Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 351 (2026) 127505

Contents lists available at ScienceDirect

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

journal homepage: www.journals.elsevier.com/spectrochimica-acta-part-a-molecular-and-biomolecular-spectroscopy

Short Communication

Detection of hazelnut rancidity inside chocolate tablets using near-infrared hyperspectral imaging

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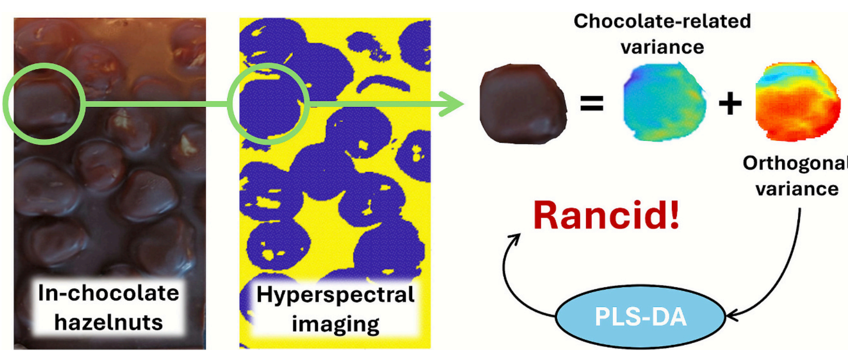
HIGHLIGHTS

- NIR-HSI detects rancid hazelnuts within intact chocolate bars.
- Spectral unmixing isolates hazelnut signal from chocolate matrix.
- ASCA: rancidity explains 13.1% of spectral variance ($p = 0.001$).
- PLS-DA on residual spectra classifies bars with 100% accuracy.
- Residual model needs fewer latent variables than raw-spectra PLS-DA.

GRAPHICAL ABSTRACT



ARTICLE INFO

Keywords:
Chemometrics
Nuts
Quality assurance
Food
Oxidation
PAT

ABSTRACT

Near-infrared hyperspectral imaging (NIR-HSI) was evaluated as a non-destructive tool to detect hazelnut rancidity directly inside commercial chocolate bars, without separating the nuts from the chocolate matrix. Chocolate bars containing fresh or deliberately oxidized hazelnuts were imaged and analysed using a spectral unmixing strategy to separate chocolate and hazelnut contributions, yielding a residual component dominated by the nut signal where rancidity-related differences became more evident. ASCA applied to the original pre-processed spectra showed that rancidity explained 13.09% of the total variance ($p = 0.001$), confirming a significant and interpretable spectral effect despite the dominant chocolate background. A PLS-DA model built on the residual spectra successfully discriminated fresh from rancid hazelnuts and correctly classified all chocolate bars in an independent validation set, using fewer latent variables than a model based on the original data. These results demonstrate the feasibility of in situ detection of hazelnut rancidity within chocolate tablets and support NIR-HSI, combined with chemometric modelling, as a promising approach for non-destructive quality control in heterogeneous confectionery products.

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https://doi.org/10.1016/j.saa.2026.127505
Received 23 November 2025; Received in revised form 3 January 2026; Accepted 19 January 2026
Available online 20 January 2026

1. Introduction

Hazelnuts (*Corylus avellana* L.) are a key ingredient in a wide range of confectionery products due to their characteristic flavour, high lipid content, and desirable contribution to the texture. However, their sensory profile is particularly susceptible to oxidative degradation. The nut lipid fraction is dominated by unsaturated fatty acids, primarily oleic and linoleic acids, which are prone to undergo peroxidation during storage and technological processing [1]. As oxidation progresses, volatile aldehydes and other secondary products lead to rancid off-flavours, diminished aroma, and ultimately compromises consumer acceptance both in the hazelnuts or in hazelnut-containing products like chocolate bars [2,3]. For this reason, ensuring the quality of hazelnuts through the entire supply chain is essential for maintaining the sensory integrity of confectionery and chocolate products [4].

Most analytical approaches for detecting hazelnut rancidity rely on destructive sampling and require isolating the nuts prior to analysis. Conventional methods such as peroxide value determination, volatile profiling, sensory evaluation, or chromatography-based assays provide reliable oxidation markers, but they are time-consuming, require sample preparation, and are not directly applicable to finished products. In industrial practice, where hazelnuts are frequently embedded within chocolate matrices, the separation of nut and chocolate complicates routine quality control and increases the risk of overlooking early oxidation defects [3].

Spectroscopic techniques have been proposed as rapid and non-destructive alternatives for assessing lipid oxidation in nuts, including near-infrared (NIR) spectroscopy and hyperspectral imaging [5,6]. Most of these applications, however, focus on raw or roasted kernels, or on bulk hazelnuts stored in modified atmosphere packaging. To date, non-invasive monitoring of hazelnut oxidation directly within commercial chocolate tablets has not been reported. The presence of the chocolate matrix introduces optical and compositional challenges, including overlapping spectral features from cocoa butter and sugars, scattering effects, and heterogeneous distribution of nut pieces [7]. Demonstrating that oxidation-related spectral signatures can still be distinguished under these conditions would provide an opportunity for realistic, in-product quality assessment.

In this short study, we investigated whether spectral markers of rancidity in hazelnuts can be detected in situ within chocolate bars, using commercial chocolate bars as a realistic model system. Fresh hazelnuts and hazelnuts deliberately oxidized under controlled storage conditions were incorporated into chocolate, and spectra were collected without separating the nut fraction. We compared spectral responses between fresh and rancid conditions to evaluate whether oxidation-related chemical differences remain detectable despite matrix interferences. The aim of this work is not to develop a full predictive model or shelf-life analysis, but to establish proof of feasibility that spectroscopic analysis can distinguish oxidation states inside finished chocolate products, enabling non-destructive quality control in industrial environments.

2. Material and methods

2.1. Samples and measurement

Commercial chocolate bars containing 25% whole hazelnuts (Ritter Sport, Germany) were used as the study matrix. Two independent sample sets were prepared: a calibration set (six bars) and a validation set (four bars) [8]. Within each set, half of the chocolate bars contained fresh hazelnuts, while the other half contained hazelnut subject to controlled artificial oxidation hazelnuts (Ritter Sport), with the same batch chocolate to avoid confounding factors. The calibration set and validation set were measured in different analytical sessions by different analysts. Each tablet was kept at 4 °C and protected from light until hyperspectral image acquisition to preserve the condition of the hazelnuts and the chocolate [5].

Hyperspectral images were acquired with a NIR line-scanning camera (950–1600 nm, 142 bands, typical spectral resolution of 4.2 nm; Headwall Photonics, MA, USA), using an array of pixel-detectors (320 in a row) positioned 30 cm above the sample, which was moved at a step size of 300 μm, yielding an approximate spatial resolution of 300 μm in both spatial dimensions. Measurements were recorded in diffuse reflectance and converted to absorbance using dark and white references [5]. For each acquisition, only a representative part of the chocolate bars was imaged: a piece of around 3 × 5 cm. After acquisition, background pixels and specular reflections were removed by PCA-based thresholding of the scores, in the mean centred data matrix.

2.2. Statistical analysis

All the statistical analysis was performed in the Matlab (R2024a, MathWorks, Natick, MA) environment. The Hyper-Tools v4.0 toolbox (Hypertools, Bilbo, Spain) [9] was used for the image processing, and the PLS_toolbox 9.0 (Eigenvector Research Inc., Manson, WA) for building multivariate models, altogether with custom-made code for managing and curation of the data.

For separating pixels corresponding mostly to chocolate from the ones that are a hazelnut-chocolate mixture, K-means clustering was used. This is an unsupervised partitioning algorithm that divides a set of observations into *k* clusters by minimising the within-cluster sum of squared distances in an iterative way [10].

For the exploratory analysis of the data, ANOVA–Simultaneous Component Analysis (ASCA) was used. ASCA is a multivariate method that separates, quantifies and helps interpret the effects of experimental factors on designed datasets by combining ANOVA with Simultaneous Component Analysis (SCA). In this study, ASCA was used to evaluate the impact of hazelnut rancidity on the overall spectral variability. The significance of each effect was assessed by permutation testing (1000 permutations) [11].

For the developing the classification model discerning fresh and rancid hazelnut containing samples, Partial Least Squares–Discriminant Analysis (PLS-DA) was employed. PLS-DA is a supervised multivariate classification method that projects spectral data into latent variables maximising covariance with the categorical response (class), adequate for highly collinear datasets like NIR spectra [12].

Spectra were pre-processed using Savitzky–Golay 1st derivative (SG, 2nd order polynomial, 15-point window) and mean-centring (MC) before modelling [13]. The calibration set was used to optimise the discriminant model, and classification performance was evaluated using the independent validation set. Model optimisation consisted of one-sample-out cross-validation for selecting the adequate preprocessing and the number of latent variables [8].

3. Results and discussion

3.1. Spectral unmixing

To better understand and ultimately discern the rancidity of hazelnut, it is important to resolve the spectral contributions of chocolate and hazelnut within the hyperspectral. For this, all six calibration-sample images were concatenated into a single dataset (Fig. 1a). This approach ensured that both products were represented across a wide range of natural variability, including differences in surface curvature, illumination, and nut-chocolate contact areas (raw and preprocessed spectral variability can be seen in Fig. S1 and Fig. S2).

K-means clustering (k = 2) was applied to the unfolded spectral matrix to perform an unsupervised differentiation of pixel types. Although hazelnut pieces are visually distinguishable because of the prominences in the surface of the chocolate bars, their spectral signatures in the NIR spectra are partially masked by the chocolate coating and by scattering effects caused by the changing surface properties and

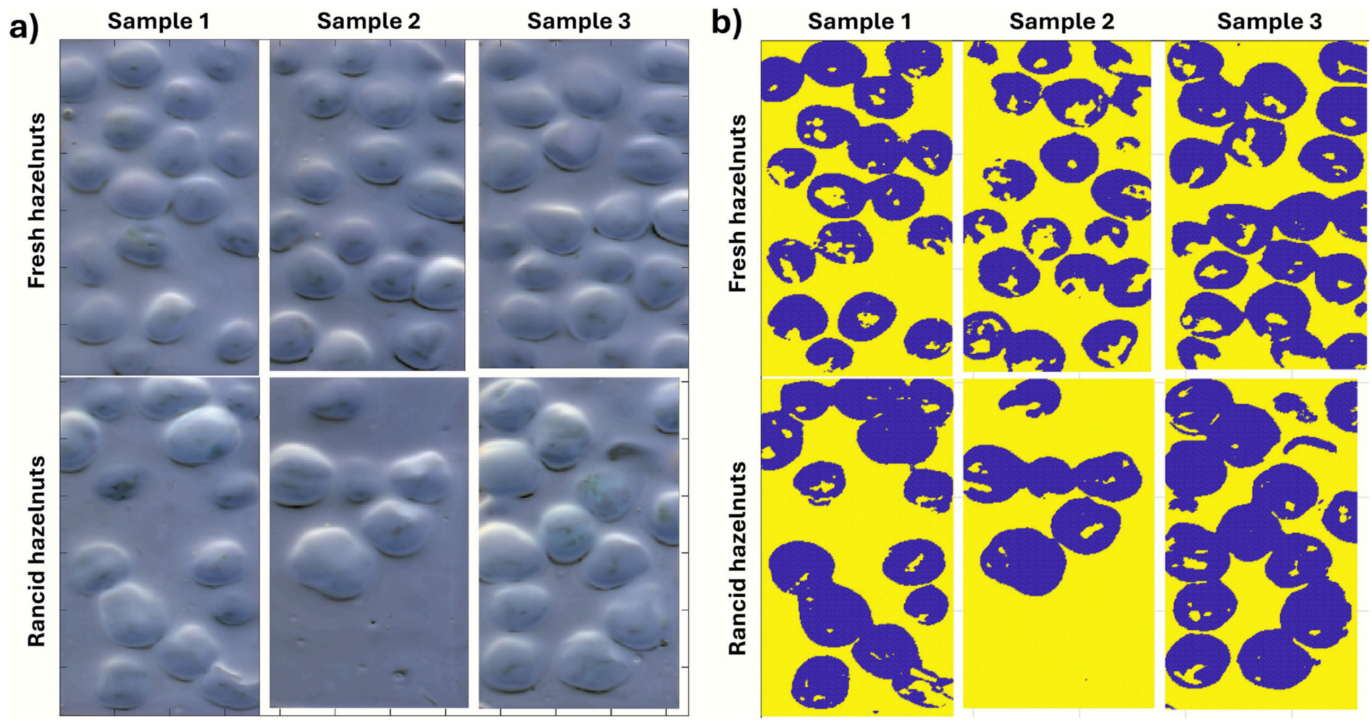

Fig. 1. Hyperspectral images acquired from the calibration set of samples. a) Fake-RGB representation of the spectra. b) The two clusters obtained from the K-means clustering.

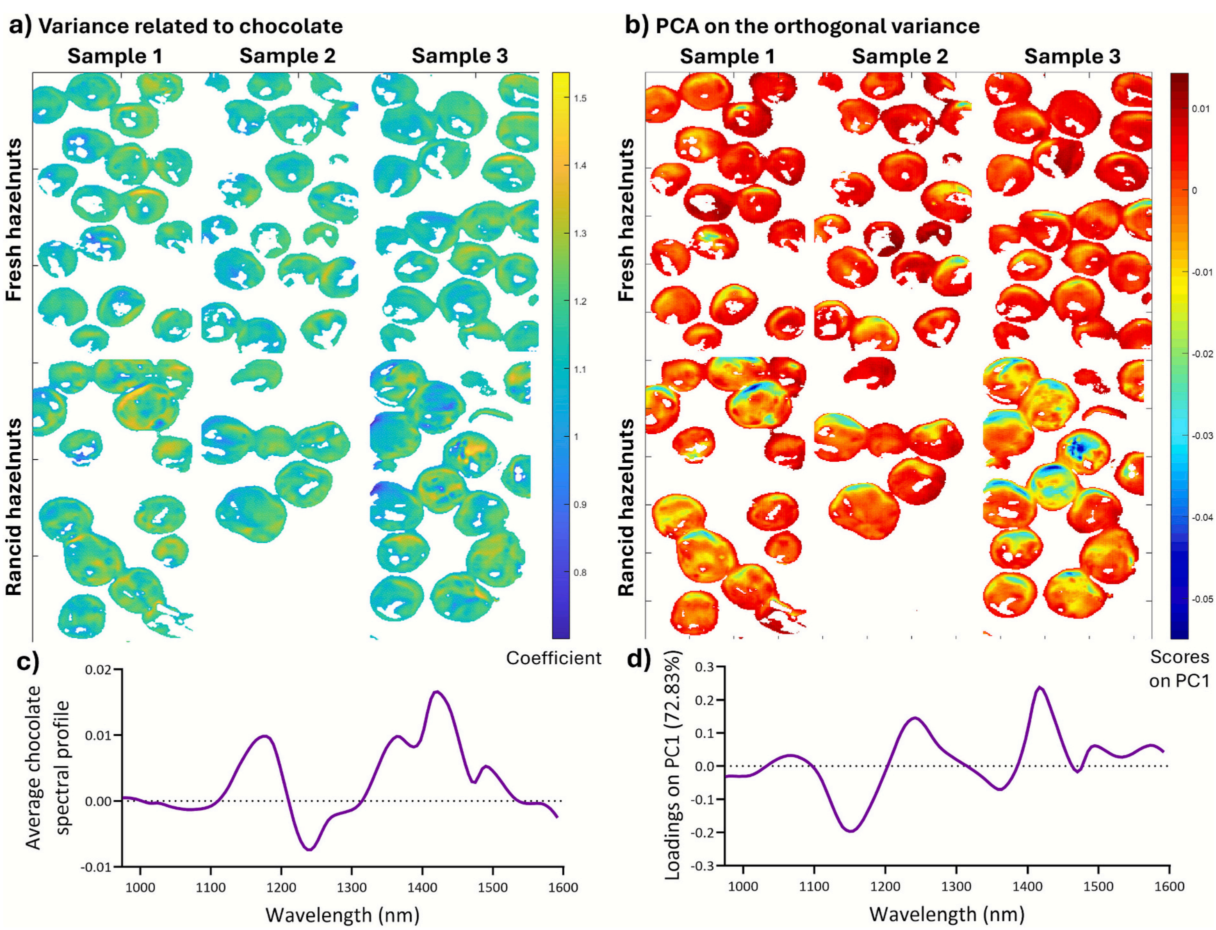

Fig. 2. RGB representation of the variance a) corresponding to the chocolate signal; and b) the residual variance after removing the chocolate-related variance. And their respective signals c) chocolate profile; d) loadings on the first PC in the residual variance.

the nut-chocolate interface. Therefore, rather than attempting to segment hazelnut directly, the clustering was designed to identify the most spectrally homogeneous material (chocolate) and isolate it from regions containing either pure hazelnut or a mixture of both components. The resulting cluster map provided a first-level separation of the tablet into chocolate-dominated and non-chocolate-dominated pixels (Fig. 1b). This map was also used for generating a mask with hazelnut-containing pixels only.

The average spectrum of the chocolate pixels was then computed (Fig. 2c). This mean profile served as a representative basis signal of the chocolate matrix, capturing the broad lipid- and carbohydrate-derived absorptions that dominate the NIR spectrum. Then, this reference spectrum was used to estimate the amount of chocolate present in each hazelnut-associated pixel, based on a least-squares projection of the chocolate mean onto every pixel spectrum. This step produced an image representing the spatial distribution of chocolate-related variance across the sample (Fig. 2a). Pixels corresponding to hazelnut pieces still contained a measurable chocolate contribution due to surface coating, internal inclusions, and partial mixing at the nut-chocolate boundary. Thus, this projection provided a relative quantification of the chocolate coating thickness across the chocolate bars; and allowed explicit removal of those contributions by subtracting the reconstructed chocolate component for each pixel. This yielded a residual dataset that contained only spectral variance orthogonal to the chocolate profile (Fig. S3). This residual variance is of particular interest because it enhances spectral features associated with hazelnut composition, including lipids and oxidation-related products, while suppressing the dominant chocolate background. This variance was explored using PCA, in which the spatial distribution of the scores (Fig. 2b) shows a difference between the fresh and rancid samples, the latter showing lower scores.

The corresponding spectral loadings (Fig. 2d) indicate the specific NIR bands contributing to this. Positive features around 1200–1220 nm and 1720–1760 nm can be attributed to first overtones and combination bands of C—H stretching in triglycerides, characteristic of fresh hazelnuts. In contrast, negative contributions near 1650–1690 nm and 1410–1450 nm are consistent with changes caused by lipid oxidation, including altered CH_2/CH_3 environments and increased contributions from carbonyl-related combination bands that emerge as triglycerides break down into aldehydes and hydroperoxides. Together, these bands reflect the chemical transition from unoxidized lipids to degradation products typical of rancidity [14].

3.2. ASCA

To evaluate and quantify whether the spectral signatures associated with hazelnut rancidity had an impact on the original preprocessed data, ASCA was applied, considering only the rancidity factor. The model revealed that this factor accounted for 13.09% of the total spectral variance (p-value = 0.001), a substantial contribution given the dominance of the chocolate matrix and the inherent heterogeneity of intact nuts embedded within chocolate.

Inspection of the SCA model revealed a strong correspondence between its latent structure and the spatial-spectral contrasts identified in the unmixing. The scores of the first Simultaneous Component (SC1, Fig. 3b) displayed similar patterns to the ones observed in the residual variance image obtained after subtraction of the chocolate contribution (Fig. 2b). This alignment indicates that the rancidity-related variance captured by ASCA is concentrated in the same hazelnut-dominated pixels highlighted by the orthogonalisation step.

The loadings associated with SC1 (Fig. 3b) further supported this interpretation. They exhibited pronounced features in spectral regions known to be sensitive to lipid composition and oxidation state consistent with the biochemical changes expected during hazelnut rancidity, as per the loading interpretation in Section 3.1. The fact that these loadings resembled those obtained from the chocolate-subtracted residual

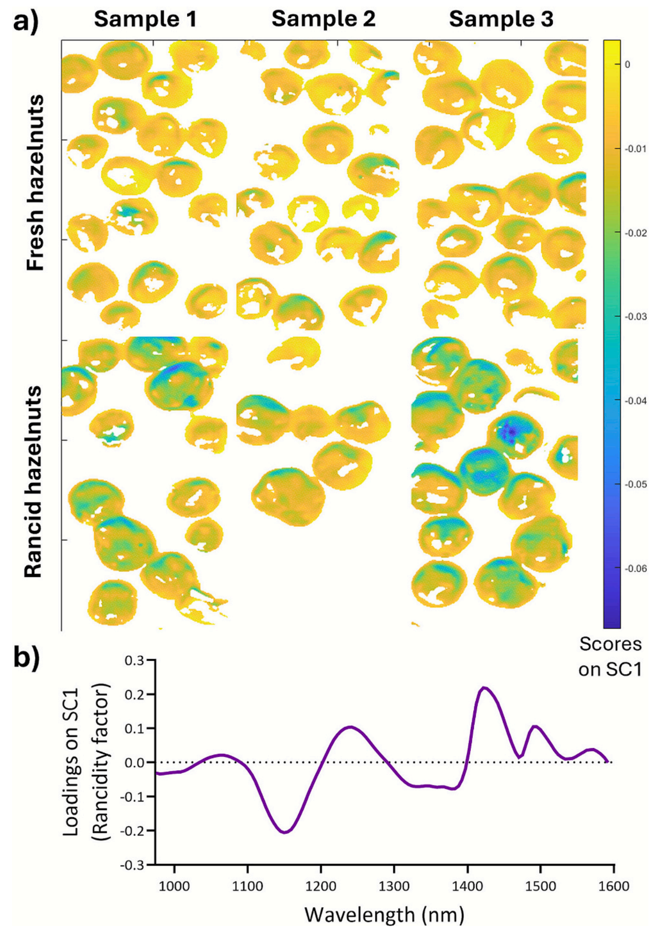

Fig. 3. a) RGB representation of the scores obtained from the SCA model on the rancidity factor, using the original preprocessed (SG 1st deriv. and MC) data. b) the corresponding loadings.

analysis (Fig. 2d) confirms that effect of rancidity can be primarily seen in the hazelnut spectral contribution rather than in the chocolate background.

3.3. Classification

To determine whether the spectral differences associated with hazelnut rancidity were strong enough for discrimination, a PLS-DA model was built using the residual variance data obtained after subtracting the chocolate contribution (Section 3.1). By focusing the model on the hazelnut-specific orthogonal component, the aim was to enhance sensitivity to chemical changes related to oxidation while reducing the confounding effect of the chocolate matrix.

The PLS-DA model was optimised using a one-sample-out cross-validation, which showed that the model with 5 latent variables (LVs) had the best performance. This model was then evaluated using the independent validation set, in which each pixel was classified into fresh/rancid (Fig. 4), and the results were combined to determine the class of each chocolate-bar by using the pixel-wise prediction as a class probability. This is, the percentage of pixels predicted as rancid is the class probability for the sample being rancid, if above 50%, it is classified as rancid. The validation results demonstrate that the model effectively differentiates fresh from rancid hazelnut-containing chocolate bars (100% accuracy chocolate-bar-wise); even though not all the pixels were predicted correctly, which can be expected due to the non-homogeneous distribution of rancidity both among-hazelnut and between-hazelnuts [5]. This pixel-wise analysis revealed that the accuracy was higher in the rancid hazelnuts than in the fresh ones, this is, the model is more prone

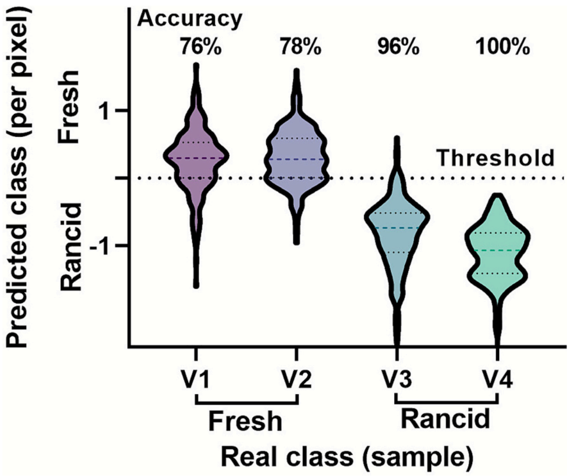

Fig. 4. Predicted values for the pixels corresponding to hazelnuts on the validation samples, using the PLS-DA model for the spectra after subtracting the chocolate-related variance. Accuracy indicates the percentage of correctly classified pixels per sample.

to Type I errors (false positives) than Type II errors (false negatives).

For comparison, an equivalent PLS-DA model was constructed using the original preprocessed spectra, without chocolate variance removal. In this case, the model required one additional LV (6 LVs) to reach similar classification accuracy and figures of merit to the model shown in Fig. 4. This makes sense as this extra LV will be used for explaining the chocolate-related variability.

4. Conclusions

This study shows that near-infrared hyperspectral imaging can detect hazelnut rancidity inside commercial chocolate tablets, without separating the nuts from the chocolate. By unmixing chocolate and hazelnut spectral contributions, we obtained a residual variance dominated by the nut fraction, where clear spectral differences between fresh and rancid hazelnuts were observed.

ASCA confirmed that rancidity has a significant effect on the original spectra, explaining 13.09% of the total variance ($p = 0.001$), with scores and loadings consistent with the contrasts revealed by the unmixing step. A PLS-DA model built on the residual spectra accurately discriminated all the fresh and rancid hazelnut-containing chocolate bars in the validation set. Altogether, this proof of concepts demonstrates the feasibility of non-destructive in situ detection of rancidity in hazelnuts embedded in chocolate, with particular consideration in the spectral unmixing, and motivate further work under more complex and industrially realistic conditions monitoring the tablets through the whole oxidation process, using different product batches and varieties of hazelnut.

Funding

J. E. thanks the Novo Nordisk Foundation grant number NNF21OC0065495. N. V.-i-V. thanks Universitat Rovira i Virgili for her grant (URV Martí i Franqués 2024-PMF-PIPF-41). Chemometrics and Sensorics for Analytical Solutions (CHEMOSENS, ref.2021 SGR 00705, Departament de Recerca i Universitats, Generalitat de Catalunya).

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

The authors would like to thank Alfred Ritter GmbH & Co. KG for kindly providing the samples and Jose Manuel Amigo for kindly lending the hyperspectral camera. During the preparation of this work the authors used ChatGPT 5 in order to edit text and improve readability. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.saa.2026.127505.

Data availability

Data will be made available on request.

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