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Use of Near-Infrared Spectroscopy and Chemometrics for the Nondestructive Identification of Concealed Damage in Raw Almonds (*Prunus dulcis*)

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ABSTRACT: Concealed damage (CD) is defined as a brown discoloration of the kernel interior (nutmeat) that appears only after moderate to high heat treatment (e.g., blanching, drying, roasting, etc.). Raw almonds with CD have no visible defects before heat treatment. Currently, there are no screening methods available for detecting CD in raw almonds. Herein, the feasibility of using near-infrared (NIR) spectroscopy between 1125 and 2153 nm for the detection of CD in almonds is demonstrated. Almond kernels with CD have less NIR absorbance in the region related with oil, protein, and carbohydrates. With the use of partial least squares discriminant analysis (PLS-DA) and selection of specific wavelengths, three classification models were developed. The calibration models have false-positive and false-negative error rates ranging between 12.4 and 16.1% and between 10.6 and 17.2%, respectively. The percent error rates ranged between 8.2 and 9.2%. Second-derivative preprocessing of the selected wavelength resulted in the most robust predictive model.

KEYWORDS: *Prunus dulcis, almond, concealed damage, near-infrared spectroscopy, partial least squares regression, discriminant analysis*

INTRODUCTION

Concealed damage (CD) in raw almonds [*Prunus dulcis* (Mill.) D.A. Webb] is defined by the industry as a brown discoloration of the kernel interior (nutmeat) that appears only after moderate to high heat treatment (e.g., blanching, drying, roasting, etc.,), as shown in Figure 1. CD may develop anytime during harvest when rain occurs or after harvest when kernels are in windrows or stockpiles and exposed to warm and moist environments.[1,2] Raw almond kernels with CD have no visible defects on the interior or exterior surface of the kernel. Additionally, there are no visible signs of CD on the surface of whole roasted kernels.[3] CD is frequently associated with a strong bitter flavor(s) that can result in immediate consumer rejection.[1] Currently, there are no screening methods available for detecting CD in raw almonds or other nuts affected by CD, and processors often do not realize nuts are damaged until after they have been roasted.[1] Under current production practices, the most common methods for detecting CD involve visual inspection of roasted almonds after they are split open. Kernels with a "dark brown" color over ∼50% of the interior of the kernel are considered to have CD.[4] A similar approach is used for hazelnuts.[5] Visual inspection and manual sorting is time-consuming, subjective, and labor-intensive and cannot be used to identify nuts with CD before heat treatments. This can result in significant product loss.

The current hypothesis is that the browning associated with CD is related to the Maillard reaction. Moisture can induced the hydrolysis of carbohydrates and potential availability of reducing sugars for Maillard browning reactions. For example, in macadamia nuts exposed to moisture during harvesting, increased levels of reducing sugars were observed in nuts with internal browning.[6] Similar observations were made in hazelnuts[7] and in almonds exposed to simulated rainfall.[2] In more recent studies, elevated levels of volatiles related to lipid oxidation and amino acid degradation were observed in almonds with CD.[8] Both lipid oxidation products and protein degradation products can serve as reactants in the Maillard browning reaction.

Near-infrared (NIR) spectroscopy is a rapid and effective method for screening foods for specific chemical and physical characteristics.[9] NIR is advantageous as a screening method because it is nondestructive, can be used on whole foods, and produces no waste. The NIR spectral region (720−2500 nm) is ideally suited for foods because it contains absorbance bands that result primarily from three chemical bonds: C−H (fats, oil, and hydrocarbons), O−H (water and alcohol), and N−H (protein). NIR spectroscopy is increasingly considered one of the more promising in-line detection methods for rapidly measuring specific chemical properties of food.[6] It has been successfully applied in detecting quality defects in macadamia kernels,[7] walnuts,[10] chestnut,[11,12] hazelnuts,[13,14] and soybean seed.[15] It has also been employed for food composition analysis, including oleic and linoleic acid content in peanut seed,[16] acidity and water content in hazelnuts,[17] and characterization of shea tree nut fat profiles.[18]

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Figure 1. Color development in raw and roasted almonds (120 °C for 90 min) exposed to 5% moisture (control) and 11% moisture (CD).

Pearson was the first to recognize the use of NIR spectroscopy for the identification of CD in raw almonds[4,19] and evaluated the transmission spectrum from 700 to 1400 nm in almonds soaked in water and dried but not roasted. In these studies, almonds were either soaked for 30 min and exposed to 95% relative humidity for 30 h (short moisture) or soaked for 60 min and exposed to 95% relative humidity for 60 h (long moisture). Almonds were then dried at either 55 or 110 °C. The higher temperature and shorter soak times produced the greatest amount of CD. Almonds with CD had enhanced absorption at 930 nm (oil absorption band). Raw almonds with CD could be distinguished from normal almonds at an error of 12.4% using principal components of the absorbance, first- and second-derivative spectra between 1000 and 1300 nm. Pearson recognized that collecting the NIR spectra over the full transmission range would be too slow to achieve desired inspection rates of 40 nuts/s and, therefore, tested the feasibility of using just six light-emitting diodes at 660, 830, 880, 890, 940, and 950 nm.[19] These data resulted in a classification error rate of 14.3% for the validation set. More recently, Nakariyakul[20,21] achieved a higher classification rate using hyperspectral transmission and focusing on a subset of absorbing bands (760, 920, 935, and 970 nm) with a false-negative (fn) error rate of 14.81%. Almonds used in this study were generated by Pearson, as described above.

Herein, we present the development of a prediction model for the classification of almonds with CD using reflectance NIR in the extended range of the NIR spectrum (1125−2153 nm) and employing data preprocessing and partial least squares discriminant analysis (PLS-DA). Almonds evaluated in this study were exposed to controlled humidity environments that produced an internal nut moisture content of ∼5% (control), 8% (mild CD), and 11% (100% CD). The percent CD in the raw almonds was validated using colorimetry as described previously.[8]

Developing a rapid in-line screening method for detecting CD in raw almonds is a critical step toward improving quality control measures in almond processing and offers the advantage of sorting almonds with CD into product lines that do not require roasting or other heat treatments.

MATERIALS AND METHODS

Sample Preparation. Dehulled raw kernels (100 lbs, var. Nonpareil) were supplied by the Nickels Soil lab (Arbuckle, CA) in September 2013. Individual vessels containing ∼100 g were exposed to conditions that produced an internal kernel moisture of 5% (actual 5.4 ± 0.2%), 8% (actual 8.6 ± 0.7%), or 11% (actual 10.4 ± 1.5%) in a controlled atmosphere (Thermo Scientific, Marietta, OH) at 45 ± 2 °C. Under these conditions, CD is observed after 24 h. The moisture content of the almonds was validated gravimetrically by drying samples (∼1 g) at 95−105 °C under vacuum to a constant weight. Moisture was determined in triplicate, and the results were averaged.

NIR Reflectance Spectra Measurement. NIR diffuse reflectance spectra were measured on single whole raw almond kernels using an extended MicroNIR 2200 spectrometer (JDSU, Milpitas, CA). The spectral range was collected from 1125 to 2153 nm using sampling intervals of 8 nm per pixel. The detector used was a 128 pixel uncooled element InGaAs (JDSU, Milpitas, CA). Reflectance spectra data (R) were converted to absorbance using the log ($1/R$) transformation. A Spectralon SRM-99 diffuse reflectance standard (Labsphere, North Sutton, NH) was used as white calibration reference. For each spectrum, 1000 scans with an integration time of 550 μs were averaged.

Data Preprocessing. NIR spectra are complex with broad overlapping NIR absorption bands, making it often difficult to identify unique spectral features related to individual chemical components within a given sample. Therefore, a mathematical treatment (preprocessing) of NIR spectra is often used to correct for unwanted systematic sample-to-sample variation (e.g., kernel shape and roughness of kernel surface), to help remove spectral baseline shift and scattering caused by particle size differences, to reduce band overlapping, and to enhance spectral differences.[22] Data preprocessing results in relevant NIR spectral data extraction without losing information while removing unwanted information (e.g., interferences or noise).[22]

After the acquisition, NIR spectra were converted to absorbance and preprocessed using either standard normal variate (SNV) or a nine-point second-order Savitzky−Golay filter (second-derivative preprocessing). These two techniques alone and a combination were compared to determine their effectiveness at removing baseline offsets. Data preprocessing was performed using R and RStudio (version

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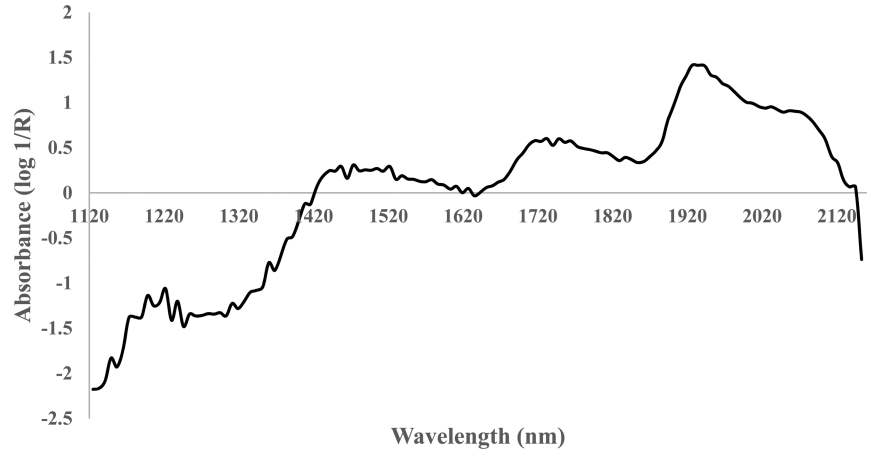

Figure 2. Mean SNV preprocessed absorbance spectra of almonds with NCD.

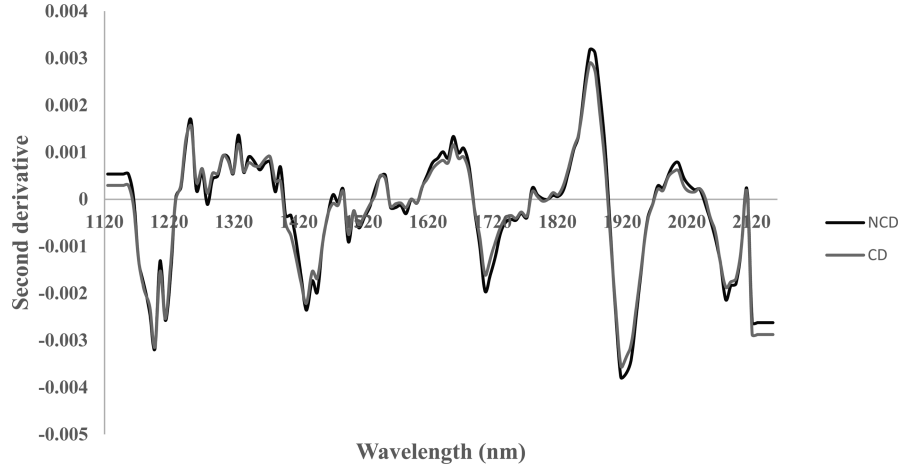

Figure 3. Comparison of the mean second-derivative (Savitzky–Golay, nine smoothing points) preprocessed spectra of almonds with NCD and CD.

0.98.1102). The following packages were used for preprocessing and PLS-DA: Chemometrics with R,[23] signal,[24] plyr,[25] dplyr,[26] and caret.[27]

Determination of CD by Colorimetry. After NIR spectra were acquired, the almonds were roasted at 120 °C for 90 min in a convection oven (Thermo Scientific, Waltham, MA). Almonds were then split in half along the natural seam, and the color of the internal kernel was measured using a ColorFlex colorimeter (HunterLab, Reston, VA) according to methods established previously.[8] The color values L^* (lightness), C (chroma), and h (hue), according to the CIE LCh color scale were recorded using a portsize of 0.4 in. with D65 optical sensor, 0° geometry, and 10° angle of vision. Almonds with CD ($L^* \leq 71$) were identified and grouped separately from those with no concealed damage (NCD; $L^* > 71$).[8]

Prediction of Almonds with CD. Preprocessed spectra (SNV, second derivative, and a combination of both) were analyzed using PLS-DA. Almonds were separated into two groups (NCD and CD) using colorimetry. The data set (855 almonds) was then randomly divided into calibration (655 almonds) and validation (200 almonds) sample sets. NCD and CD almonds were assigned constant values of 0 and 1 for a two-class model, respectively.

For the calibration model, repeated cross-validation was used to find the best model. Calibration models were evaluated on the basis of the percentage false positive (% fp), percentage false negative (% fn), and percentage error rate (% ER). A fn was defined as the percentage of NCD almonds classified as those with CD, while fp was defined as CD almonds classified as NCD. The % ER represents the percentage of total almonds incorrectly classified by the predictive method.[4,12]

RESULTS AND DISCUSSION

A representative NIR spectrum (1125–2153 nm) of the NCD almonds, after SNV preprocessing, is shown in Figure 2. The spectrum is characterized by broad and unresolved absorption bands and is similar to spectra for peanut,[28] walnut,[10]

Table 1. Results of the PLS-DA Model Using SNV, Second-Derivative, and SNV and Second-Derivative Preprocessing

	SNV	second derivative	second derivative + SNV
	(a) Calibration Model		
wavelength selected (nm)	1408–1465 1902–1959	1408–1465 1692–1740 1902–1959 2064–2104	1408–1465 1692–1740 1902–1959
number of latent variables	4	7	4
ROC[a]/% ER	0.908/9.2	0.918/8.2	0.918/8.2
specificity/% fn	0.839/16.1	0.876/12.4	0.840/16.0
selectivity/% fp	0.874/12.6	0.828/17.2	0.894/10.6
	(b) Validation Model		
% ER	9	7	9
% fp	8	8	9
% fn	11	6	7

[a]Area under the receiver operating characteristics.

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Table 2. Comparison of NIR Validation Results between Methods Used in the Classification of Almond with CD

	Pearson[19]	Nakariyakul[20]	Nakariyakul[21]	results obtained herein[a]
range (nm)	700−1400	700−1400 (selected wavelength)	700−1400 (selected wavelength)	1125−2153 (selected wavelength)
% ER	12.4−27.5	5.8	8.8	8.2−9.2
% fp	0.7−5.4	2.91−3.41	0.58−1.74	12.4−16.1
% fn	11.1−23.8	14.81−62.96	31.48−53.70	10.6−17.2

[a]On the basis of calibration models.

macadamia,[7] and shea nut.[18] To enhance spectral features and compensate for baseline offsets, a second derivative of the absorbance data, with respect to wavelength, was calculated. In the second-derivative data, absorbance maxima are converted to minima (Figure 3). The NIR spectra obtained after applying the second derivative were characterized by 10 absorption bands. These bands correlate with the major constituents of raw almonds: lipid (50%), carbohydrates (~22%), and protein (~21%).[29] The absorption bands between 1165 and 1238 nm, between 1692 and 1740 nm, and between 2064 and 2104 nm are associated with lipids. These include the C−H (−CH) second overtone stretching band (1200−1214 nm),[30] the C−H ($-CH_2$) first overtone stretching band (1700−1724 nm),[6,31] and the C−H combination band (~2098 nm).[32] The absorption bands between 1408 and 1462 nm and between 1902 and 1959 nm are associated with the H−OH second overtone of water[18] as well with protein. The absorption bands between 1692 and 1740 nm and between 2064 and 2104 nm are associated with the absorption of protein (~1700−1850 nm) and amino acids (~2080 nm), respectively,[32] and the region between 1902 and 1959 nm correlates with water and amides (~1910−1920 nm).[32] Additionally, the absorption band between 2064 and 2104 nm can be associated with the O−H and carboxylic group (C═O−O) bands of carbohydrates.[31]

An overlay of the averaged second-derivative spectra for almonds classified as NCD and CD is also given in Figure 3. The main differences between the NCD and CD spectra occur at 1432, 1457, 1505, 1513, 1708, 1918, 2080, and 2096 nm. The absorption bands at 1432, 1457, 1505, 1513, and 1918 nm correspond to protein;[33] the absorption band at 1708 nm corresponds to free fatty acids and oil;[12,33] and the absorption bands at 2080 and 2096 nm correspond to carbohydrates. Almonds with CD present less absorbance in these regions, indicating that kernels display decreased levels of lipids, protein, and carbohydrates compared to controls. These results correspond to observations of King et al.,[34] who reported that almonds with CD have lower crude fat (oil) and total carbohydrates compared to almonds with NCD. Additionally, we recently demonstrated higher levels of volatiles related to lipid oxidation and amino acid degradation in almonds with CD compared to almonds with NCD.[8] Taken together, these results indicate the metabolic processes that activate the degradation of proteins, carbohydrates, and lipids are involved in the development of CD. The free amino acids, sugars, and products from the oxidation of lipids would be substrates for the Maillard reaction and support the hypothesis that the Maillard reaction is involved in the formation of CD in almonds.

Initially, multiple PLS-DA models were evaluated using the full wavelength region from 1125 to 2153 nm after data preprocessing (SNV, second derivative, and SNV and second derivative). In general, the best predictive models give low percentage error rates (i.e., the highest percentage of correct classification). Herein, we found that using the full wavelength region resulted in models with high percentage error rates, and therefore, PLS-DA models were developed using only relevant portions of the NIR spectra. Table 1 summarize the prediction performance of the calibration models and validation models, which were selected because they had the lowest % ER, % fp, and % fn rates. A large data set (200 samples) was analyzed to optimize the prediction models. The lowest % ER (8.2%) was obtained using only second-derivative preprocessing compared to 9.2% when using SNV preprocessing and 8.2% when using SNV and second derivative preprocessing. Although the % fp rate was higher for this model (17.2%) compared to the SNV (12.6%) and SNV and second-derivative preprocessing (10.6%), the % fn was significantly lower (12.4%) compared to these models (16%).

Previous studies employing infrared (IR) spectroscopy to build models to discriminate differences between CD and NCD focused on the absorbance range between 700 and 1400 nm[5] and selected wavelengths within the 700−1400 nm absorbance range.[20,21] Comparisons of these results to results obtained herein are summarized in Table 2. Although the rates of % fp were lower across these studies (0.7−5.4%) compared to our results (12.4−16.1%), the rates of % fn were significantly higher (11.1−62.96%) than those obtained using our predictive models (10.6−17.2%). Additionally, the % ER ranged from 5.8 to 27.5%, whereas our predictive models gave a much narrower range of 8.2−9.2%. The three PLS-DA models presented herein offer significant improvements in the prediction capabilities and are able to identify almonds with CD with 90.8−91.8% certainty based on calibration models. Although any of the three models presented could be considered for further development of a rapid in-line screening method for detecting CD in raw almonds, the PLS-DA model based on the second-derivative spectra and using four wavelength ranges (i.e., 1408−1462, 1692−1740, 1902−1959, and 2064−2104 nm) gives the lowest rate of % fn and may be the best choice for further method development.

Our results indicate that these PLS-DA predictive models offer advantages over previously reported models and that CD is related to the degradation of lipids, carbohydrates, and proteins in almonds.

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Notes

The authors declare no competing financial interest.

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■ ABBREVIATIONS USED

CD, concealed damage; NCD, no concealed damage; NIR, near infrared; SNV, standard normal variate; PLS, partial least squares; DA, discriminant analysis; fp, false positive; fn, false negative; % ER, percent error rate

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