorption bands near 1,400–1,440 nm and 1,900–1,950 nm are often applied for the quantitative analysis of water content in foods. A range of 1,600–2,500 nm was used in our analysis because information on oil and fatty acid composition is concentrated in this NIR region. Figure 2 shows the derivative spectra of in-shell Virginia and Valencia peanuts. In this figure, the NIR spectra show the peaks at 1,722, 1,735, 1,757, 1,768, 1,787, 2,127 and 2,144 nm for saturated and *trans* unsaturated fatty acids. The peaks at around 1,660 and 2,145 nm are due to *cis* unsaturation. All of these peaks appeared more clearly than in the primary spectra (Fig. 1). Figure 3 shows the regression coefficients of the calibration models obtained using the absorbance and its derivative developed using PLS. The wavelengths corresponding to many of the peaks appearing in this figure are related to the total oil and fatty acid compositions of the peanuts. The peaks at 1,600–1,800 nm and 2,100–2,400 nm contributed significantly to the regression coefficients of the calibration equation developed using the reference values obtained from the Soxtec and GC methods. Concentrations of total oil and fatty acid percentages are given in Tables 1 and 2, along with corresponding moisture percentages. R^2 and SEC values of these regression curves are given in Table 3. The RPD and SEP values of the validation set obtained using the calibration regression equation are given in Table 4.

Total Oil Calibration and Prediction

The NIR regions selected for total oil measurements were 1,600–1,800 nm and 2,100–2,400 nm, which correspond to the oil absorption bands in the NIR region [17]. Table 2 shows the fitness measures for the calibration groups. Calibration models developed using absorbance and reflectance gave an R^2 value of 0.99 for both peanut types with low SEC values. Table 3 shows the fitness measures

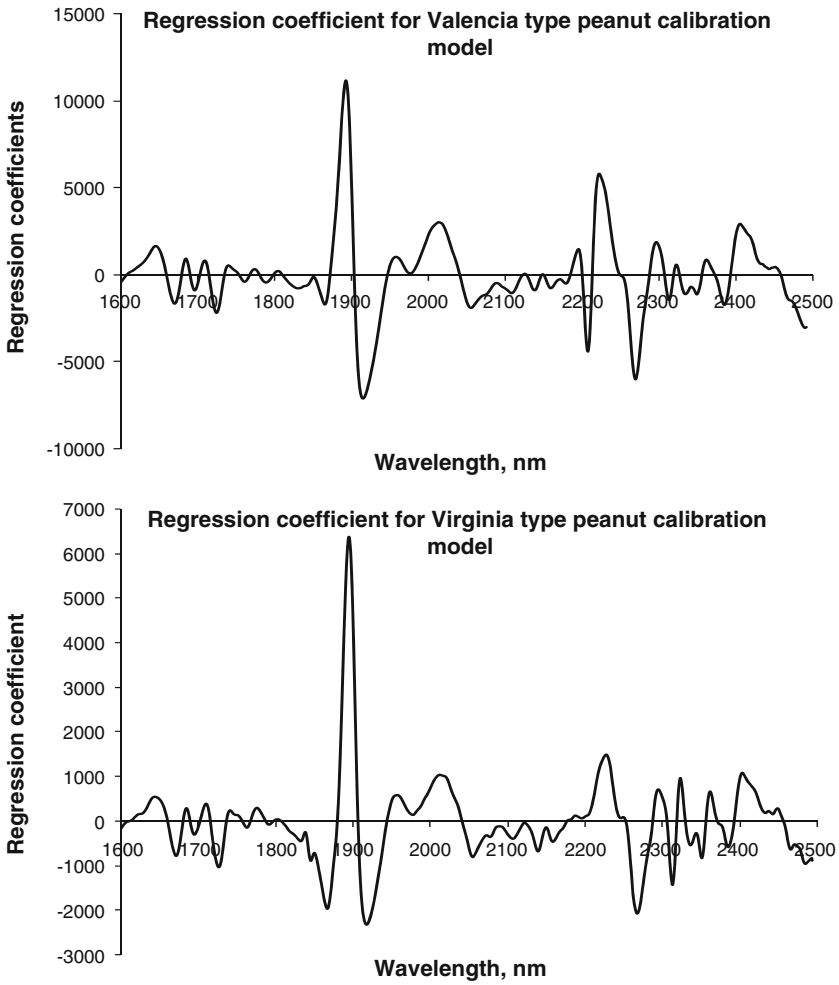

Fig. 3 Representative graphs of the regression coefficients of the calibration models used for total oil prediction

for the validation groups. RPD values were calculated to find the goodness of fit of the calibration model. For Virginia-type in-shell peanuts, RPD values of >5.0 were obtained using both absorbance and reflectance data, which showed that these models should work well for quality control and analysis. Based on the SEP values of 2.77 for absorbance and 1.65 for reflectance, the model developed from the reflectance data was selected as the best model for predicting the total oil of the Virginia-type peanuts. For Valencia-type in-shell peanuts, neither the absorbance nor the reflectance data models were suitable for quality control and analysis. The model developed using absorbance data gave an RPD value of 3.01, so it could be used for the initial screening of peanuts. Though the reflectance model's RPD value of 2.77 was not less than 1.0, it could not be considered a valid model for total oil prediction.

A graphical comparison between the reference and NIR-predicted values obtained using regression equations and validation datasets is shown in Fig. 4. This figure shows the predicted total oil percentage values obtained from 30 replicates of a validation set and three replicates of Soxtec-measured values. Excellent correlation between the predicted and reference total oil values of Valencia- and Virginia-type in-shell peanuts was achieved. Both NIR absorption and reflection derivative data resulted in R^2 values in excess of 95% with the exception of the reflection derivative data of Valencia-type peanuts. For Valencia-type peanuts, the absorption derivative model fitted the data very well, with an R^2 value of over 98%, but the R^2 value for the reflectance derivative model was only 86%. Based on the SEP of 4.58 and RPD of 2.77, as shown in Table 3, for Valencia in-shell peanuts, the model developed using reflection derivative data cannot be considered a valid model for initial screening or quality control and analysis.

Fatty Acids

The NIR region selected for fatty acid analysis was 1,600–1,800 nm because this region contains absorption bands for *cis* unsaturation and fatty acid carbon chains [18]. The relative amounts of the individual fatty acids were less than the total oil and moisture concentrations. Thus, the spectral characteristics were dominated by the oil and moisture

Table 1 Fatty acid and oil concentrations of peanuts measured by standard analytical methods and the NIR method for the calibration groups

MC %	Total oil %		Oleic acid		Linoleic acid		Linolenic acid		Palmitic acid		Stearic acid	
	Soxtec	NIR	GC[a]	NIR	GC[a]	NIR	GC[a]	NIR	GC[a]	NIR	GC[a]	NIR
Valencia												
6.18	46.43	46.43	54.57	54.53	22.26	22.38	1.18	1.17	11.39	11.40	3.37	3.37
10.07	44.43	44.41	47.45	47.52	29.71	29.53	1.23	1.23	11.03	11.02	3.32	3.31
13.10	43.74	43.75	39.95	39.90	36.84	36.91	1.28	1.28	11.03	11.04	3.13	3.13
15.74	43.09	43.08	40.13	40.18	37.00	36.97	1.28	1.29	10.85	10.86	3.20	3.19
18.28	42.47	42.47	52.28	52.25	25.37	25.32	1.27	1.13	10.21	10.20	3.72	3.73
19.33	40.82	40.84	51.62	51.57	26.87	26.88	1.11	1.11	10.25	10.26	3.41	3.42
21.69	38.38	38.37	51.29	51.35	27.10	27.18	1.11	1.11	10.33	10.32	3.40	3.40
Virginia												
6.90	46.24	46.24	64.44	64.43	15.90	15.89	1.29	1.29	7.70	7.69	3.46	3.45
10.80	44.12	44.12	64.36	64.37	15.91	15.91	1.39	1.39	7.53	7.54	3.67	3.67
14.90	42.01	42.00	63.79	63.78	14.66	14.66	1.24	1.24	7.36	7.35	3.85	3.86
15.80	38.48	38.48	65.31	65.30	15.33	15.33	1.25	1.25	7.80	7.80	3.49	3.48
19.40	35.18	35.18	63.89	63.92	16.61	16.61	1.30	1.30	8.27	8.29	3.23	3.24
22.28	34.37	34.37	64.57	64.56	16.06	16.06	1.21	1.21	8.20	8.19	3.49	3.49
23.70	35.02	35.02	66.22	66.22	15.22	15.22	1.32	1.32	7.81	7.80	3.46	3.46
26.70	30.75	30.75	65.46	65.46	15.18	15.18	1.33	1.33	7.67	7.67	3.33	3.33

MC, moisture content

[a] All values are averages of three replicates

Table 2 Fatty acid and oil concentrations of peanuts, as measured by standard analytical methods, for the validation groups (all values are averages of three replicates)

Moisture content (%)	Total oil (%)	Oleic acid	Linoleic acid	Linolenic acid	Palmitic acid	Stearic acid
Valencia						
7.40	45.16	53.22	25.65	1.01	12.41	3.14
12.18	44.07	51.62	27.89	1.10	10.12	3.14
14.61	43.27	51.95	26.63	1.12	10.16	3.43
18.77	42.43	40.32	37.17	1.29	10.66	3.26
20.90	39.60	51.45	26.98	1.11	10.29	3.41
Virginia						
7.60	45.12	63.14	17.13	1.40	7.66	3.49
11.30	43.97	63.41	15.22	1.26	7.51	3.29
14.05	42.23	63.26	16.52	1.35	7.50	3.53
15.00	41.94	61.64	18.12	1.30	7.93	3.37
15.44	41.45	64.79	15.61	1.24	7.83	3.72
18.81	38.62	64.53	15.35	1.23	8.17	3.65
22.80	34.37	61.63	11.36	1.24	9.21	4.60

Table 3 Fitness measurements for total oil and fatty acids of the calibration groups

Composition	Absorbance derivative spectra						Reflectance derivative spectra					
	Virginia			Valencia			Virginia			Valencia		
	R^2	SEC	Bias	R^2	SEC	Bias	R^2	SEC	Bias	R^2	SEC	Bias
Total oil	0.99	0.005	-3×10^{-5}	0.99	0.01	-1×10^{-3}	0.99	0.03	-3×10^{-4}	0.99	0.03	-4×10^{-3}
Oleic	0.99	0.015	5×10^{-5}	0.99	0.15	$+1 \times 10^{-2}$	0.99	0.05	2×10^{-4}	0.99	0.05	$+1 \times 10^{-2}$
Linoleic	0.99	1×10^{-4}	1×10^{-7}	0.99	0.17	-1×10^{-2}	0.99	2×10^{-4}	2.5×10^{-6}	0.99	0.11	$+3 \times 10^{-2}$
Linolenic	0.99	5×10^{-5}	3.4×10^{-7}	0.99	0.002	-1.4×10^{-5}	0.99	3×10^{-5}	$+5 \times 10^{-7}$	0.99	0.002	-6×10^{-5}
Palmitic	0.99	0.006	-1×10^{-5}	0.99	0.002	-3.3×10^{-6}	0.99	0.006	-8×10^{-5}	0.99	0.01	-1×10^{-2}
Stearic	0.99	0.004	3×10^{-6}	0.99	0.01	5.3×10^{-5}	0.99	0.007	-5×10^{-5}	0.99	0.002	$-6. \times 10^{-5}$

Table 4 Fitness measurements for total oil and fatty acids of validation groups

Composition	Absorbance derivative spectra						Reflectance derivative spectra					
	Virginia			Valencia			Virginia			Valencia		
	RPD	SEP	Bias	RPD	SEP	Bias	RPD	SEP	Bias	RPD	SEP	Bias
Total oil	6.2	2.77	−2.6	3.01	2.76	−1.42	6.06	1.65	−2.02	2.77	4.58	−1.75
Oleic	3.62	3.07	+1.3	3.41	4.15	−2.94	3.42	0.56	−0.20	3.72	4.48	−3.56
Linoleic	3.21	2.06	+0.05	2.50	0.18	+0.03	3.50	2.03	−0.32	2.30	7.66	−0.83
Linolenic	3.78	0.05	+0.01	3.02	6.19	−0.61	4.51	0.07	−0.03	2.80	0.23	+0.02
Palmitic	3.74	0.79	−0.16	2.90	1.01	−0.34	3.27	0.69	−0.40	2.85	1.56	−0.44
Stearic	3.36	0.51	−0.15	3.05	0.37	−0.015	3.01	0.52	−0.23	3.02	0.53	−0.05

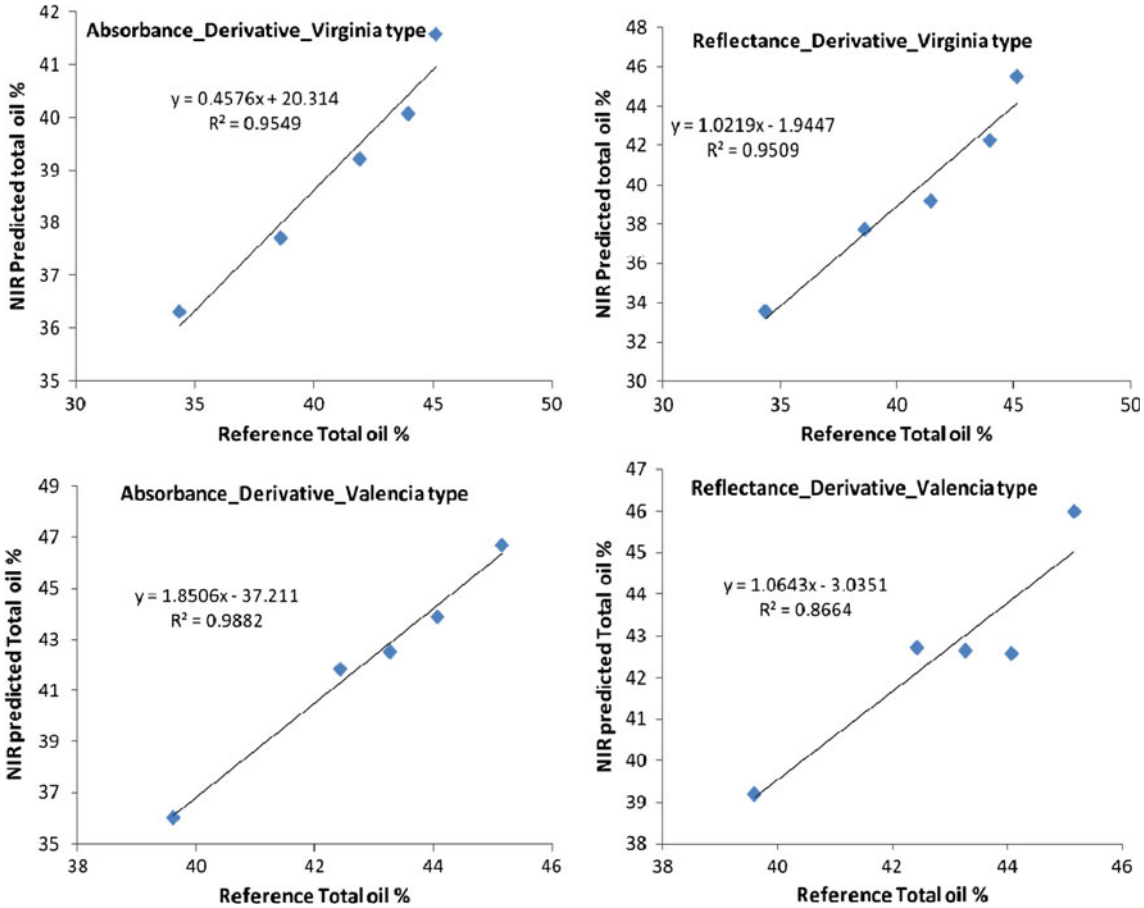

Fig. 4 Comparison of wt% total oil values predicted by NIR and measured by Soxtec for Virginia- and Valencia-type in-shell peanuts

concentrations. Therefore, the second derivatives of the NIR spectral data were used to determine the fatty acids. The predominant fatty acids present in the peanuts taken for analysis included oleic, linoleic, linolenic, palmitic and stearic acids. Table 1 shows the GC- and NIR-measured fatty acid concentration percentages of the calibration group of each type of peanut, and Table 2 shows the GC-measured value of the validation group of each type of peanut. Table 3 shows the fitness measures of the calibration groups. Calibration models developed using absorbance and reflectance gave R^2 values of 0.99 for both peanut types and all fatty acids. Their SEC values were also low. Based on the guidelines for interpreting R^2 outlined by Williams and Norris [19], NIR calibration equations for fatty acids were usable for quality assurance applications.

Table 4 shows the fitness measures for the validation group peanuts. The predictive ability of fatty acids based

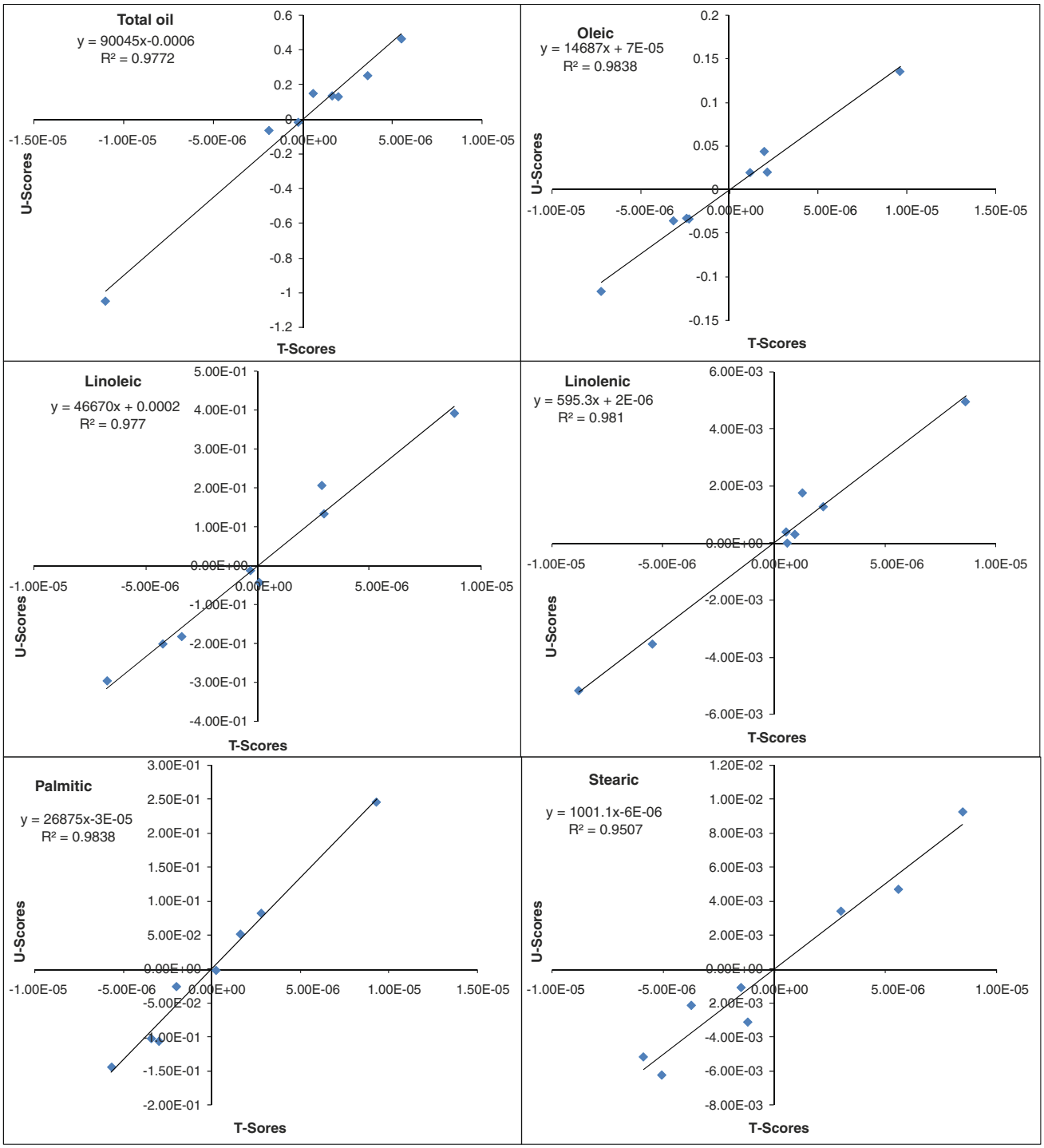

Fig. 5 Outliers for the relationship between Virginia-type peanut composition (*Y*) and wavelength (*X*)

on their RPD values varies from 2.3 to 3.41 for Valencia-type and 3.01 to 4.51 for Virginia-type peanuts. Models for the fatty acids had lower predictive power (low RPD values), and no model could be used for quality control and analysis. However, they could still be used for sample screening, except for the palmitic and linoleic acids in Valencia-type peanuts. A previous study by Pazdernik et al. [20] on the applicability of NIR spectroscopy to fatty acid composition determination in soybeans resulted in validation R^2 values of 0.18 (palmitic), 0.54 (stearic), 0.38 (oleic), 0.52 (linoleic), and 0.56 (linolenic) for whole-seed samples. For Virginia-type in-shell peanuts, both absorbance and reflectance data models gave RPD values of greater than 3.01 for all five fatty acids selected, which is

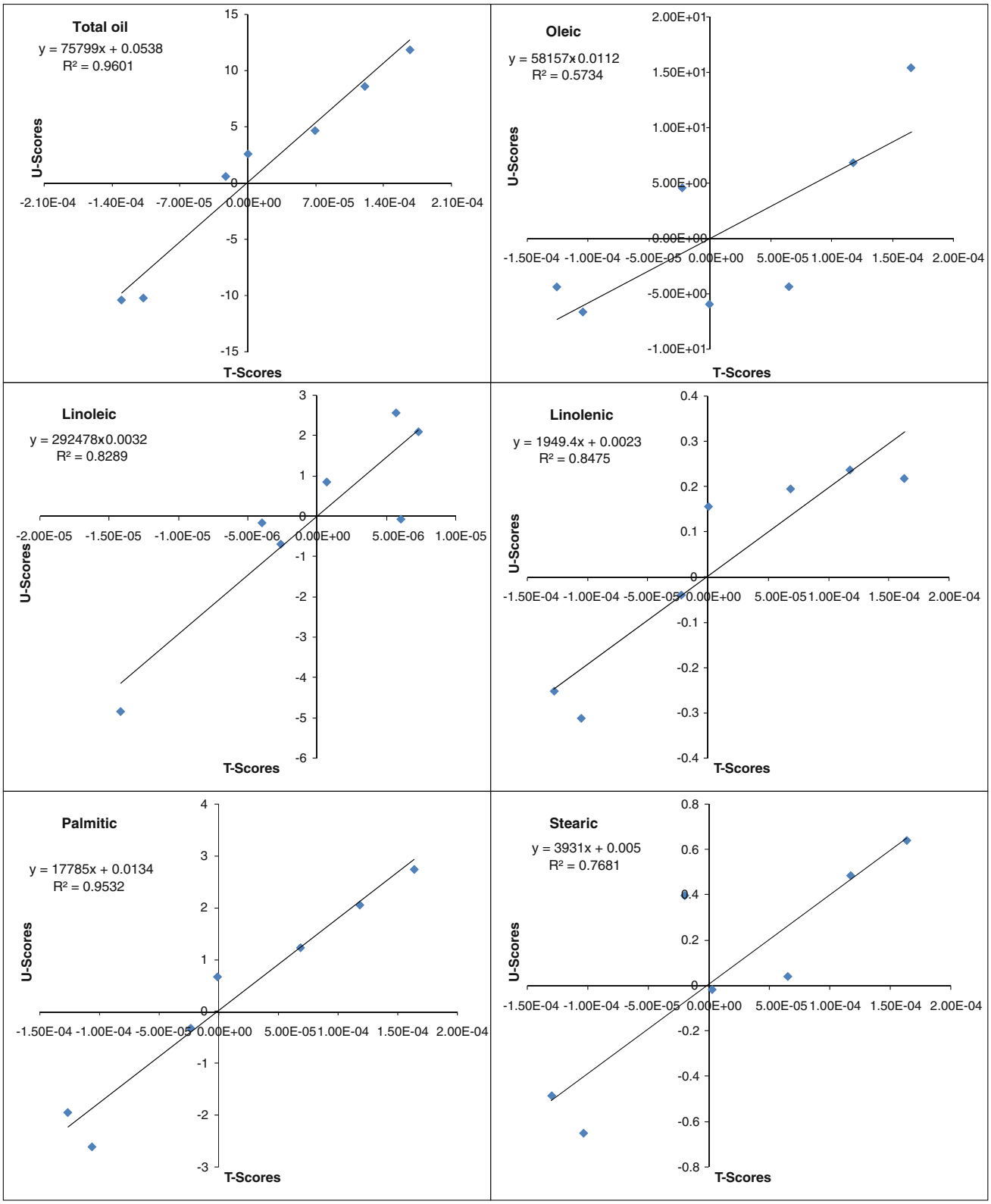

Fig. 6 Outliers for the relationship between Valencia-type peanut composition (*Y*) and wavelength (*X*)

suitable for the initial screening of peanuts. For Valencia-type peanuts, both models were suitable for screening purposes based on the RPD values for oleic and stearic acids. For linolenic acid, only the absorbance model could be used. No model is valid for linoleic and palmitic acids in Valencia-type peanuts. However, since models for these

fatty acids had lower RPD values, they could still be used for sample screening—an essential task in breeding. Most of the variation in the RPD values of NIR calibration models could be explained by the standard deviation of the reference data used in the calibration group. Therefore, by introducing a larger number of samples with very high and low values of fatty acids into the corresponding calibration data sets, the predictive ability of NIR spectroscopy for these constituents can be improved. Validation results also showed that RPD values of the NIR calibration equations were not dependent on the correlation between the total oil and the relative fatty acid concentration.

The relationship between the peanut composition—i.e., total oil and fatty acids (Y)—and the wavelength (X) in the NIR region can be explained by plotting the T and U scores of the calibration model developed using PLS regression (Figs. 5, 6). Regression was done to describe and interpret the relationship between the X and Y variables and to predict the Y values of new samples from the values of the X variable. Figure 5 shows the T and U scores of the PLS calibration model developed for Virginia-type peanut total oil and fatty acids. The basic assumption used in PLS analysis was that the relationship between the X and Y variables is linear. Any deviation from that assumption could result in calibration or prediction error. The linearity was evaluated using an X–Y outlier plot (Fig. 5). This shows that all of the components (Y) have linear relationships with wavelength (X); the regression coefficients are more than 97%, except for stearic acid (95%). This explains the accuracy of the calibration models that were developed to predict peanut composition. Figure 6 shows the T and U scores of the PLS calibration model developed for Valencia-type peanut total oil and fatty acids. Except for oleic acid, all of the other acids gave high regression coefficients of more than 77%. Oleic acid shows some outliers that were not fitted well by the model. Though it did not show much linearity, the calibration model developed for oleic acid gave a coefficient of determination for prediction of 0.99 (Table 2).

Conclusions

NIR reflectance spectroscopy could be a useful tool for the analysis of total oil and fatty acid concentrations of in-shell peanuts with minimal sample preparation. NIR measurement is procedurally very simple, considerably reducing the time required for composition measurements compared to standard analytical procedures. The use of NIR spectroscopy as described in this paper would result in significant savings in time and labor during the grading and processing of peanuts. RPD values of Virginia-type in-shell peanuts showed that the calibration models developed using both reflection and absorption derivative data were good enough to be able to use them to accurately predict total oil and fatty acid percentages. For Valencia in-shell peanuts, parameters such as total oil, oleic, linolenic and stearic acids gave safe RPD values, above 3. With further improvements to the analysis of NIR data, it will be possible to predict the fatty acid composition with sufficient accuracy for quality control purposes.

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