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Discrimination of centre composition in panned chocolate goods using near infrared spectroscopy

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Abstract

Non-destructively identifying the centre composition of panned chocolate goods may be useful in quality assurance settings. However, no studies to date have investigated this topic. In this study, NIR spectra (1000-2500 nm) were collected from chocolate-coated peanuts and chocolate-coated sultanas (n=170 of each) in order to investigate the prospect of non-invasively detecting the composition of the centre. Principal component analysis (PCA) confirmed that the spectra of these samples were distinct from one another. Partial least squares discriminant analysis (PLS-DA) model showed a high level of separation between chocolate-coated peanuts and sultanas in the training set ($R^2 = 0.95$; RPD = 4.4). Discrimination between peanut and sultana samples from an independent test set was also possible, although with slightly less distinct separation between the sample types. A SIMCA model was also able to differentiate between the two sample types, albeit with higher levels of misclassification compared to PLS-DA. Incorporating samples from different manufacturers may be useful for improving the broader applicability of the model.

Keywords

Quality assurance; peanuts; cocoa; PLS-DA.

Introduction

Chocolate-coated nuts and fruit are a common snack food in Western society. The first commercial chocolate-coated peanuts are believed to have been produced by Blumenthal Brothers Chocolate & Cocoa Company in North Carolina in 1925, sold under the product name “Goobers”. Currently, the chocolate industry in Europe alone is valued at over $51 billion USD, with 90% of small and medium sized chocolate manufacturers in this region focusing almost exclusively on the production of filled chocolate products, which include coated nuts and fruit.[1]

Such chocolate-coated produce is usually manufactured through a process known as “chocolate panning”, whereby the chocolate coating is sequentially layered onto the centre in a rotating pan or drum.[2] Between each layer, adequate time is allowed for solidification, before addition of further layers until the desired size is reached.[3] The final product is then polished, glazed and varnished to seal the product, and to prevent the chocolate from melting on the consumer’s fingers.[4] For more information on the manufacturing process, the reader is referred to several recent reviews that cover this topic.[3-5]

Recent research on chocolate-coated produce has investigated the use of peanut skins for increasing the antioxidant and phenolic content of peanut coatings[6] and investigated the optimum package types for long-term storage of chocolate-coated fruits and nuts.[7] In another recent study, Raman spectroscopy was used to detect chocolate bloom on a range of chocolate samples, including chocolate covered macadamia nuts.[8] Detection of chocolate bloom is an important aspect of the quality assurance process, as its presence reduces the shelf-life of product and affects consumer acceptability.[9] Other problems that can occur with panned chocolates include incomplete or poor coverage, rough surfaces, peeling of the chocolate coating, crushed centres, and the production of “doubles”.[3]

Another aspect of quality assurance is determining the centre composition in the final chocolate-coated product. As shown in Figure 1, different products such as chocolate-coated peanuts and sultanas can be visually similar, making it difficult to confirm the identity of the manufactured product without resorting to destructive means. However, one non-invasive analytical technique which could show promise for this application is near infrared (NIR) spectroscopy, which uses electromagnetic wavelengths between 800-2500 nm to non-destructively gather chemical information about the sample composition. The penetration depth of infrared light is wavelength dependent, with a depth of 0.5-2.5 mm found in wheat flour between 1100–1350 nm.[10] However, the penetration depth may be different for the chocolate matrix.[11] As chocolate coatings are usually 1-2 mm thick, the NIR signal may include some information relating to the composition of the chocolate-coated centre. Notably, NIR spectroscopy has previously been applied to the detection of internal defects in intact macadamia kernels,[12, 13] demonstrating that this technique can be used to detect the internal nut composition through the kernel thickness.

Figure 1. The appearance of chocolate-coated peanuts and sultanas.

Near infrared spectroscopy has a long and successful history of use for quality assurance and process control in the food industry.[14-17] Although NIR spectroscopy has been used for various aspects of the quality assurance of chocolate, including prediction of sucrose content,[18] measurement of viscosity,[19] discrimination of chocolate varieties[20] and detection of contaminants including insects[21] and cocoa shell.[22] However, there does not appear to be any work to date investigating the non-destructive discrimination of the identity of chocolate-coated centres. This ability could be potentially useful for confirming product identity in post-manufacture settings. Consequently, the aim of this paper was to investigate the potential use of NIR spectroscopy for non-destructively discriminating between chocolate-coated peanuts and sultanas.

Methods

For calibration purposes, two batches of chocolate-coated peanuts and two batches of chocolate-coated sultanas (all Cadbury brand) were purchased from local grocery stores. For the peanuts, 120 samples were analysed from the first batch and 50 from the second batch, while 115 samples were analysed from the first batch of coated sultanas and 65 samples from the second batch. For the unknown samples (test set), a container of mixed Cadbury chocolate-coated fruit & nut was used. This product comprises chocolate-coated peanuts, sultanas, and almonds in a ratio of approximately 8:2:1. For the purposes of this study, the almonds were excluded from analysis.

The NIR spectra were acquired using the integrating sphere on a Thermo Scientific Antaris II FT-NIR Analyzer (Thermo Scientific, Watham, MA, USA), operating at wavelengths between 1000-2500 nm (10,000-4,000 cm^{-1}). The spectral resolution was 8 cm^{-1}, with 16 scans averaged for each spectra. The chocolate-coated samples were placed directly on top of the integrating sphere port, allowing spectra to be collected from the sample in reflectance mode. Although stray light was not eliminated, its potential effects were minimised by conducting all analyses in a controlled room with indirect fluorescent lighting. Spectra were collected in triplicate for each sample (removing and replacing the sample each time) and exported in *.csv format. Partial least squares discriminant analysis (PLS-DA) was performed in R Studio running R 4.0.5,[23] using the spectrolab, prospectr and plsr packages. SIMCA was performed using the mdatools package.[24] Pre-processing methods included SNV normalisation and 1st derivative using a Savitzky-Golay algorithm with 11 smoothing points. For the purposes of this portion of the study, the peanut-containing samples were coded as a value of “1”, while the sultana-containing samples were coded as “-1”. Consequently, the mean “reference value” of the calibration set was 0.00 and the standard deviation of the dataset was 1.00.

The experimental work was performed in several stages. The first step was to confirm whether NIR could in fact penetrate through the thickness of the chocolate coating. In order to assess this, NIR spectra were collected in triplicate from intact chocolate-coated peanut and sultana samples (n=5 samples for each). The chocolates were then cut open and the centre removed, before NIR spectra were collected from the hollow samples.

The second stage was to determine whether there was a detectable difference in the NIR spectra of the nut and fruit cores, which would be a necessary prerequisite to allow discrimination of these samples using NIR spectroscopy. Spectra were collected from one each of the peanut and sultana cores isolated in the previous step.

The third and major aim of the experimental work involved collecting NIR spectra from larger numbers of chocolate-coated peanuts and chocolate-coated sultanas (n=170 samples for each; sourced from two independent batches for each sample type). The data were used to create a discriminant calibration model.

Finally, an independent test set was used to confirm the accuracy of the calibration model. As previously mentioned, the test set was drawn from a mixed container of Cadbury chocolate-coated fruit & nut, from a different manufacturing batch to either the peanut or sultana samples (n=50 samples). Following collection of the NIR spectra, the identity of the centre composition (i.e. peanut or sultana) was confirmed by destructive organoleptic analysis (100% accuracy).

Results and Discussion

NIR spectra of intact and hollow chocolates

The mean NIR spectra of the intact and hollowed chocolate samples are shown in Figure 2. Overall, the appearance of the spectrum followed previous work on chocolate samples.[18, 25] The major peaks were located at 1215 nm (C-H second overtone), 1437 nm (O-H second overtone), 1729 nm (C-H first overtone), 1765 nm (C-H stretch first overtone), 1932 nm (amide first overtone) and 2083 nm (O-H combination), with smaller but sharp peaks at 1395 nm (C-H combination first overtone), 1692 nm (C-H first overtone) and 2019 nm (O-H asymmetric stretch).

There was some difference observed in the NIR signal between the intact and hollow samples, particularly for the peanut samples (Figure 2), most notably between 1300-2000 nm. However, there was less difference between the spectra from the intact and hollow sultana samples. Exploratory principal component analysis performed on the spectra revealed that the spectra for the hollow and intact sultana samples were quite similar to one another, while those for hollow and intact peanut samples were more distinct (Figure 3). This suggested that the peanut centres may be easier to detect through the chocolate coating using NIR spectroscopy compared to the sultana centres. However, the mean thickness of the chocolate layer did not vary significantly between the peanut samples (mean thickness of 1.9 ± 0.2 mm; n=5) and the sultana samples (mean thickness of 2.0 ± 0.2 mm; n=5) ($t_{7.99} = -1.129$, $P > 0.05$), indicating that the difficulty detecting in detecting the sultana cores is due to the greater similarity between their NIR spectra and the NIR spectra of the chocolate coating.

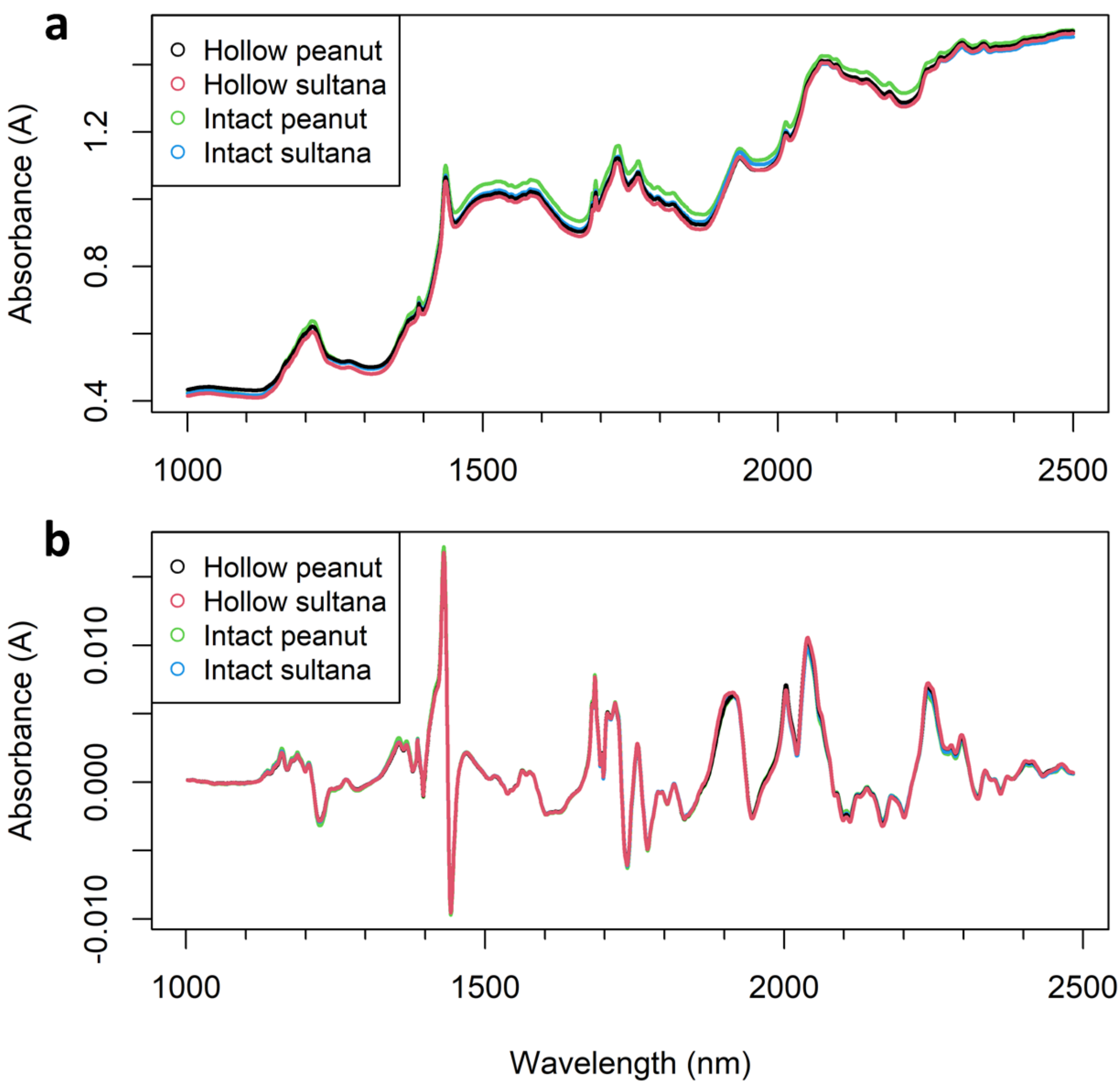

Figure 2. (a) Mean NIR spectra of chocolate-coated peanut and sultana samples, in addition to spectra from the same samples with the centres removed (n=15 spectra for each). (b) First derivative of the spectra.

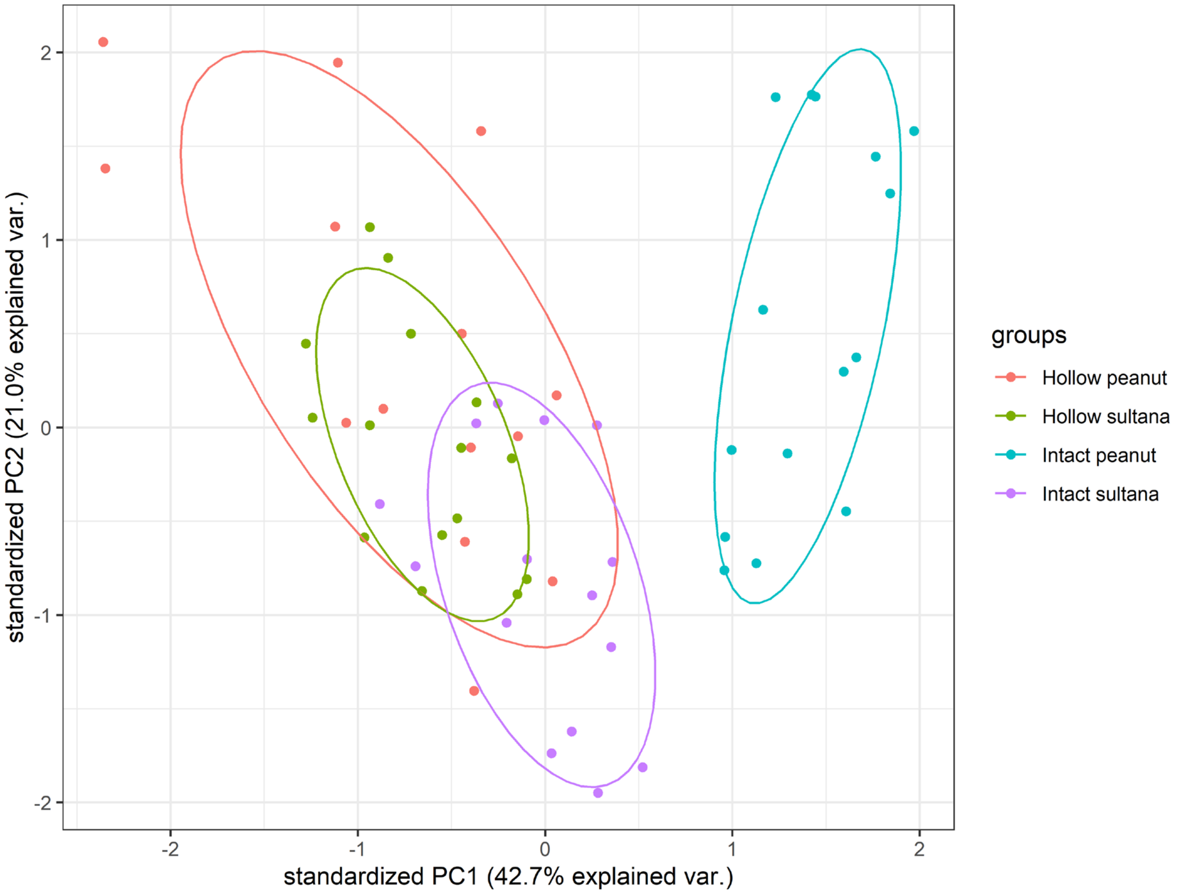

Figure 3. Scores plot showing the results of PCA performed on the first derivative of the intact and hollow sample spectra. Spectra are grouped by centre type (peanut or sultana) and hollow/intact.

NIR spectra of peanut and sultana centres

There was a clear difference in the NIR spectra of the non-coated peanut and sultana centres. The sultana spectra showed greater absorbance across the spectrum (Figure 4a), likely due to increased moisture content of the sample, as well as greater surface contact between the sample and the integrating sphere interface. The sultana spectra were dominated by water bands at 1200 and 1900-2100 nm, as well as a peak in the 1440 nm region due to sugars.[26] The peanut spectra were similar to that reported in previous work, with major peaks attributable to oil/fatty acids, protein and water.[27] The difference in spectral signatures was quite evident in the first derivative of the spectra (Figure

4b), confirming that if NIR spectroscopy can sufficiently penetrate through the thickness of the chocolate coating, then discrimination between these inclusion types should be feasible.

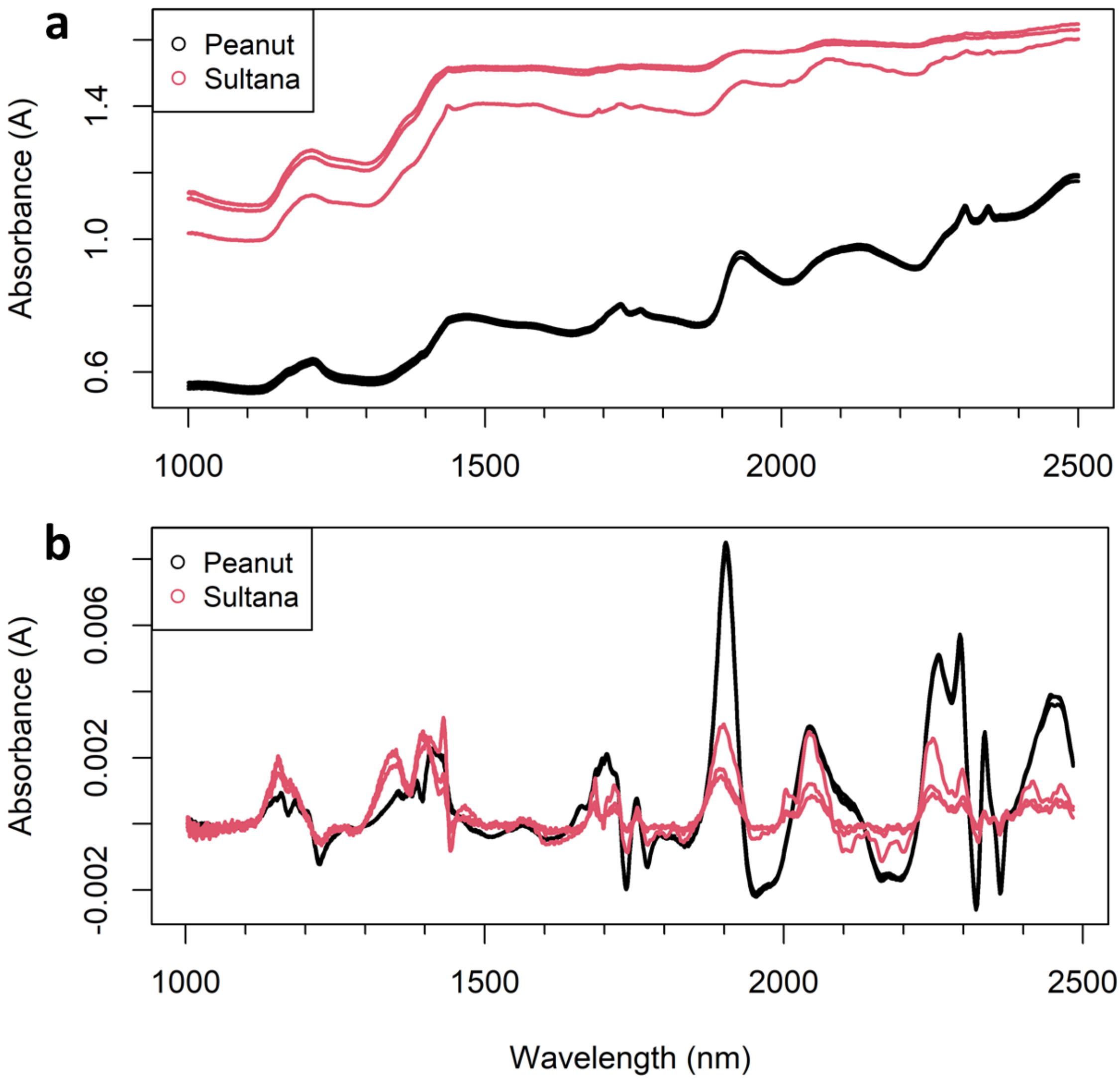

Figure 4. (a) NIR spectra of the uncoated peanut and sultana centres. (b) First derivative of the NIR spectra of the uncoated peanut and sultana centres.

Discrimination between chocolate-coated peanuts and sultanas

In the main portion of this study, NIR spectra were collected in triplicate from a total of 170 chocolate-coated peanuts (n=510 spectra) and 170 chocolate-coated sultanas (n=510 spectra), from a total of four different manufacturing batches. There was minimal variation visible between the first derivative of these spectra (calculated using the Savitzky-Golay algorithm with 11 smoothing points), as seen in Figure 5. However, principal component analysis performed on the first derivative showed relatively clear separation of these sample types across the first two principal components (PC-1 and PC-2) (Figure 6). There was some spectral variance between the two different manufacturing batches of each sample type, which was primarily found across PC-1 (Figure 6).

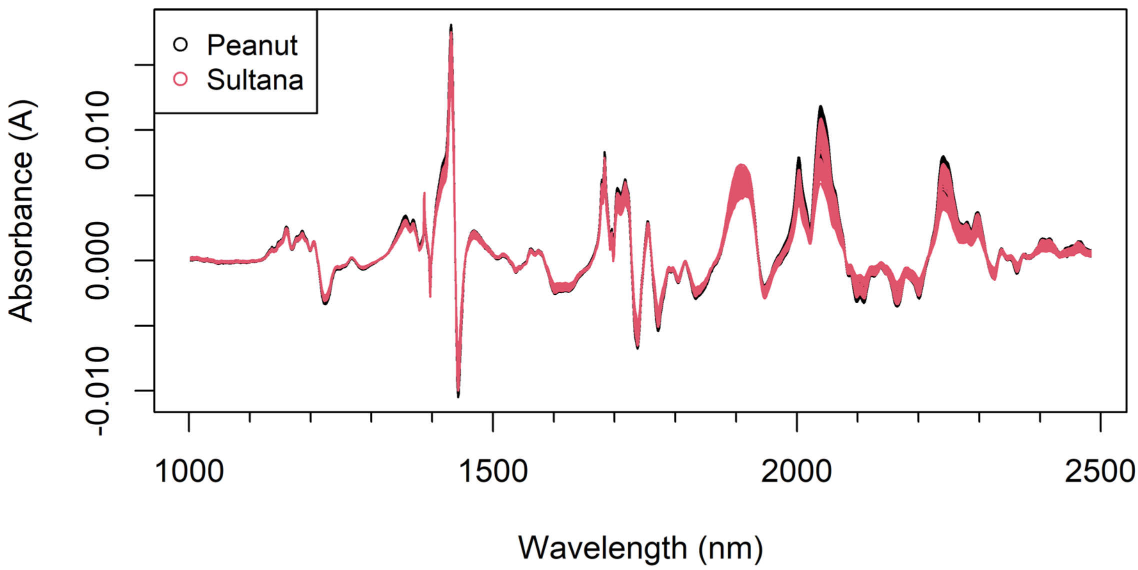

Figure 5. First derivative of the NIR spectra for the chocolate-coated peanut and sultana samples.

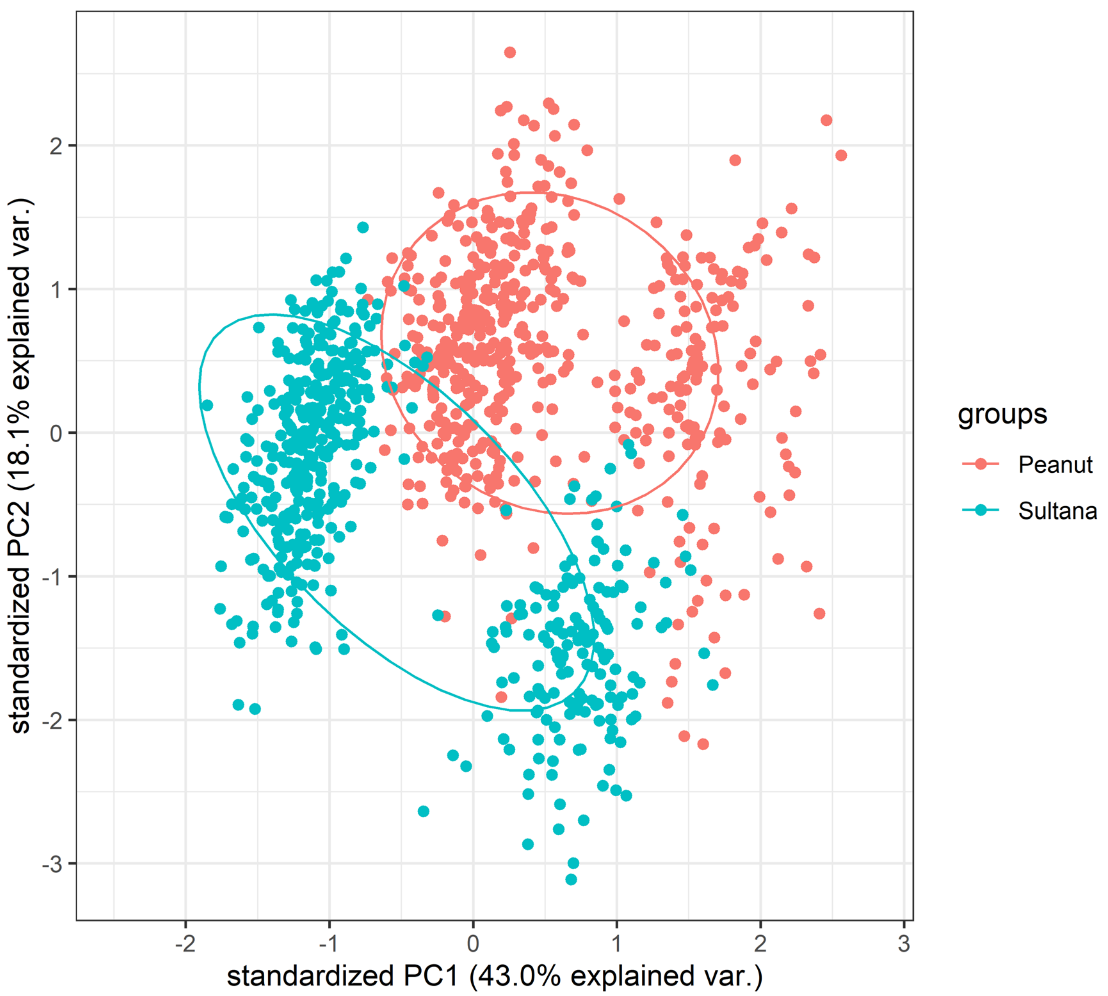

Figure 6. Scores plot showing the results of PCA performed on the first derivative of the NIR spectra.

Subsequently, partial least squares discriminant analysis (PLS-DA) was performed on the first derivative of the NIR spectra, using leave-one-out (LOO) cross-validation to optimise the number of latent variables.[28] The model performance as a function of the number of latent variables is presented in Table 1. To avoid over-fitting the model,[29] the RMSECV scree plot (Figure 7) was used to select 3 components as the optimum number of latent variables. The R^2_{cv} of this model was 0.949, with an RMSECV of 0.225 and RPD value of 4.44.

Table 1. Performance of the PLS-DA model using different numbers of latent variables.

Latent variables	Variance explained (%)		RMSECV	R^2_{CV}	RPD
	Spectra	Reference			
1	88.4	14.2	0.928	0.139	1.08
2	92.6	71.4	0.539	0.710	1.86
3	93.7	95.1	0.225	0.949	4.44
4	97.2	95.9	0.205	0.958	4.88
5	97.5	97.2	0.175	0.969	5.71
6	97.8	97.7	0.160	0.974	6.25
7	98.0	97.9	0.152	0.977	6.58
8	98.3	98.1	0.149	0.978	6.71
9	98.7	98.2	0.145	0.979	6.90
10	99.0	98.3	0.143	0.980	6.99

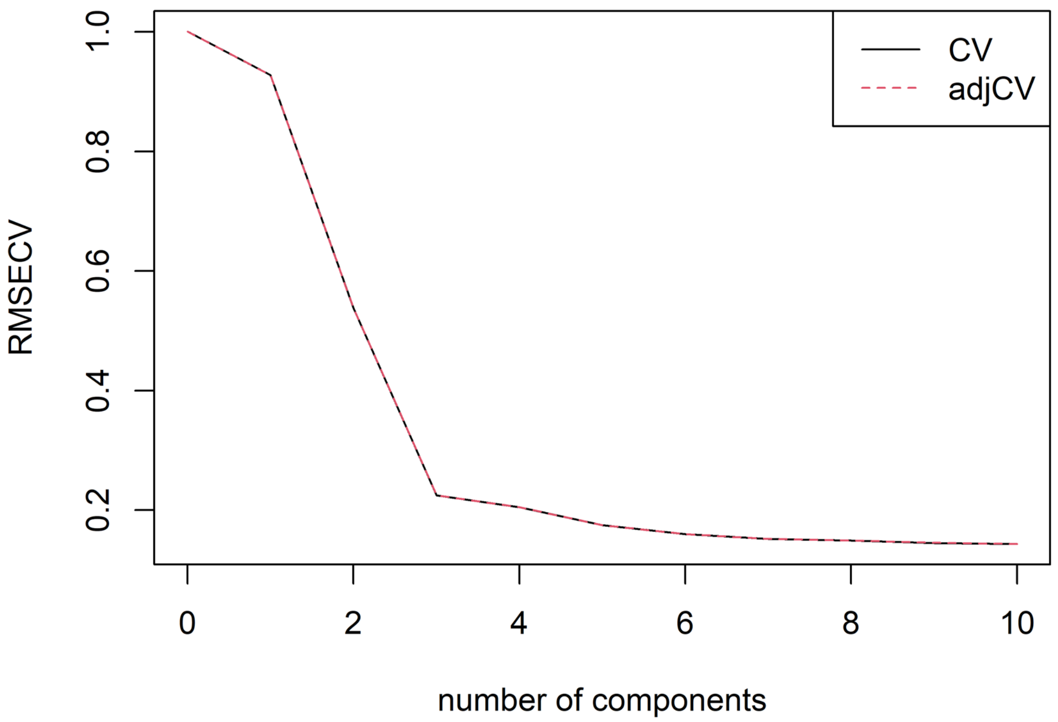

Figure 7. Scree plot showing the RMSECV values for different numbers of model components.

The cross-validated model predictions are shown in Figure 8. During the cross-validation process, all of the sultana samples were identified as belonging to the correct class, while three of the peanut spectra (from two different samples) were misclassified as being sultanas (Figure 8).

Examination of the loadings plot for the first component of the PLS-DA model (which explained 88% of the total spectral variance) revealed the most influential wavelengths to be located at 2040, 1431, 1685 and 2245 nm (Figure 9). These were attributed to the peaks resulting from O-H asymmetric stretch (2040 nm), O-H second overtone (1431 nm), C-H first overtone (1685 nm) and bonds associated with saturated and unsaturated triglycerides (2245 nm).[18, 25]

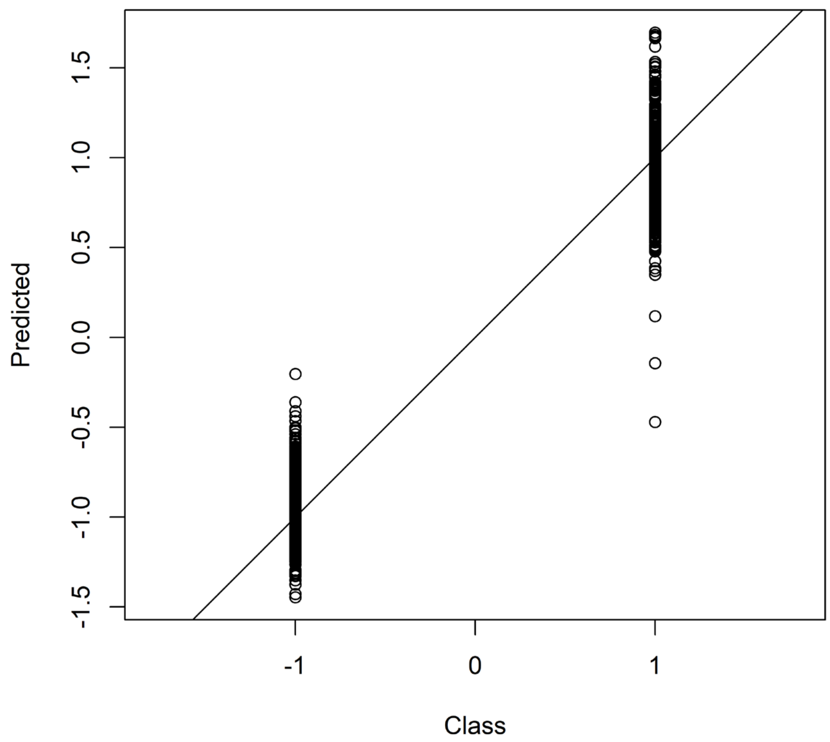

Figure 8. Cross-validated predictions of the PLS-DA model (3 components) calculated using the leave-one-out method. 1 = peanut, -1 = sultana

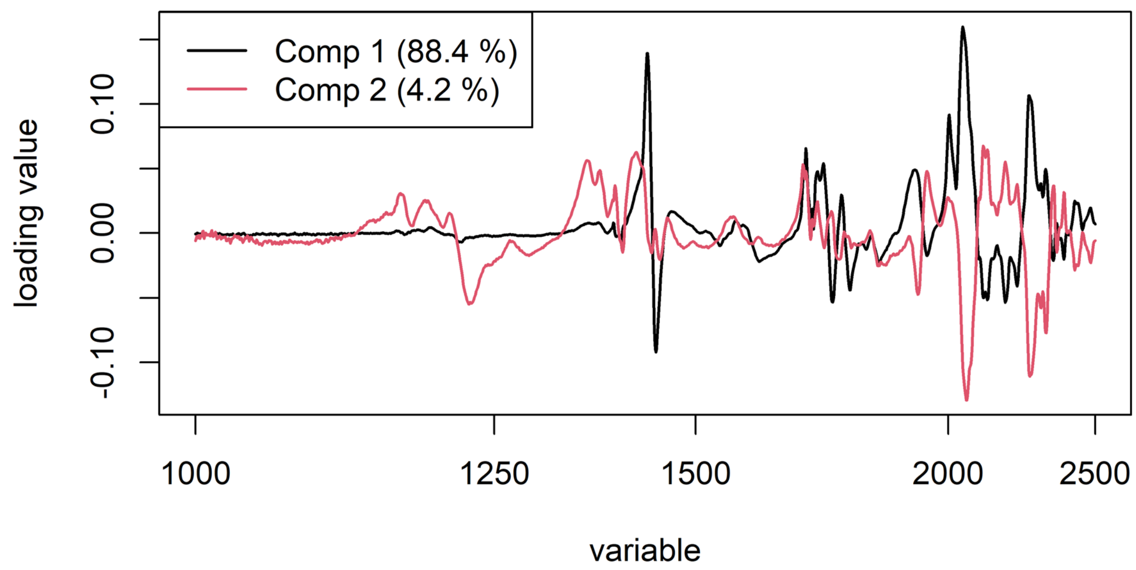

Figure 9. Loadings plot for the first two components of the PLS-DA model.

Independent test set

Finally, the PLS-DA model was applied to an independent test set, comprising 50 unknown samples of chocolate-coated peanuts or sultanas (comprising 11 sultana and 39 peanut samples for a total of n=150 spectra). All peanut samples were correctly classified (i.e. had a score > 0), while one spectra from one sultana sample was mis-classified as a peanut spectra (0.7% error). The PLS-DA prediction results for the chocolate-coated sultana samples gave a mean score of -0.29 ± 0.13, compared to a mean score of 0.61 ± 0.20 for the peanut samples (Figure 10), suggesting slightly poorer ability to discriminate between sample types in the independent test set. Nevertheless, the sample types were still clearly distinguishable from one another. It is possible that minor differences in the chocolate composition between the training and test batches may contribute to some of this error; however, the inclusion of multiple batches in the training set would be anticipated to reduce this effect. The risk of model over-fitting was considered low, given that the optimum number of components was chosen using the RMSECV scree plot to provide the best trade-off between the number of components and model accuracy. Using a higher or lower number of components did not improve the accuracy of the model performance on the independent test set, suggesting that under- or over-fitting was not an issue.

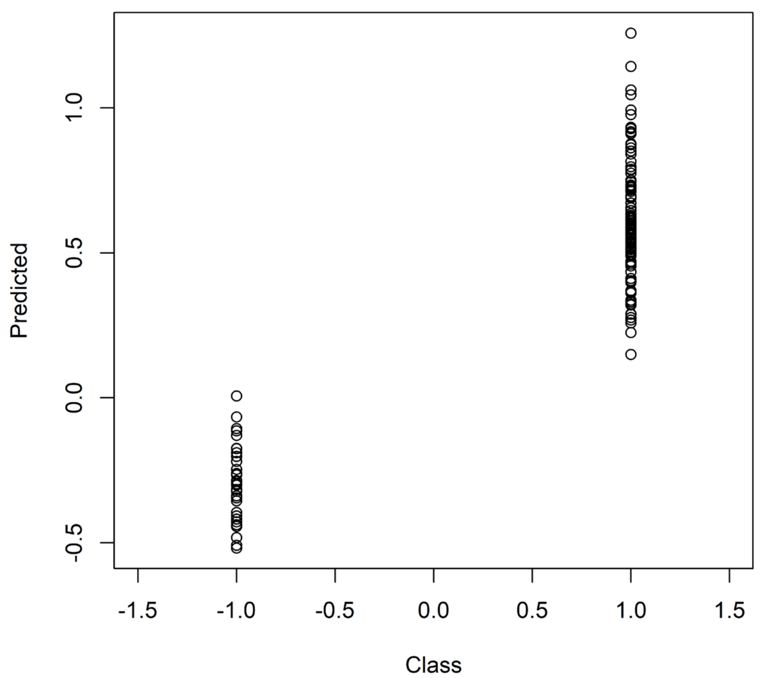

Figure 10. Prediction results for the application of the PLS-DA model to the independent test set. Each sultana-containing sample is indicated by a red ellipse. 1 = peanut, -1 = sultana

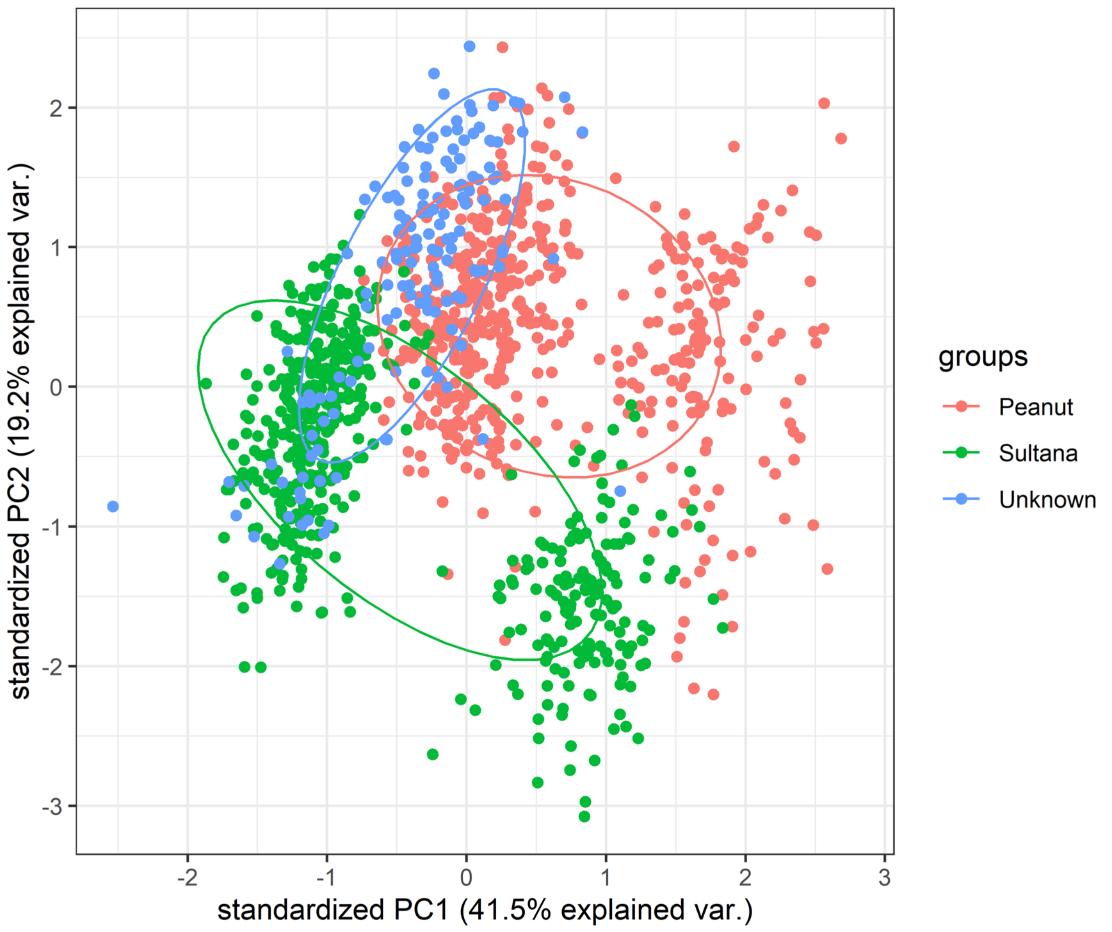

Figure 11. Scores plot showing a PCA performed on the first derivative of the NIR spectra from the independent test set, projected onto the PCA of the spectra from the calibration set.

SIMCA

As the unknown spectra showed considerable overlap when included in the PCA of the calibration spectra (Figure 11), soft independent modelling by class analogy (SIMCA) was investigated as an alternative classification method. A model created on the chocolate-coated peanut samples showed an optimum number of three components (Figure 12), with a classification accuracy of 0.959. When this model was extended to the full dataset, it showed a specificity of 0.836, sensitivity of 0.959 and accuracy of 0.890. The SIMCA model was able to correctly classify all of the chocolate-coated sultana samples, as well as correctly classify 94% of the peanuts and sultanas from the independent test set (Table 2). Similar to previous studies which have compared the performance of SIMCA and PLS-DA,[30, 31] both models appeared suitable for the discrimination of chocolate-coated peanuts and sultanas from their NIR spectra. However, the SIMCA results found here were slightly poorer than those from PLS-DA, supporting the use of the latter technique for future work.

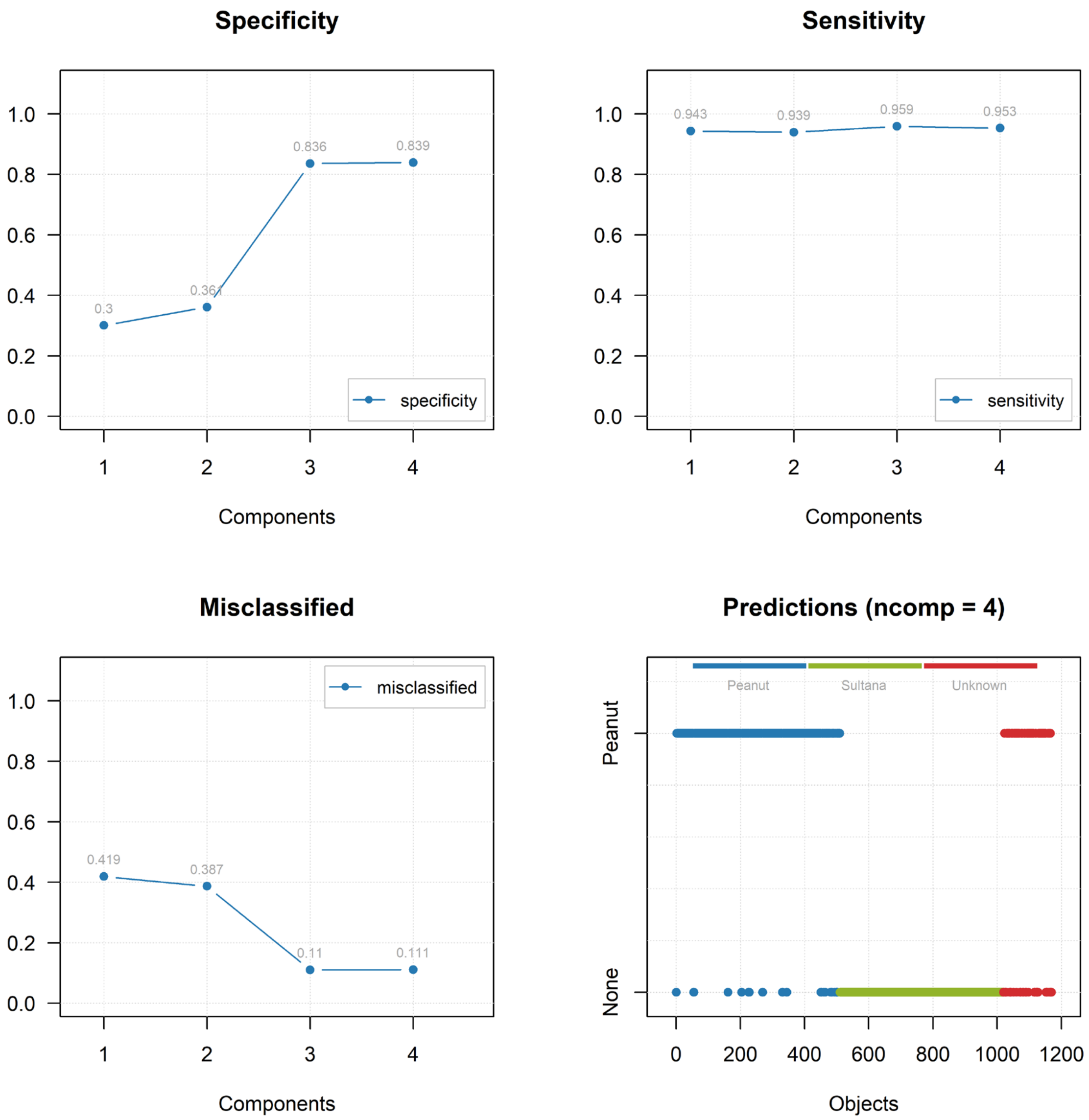

Figure 12. Summary of SIMCA results for the detection of chocolate-coated peanut samples.

Table 2. Confusion matrix for the SIMCA model (3 components).

	Real class	**Predicted class**	
		Peanut	Sultana
Calibration set	Peanut	489	21
	Sultana	0	509
Independent test set	Peanut	108	9
	Sultana	0	33

Overall, the results suggest that NIR spectroscopy has the ability to discriminate between chocolate-coated peanut and sultana samples with a high level of accuracy. However, creation of a calibration model incorporating the chemical variability found across different brands of these products may be beneficial for ensuring a high level of robustness.

Although beyond the scope of this study, future work could also investigate the use of NIR spectroscopy for the quality determination of panned chocolate goods, namely the quality of the chocolate and core (peanut or sultana) used in the manufacturing process. This could allow detection of potential adulteration of panned chocolate products with low quality peanuts or sultanas. Other researchers have used hyperspectral imaging to detect adulteration of chocolate powder with non-cocoa products.[11] Furthermore, NIR spectroscopy may be able to simultaneously profile the fatty acid composition[28, 32] or sucrose content[18] of the chocolate layer, allowing identification of products made from lower quality chocolate.

Conclusion

This study investigated the potential of NIR spectroscopy for the discrimination of the centre composition of panned chocolate goods for the first time. The NIR spectra showed a high level of separation between chocolate-coated peanuts and sultanas in the training set. Similarly, NIR spectroscopy could discriminate between the peanut and sultana samples in an independent test set, although the separation between samples was not as distinct. The robustness of this model may be improved by incorporating samples from different manufacturers. Nevertheless, this proof-of-concept study demonstrates the power of NIR spectroscopy for confirming product identity in post-manufacture quality assurance settings. Future work could extend this to the quality analysis of the peanuts or sultanas used in the manufacture of panned chocolate goods.

Declarations

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Declaration of Conflicting Interests

The author declares that there is no conflict of interest.

Availability of data

The dataset is available in the online Supplemental materials.

Code availability

The code used for the analyses presented in this study are available in the online Supplemental materials.

References

1. Depypere F, Delbaere C, De Clercq N, et al. Fat bloom and cracking of filled chocolates: issues for the European manufacturer? *New Food* 2009; 12: 9-12.
2. Geschwindner G and Drouven H. 18 - Manufacturing processes: chocolate panning and inclusions. In: Talbot G (ed) *Science and Technology of Enrobed and Filled Chocolate, Confectionery and Bakery Products*. Woodhead Publishing, 2009, pp.397-413.
3. Hartel RW, von Elbe JH and Hofberger R. Chocolate Panning. *Confectionery Science and Technology*. Cham: Springer International Publishing, 2018, pp.501-510.
4. Gutiérrez TJ. State-of-the-Art Chocolate Manufacture: A Review. *Comprehensive Reviews in Food Science and Food Safety* 2017; 16: 1313-1344. DOI: 10.1111/1541-4337.12301.
5. Aebi M. Chocolate panning. *Beckett's Industrial Chocolate Manufacture and Use*. 2017, pp.431-449.
6. Christman LM, Dean LL, Bueno Almeida C, et al. Acceptability of Peanut Skins as a Natural Antioxidant in Flavored Coated Peanuts. *Journal of Food Science* 2018; 83: 2571-2577. DOI: 10.1111/1750-3841.14323.
7. Kita A, Lachowicz S and Filutowska P. Effects of package type on the quality of fruits and nuts panned in chocolate during long-time storage. *LWT-Food Science and Technology* 2020; 125: 109212. DOI: 10.1016/j.lwt.2020.109212.
8. Heuler J, He S, Ambardar S, et al. Point-of-care detection, characterization, and removal of chocolate bloom using a handheld Raman spectrometer. *Scientific Reports* 2020; 10: 9833. DOI: 10.1038/s41598-020-66820-1.
9. Delbaere C, Van de Walle D, Depypere F, et al. Relationship between chocolate microstructure, oil migration, and fat bloom in filled chocolates. *European Journal of Lipid Science and Technology* 2016; 118: 1800-1826. DOI: 10.1002/ejlt.201600164.
10. Laborde A, Jaillais B, Bendoula R, et al. A partial least squares-based approach to assess the light penetration depth in wheat flour by near infrared hyperspectral imaging. *J Near Infrared Spectrosc* 2020; 28: 25-36. DOI: 10.1177/0967033519891594.
11. Laborde A, Puig-Castellví F, Jouan-Rimbaud Bouveresse D, et al. Detection of chocolate powder adulteration with peanut using near-infrared hyperspectral imaging and Multivariate Curve Resolution. *Food Control* 2021; 119: 107454. DOI: 10.1016/j.foodcont.2020.107454.
12. Rahman A, Wang S, Yan J, et al. Intact macadamia nut quality assessment using near-infrared spectroscopy and multivariate analysis. *Journal of Food Composition and Analysis* 2021; 102: 104033. DOI: 10.1016/j.jfca.2021.104033.
13. Carvalho LCd, Verbi Pereira FM, Morais CdLMd, et al. Assessment of macadamia kernel quality defects by means of near infrared spectroscopy (NIRS) and nuclear magnetic resonance (NMR). *Food Control* 2019; 106: 106695. DOI: 10.1016/j.foodcont.2019.06.021.
14. Johnson JB. An overview of near-infrared spectroscopy (NIRS) for the detection of insect pests in stored grains. *Journal of Stored Products Research* 2020; 86: 101558. DOI: 10.1016/j.jspr.2019.101558.
15. Grassi S and Alamprese C. Advances in NIR spectroscopy applied to process analytical technology in food industries. *Current Opinion in Food Science* 2018; 22: 17-21. DOI: 10.1016/j.cofs.2017.12.008.
16. Cortés V, Blasco J, Aleixos N, et al. Monitoring strategies for quality control of agricultural products using visible and near-infrared spectroscopy: A review. *Trends in Food Science & Technology* 2019; 85: 138-148. DOI: 10.1016/j.tifs.2019.01.015.
17. Johnson JB, Walsh K and Naiker M. Application of infrared spectroscopy for the prediction of nutritional content and quality assessment of faba bean (*Vicia faba* L.). *Legume Science* 2020; n/a: e40. DOI: 10.1002/leg3.40.
18. da Costa Filho PA. Rapid determination of sucrose in chocolate mass using near infrared spectroscopy. *Analytica Chimica Acta* 2009; 631: 206-211. DOI: 10.1016/j.aca.2008.10.049.

19. Bolliger S, Zeng Y and Windhab EJ. In-line measurement of tempered cocoa butter and chocolate by means of near-infrared spectroscopy. *Journal of the American Oil Chemists' Society* 1999; 76: 659-667. DOI: 10.1007/s11746-999-0157-5.

20. Bin Z, Lei D, Qiao G, et al. Fast discrimination of chocolate varieties using near infrared spectroscopy. In: *2008 IEEE International Conference on Automation and Logistics* 1-3 Sept. 2008 2008, pp.730-735.

21. Ma T, Kobori H, Katayama N, et al. Non-Destructive Inspection of Insects in Chocolate Using near Infrared Multispectral Imaging. *J Near Infrared Spectrosc* 2016; 24: 391-397.

22. Quelal-Vásconez MA, Lerma-García MJ, Pérez-Esteve É, et al. Fast detection of cocoa shell in cocoa powders by near infrared spectroscopy and multivariate analysis. *Food Control* 2019; 99: 68-72. DOI: 10.1016/j.foodcont.2018.12.028.

23. R Core Team. R: A language and environment for statistical computing. version 4.0.2 ed. Vienna, Austria: R Foundation for Statistical Computing, 2020.

24. Kucheryavskiy S. mdatools – R package for chemometrics. *Chemometrics and Intelligent Laboratory Systems* 2020; 198: 103937. DOI: 10.1016/j.chemolab.2020.103937.

25. Moros J, Iñón FA, Garrigues S, et al. Near-infrared diffuse reflectance spectroscopy and neural networks for measuring nutritional parameters in chocolate samples. *Analytica Chimica Acta* 2007; 584: 215-222. DOI: 10.1016/j.aca.2006.11.020.

26. Huxsoll CC. Assessment of near infrared (NIR) diffuse reflectance analysis for measuring moisture and water activity in raisins. *Journal of Food Processing and Preservation* 2000; 24: 315-333. DOI: 10.1111/j.1745-4549.2000.tb00422.x.

27. Tao F, Yao H, Hruska Z, et al. Use of Visible–Near-Infrared (Vis-NIR) Spectroscopy to Detect Aflatoxin B1 on Peanut Kernels. *Applied Spectroscopy* 2019; 73: 415-423. DOI: 10.1177/0003702819829725.

28. Gatti RF, de Santana FB, Poppi RJ, et al. Portable NIR spectrometer for quick identification of fat bloom in chocolates. *Food Chemistry* 2021; 342: 128267. DOI: 10.1016/j.foodchem.2020.128267.

29. de Andrade BM, de Gois JS, Xavier VL, et al. Comparison of the performance of multiclass classifiers in chemical data: Addressing the problem of overfitting with the permutation test. *Chemometrics and Intelligent Laboratory Systems* 2020; 201: 104013. DOI: 10.1016/j.chemolab.2020.104013.

30. Hao Y, Sun X, Gao R, et al. Application of visible and near infrared spectroscopy to identification of navel orange varieties using SIMCA and PLS-DA methods. *Transactions of the Chinese Society of Agricultural Engineering* 2010; 26: 373-377.

31. Vitale R, Bevilacqua M, Bucci R, et al. A rapid and non-invasive method for authenticating the origin of pistachio samples by NIR spectroscopy and chemometrics. *Chemometrics and Intelligent Laboratory Systems* 2013; 121: 90-99. DOI: 10.1016/j.chemolab.2012.11.019.

32. Amorim TL, Duarte LM, de Oliveira MAL, et al. Prediction of Fatty Acids in Chocolates with an Emphasis on C18:1 trans Fatty Acid Positional Isomers Using ATR-FTIR Associated with Multivariate Calibration. *Journal of Agricultural and Food Chemistry* 2020; 68: 10893-10901. DOI: 10.1021/acs.jafc.0c04316.