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A novel and sustainable analytical strategy to control the origin and mitigate the fake coffee from *Coffea canephora* in Brazil

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ABSTRACT

The increasing price of coffee, mainly in Brazil, has led to the production and sale of coffee substitutes made from alternative ingredients such as coffee husks, soy, corn, and açaí, among others. They are becoming known as fake coffee. *Coffea canephora* from Brazilian terroirs has attracted growing attention, but this heightened focus has also made it a prime target for intentional fraud, affecting both its pricing and credibility. This study explores the use of reflectance spectroscopy based on near-infrared region to verify the authenticity of the Conilon variety from Espírito Santo (80 pure samples and 640 adulterated samples) and the Robusta variety from Rondônia, sourced from both indigenous (80 pure samples and 640 adulterated samples) and non-indigenous producers (80 pure samples and 640 adulterated samples). Data-Driven Soft Independent Modeling of Class Analogy (DD-SIMCA) authenticated these coffees by geographical origins and detected adulterants such as açaí seeds, corn, soybean, arabica coffee, coffee husks, and spent coffee grounds. Espírito Santo Conilon was tested as an adulterant for Rondônia samples. Multi-class Partial Least Squares Discriminant Analysis (PLS-DA) differentiated these adulterants implementing a Monte Carlo cross-validation with 20 % data hold-out. The developed method achieved 100 % accuracy with DD-SIMCA and 99.6 % with PLS-DA, detecting up to 10 % w/w of adulteration. These results surpass both previous studies on coffee adulteration detection using NIRS and other analytical techniques in terms of accuracy.

1. Introduction

Food control becomes increasingly important during periods of rising inflation in developing countries, as inflation often drives the creation of imitation products designed to reduce costs. In Brazil, for example, the increasing price of coffee has led to the production and sale of coffee substitutes made from alternative ingredients such as coffee husks, soy, corn, and açaí, among others. They are often blending coffee with other materials or even entirely non-coffee ingredients. The potential health and economic consequences of consuming fake coffee remain uncertain, making the identification of such practices essential.

When the questions involving coffee integrity are raised, a primary concern revolves around its purity. In such a scenario, food fraud remains a consistent worry for both consumers and companies, whether it is perpetrated intentionally or inadvertently. Underscoring the ongoing efforts to combat this issue, scientists and regulatory agencies are actively engaged in developing methods to detect adulteration in coffee (Toci et al., 2016). In this persistent fraudulent practice, coffee is blended with cheaper food items like corn, soybeans, açaí seeds, or even with by-products from the coffee industry such as coffee husks or spent

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coffee grounds (Correia et al., 2016, 2018; Milani et al., 2020; Pizarro et al., 2007).

Detecting adulteration in ground roasted coffee, whether specialty, gourmet, or traditional, poses a significant challenge due to the complexity of distinguishing substances after roasting and grinding. Many non-coffee substances and by-products closely mimic the appearance of ground roasted coffee, making visual detection difficult (Toci et al., 2016). Recently, Baqueta, Postigo, et al. (2024) investigated the adulteration of specialty Coffea canephora coffee, characterized by sensory scores exceeding 80 points on a 100-point scale, with traditional Coffea arabica coffee and low-quality Canephora coffee, both of which typically exhibit lower sensory scores. Notably, the incorporation of these coffee-based matrices constitutes a more sophisticated form of adulteration in specialty Canephora coffee, as their chemical compositions are more similar to the original product compared to other low-quality adulterants, such as açaí, corn, soybean, coffee husks, and spent coffee grounds, thereby increasing the challenges associated with their detection.

Detecting adulteration in ground roasted coffee presents a significant challenge due to the complexity of distinguishing substances post-roasting and grinding. Many non-coffee substances and by-products closely resemble ground roasted coffee, making visual detection difficult. Traditional methods of fraud detection in coffee primarily rely on optical and electron microscopy, sometimes in conjunction with physicochemical analyses like moisture content, mineral residues, and ether extractable substances. However, microscopy procedures are often slow and subjective, lacking immediate and reliable results, while wet chemical analysis is labor-intensive and damages the samples.

Recent reviews have been addressed to alternative analytical methods for detecting coffee adulteration, including liquid and gas chromatography, DNA-based methods, mass spectrometry, atomic spectrometry, digital imaging, and numerous spectroscopic techniques such as nuclear magnetic resonance (NMR), molecular fluorescence, X-ray fluorescence, ultraviolet–visible (UV–Vis), Raman, mid-infrared (MIR), and near-infrared (NIR) spectroscopy (Couto et al., 2023; Perez et al., 2023; Munyendo et al., 2022; Ferreira et al., 2021; Baqueta et al., 2020; Wang et al., 2020). However, most of these methods still necessitate sample preparation techniques. Nonetheless, non-destructive techniques like NIR spectroscopy allow for direct sample analysis much faster than other methods, and its significance in verifying coffee authenticity has been noteworthy (Araújo et al., 2021, 2024; Boadu et al., 2023; Nóbrega et al., 2023; Couto et al., 2022; Correia et al., 2018; Barbin et al., 2014).

Due to the lower price of *Coffea canephora*, it has been explored as a common adulterant of *Coffea arabica*, thus justifying the predominance of the scientific literature on coffee adulteration. However, in recent years, the coffee industry has begun to recognize the high-quality potential of specialty Canephora coffees (Baqueta, Postigo, et al., 2024). As a result, there has been a surge in demand for these coffees, especially those sourced from unique geographical regions (Baqueta et al., 2025). In Brazil, the States of Rondônia and Espírito Santo are the main producers of high-quality Canephora coffees. Rondônia coffees are Robusta variety Canephora coffees produced by both indigenous and non-indigenous coffee producers in the Western Brazilian Amazon (Zacharias et al., 2021), while Espírito Santo coffees are of the Conilon variety (Agnoletti et al., 2023). These three national producers (Rondônia indigenous, Rondônia non-indigenous, and Espírito Santo) have obtained geographical indication certifications (Brazil, 2021), underscoring the importance of identifying distinct characteristics of these coffees to market them as "single geographical origin" products.

In this study, for the first time, non-destructive direct NIR spectroscopic analysis was employed to authenticate the geographical origins of specialty Brazilian Canephora coffees using Data-Driven Soft Independent Modeling of Class Analogy (DD-SIMCA) and to discriminate against multiple adulterants using Partial Least Squares Discriminant Analysis (PLS-DA). The adulteration of indigenous Rondônia, non-indigenous Rondônia, and Espírito Santo specialty Canephora coffees involved the addition of different ground roasted items such as açaí, corn, soybean, arabica coffee, low-quality Canephora coffee, coffee husks, and spent coffee grounds. Additionally, indigenous and non-indigenous Rondônia Robusta coffees were adulterated with Espírito Santo Conilon coffees to emphasize the idea of using the closest analogues of the target class to validate the chemometric models, which aligns with the Nearest of Kin (NoK) concept (Rodionova et al., 2019).

2. Materials and methods

2.1. Coffee samples

A total of 240 green Canephora coffee samples, with 80 samples each originating from indigenous Rondônia, non-indigenous Rondônia, and Espírito Santo, were generously provided by the Brazilian Company of Farming Research (EMBRAPA, Research Center of Rondônia). They were selected to represent the diversity of production in each region. For indigenous and non-indigenous Rondônia, the samples were collected from different communities and farms to capture variability in agricultural practices and environments. For Espírito Santo, samples were chosen to reflect the main producing areas of the state. This approach ensured a representative set of green Canephora coffees for each origin while maintaining balance across the groups. The Rondônia samples comprised the Amazonian Robusta variety, while the Espírito Santo samples were of the Conilon variety. These samples underwent medium roasting in a Probat sample roaster following the protocol outlined by the Uganda Coffee Development Authority (UCDA, 2010), with temperatures ranging from 160 °C to 190 °C over a duration of 7.5–9 min.

2.2. Preparation of the adulterated coffee samples

Corn and soybeans were purchased from local markets in Campinas, São Paulo, Brazil, while Arabica coffee cultivated in Pedregulho, São Paulo, Brazil, and low-quality Canephora from Londrina, Paraná, Brazil, were provided by coffee industries. Three samples of each adulterant type (300 g each) were obtained and combined to prepare a representative composite sample. Canephora coffee husks were supplied by EMBRAPA Rondônia. Pulped açaí seeds, obtained from a local manufacturer in Belém, Pará, Brazil, were kept frozen at −12 °C until required. All raw materials underwent roasting in a manner similar to pure samples, with variations in temperature and time to achieve a comparable roasted coffee profile based on previous studies (Milani et al., 2020; Reis et al., 2017). Spent coffee grounds, obtained from water extraction of authentic coffee samples, were dried in a convection oven (Model 520-C, Fanem, São Paulo, Brazil) at 100 °C for 5 h to attain a moisture content similar to ground roasted coffee (~5 % w w^{-1}). Pure Espírito Santo samples were also tested as an adulterant for Rondônia samples to verify the robustness of the models in differentiating them from those produced in the Amazonian terroirs of Rondônia. The roasted coffee and adulterants were milled and then passed through a 20-mesh sieve for particle size standardization. Ten pure coffee samples, randomly selected from each group of 80, were deliberately mixed with increasing proportions (10 %, 20 %, 30 %, 40 %, 50 %, 60 %, and 70 % w w^{-1}) of adulterants, resulting in a total of 1840 adulterated samples. Fig. 1 illustrates the sample composition, including the number of pure and adulterated samples, and depicts the appearance of adulterants before and after roasting. Visually, the pure ground adulterants closely resembled pure ground roasted coffee post-roasting and grinding.

2.3. Instrumentation

All pure and adulterated samples underwent direct analysis using a PerkinElmer FT-NIR spectrophotometer model Spectrum™ 100N, equipped with an InGaAs detector, within the range of 10,000–4000 cm^{-1}. The equipment was set to operate in reflectance mode, with 32

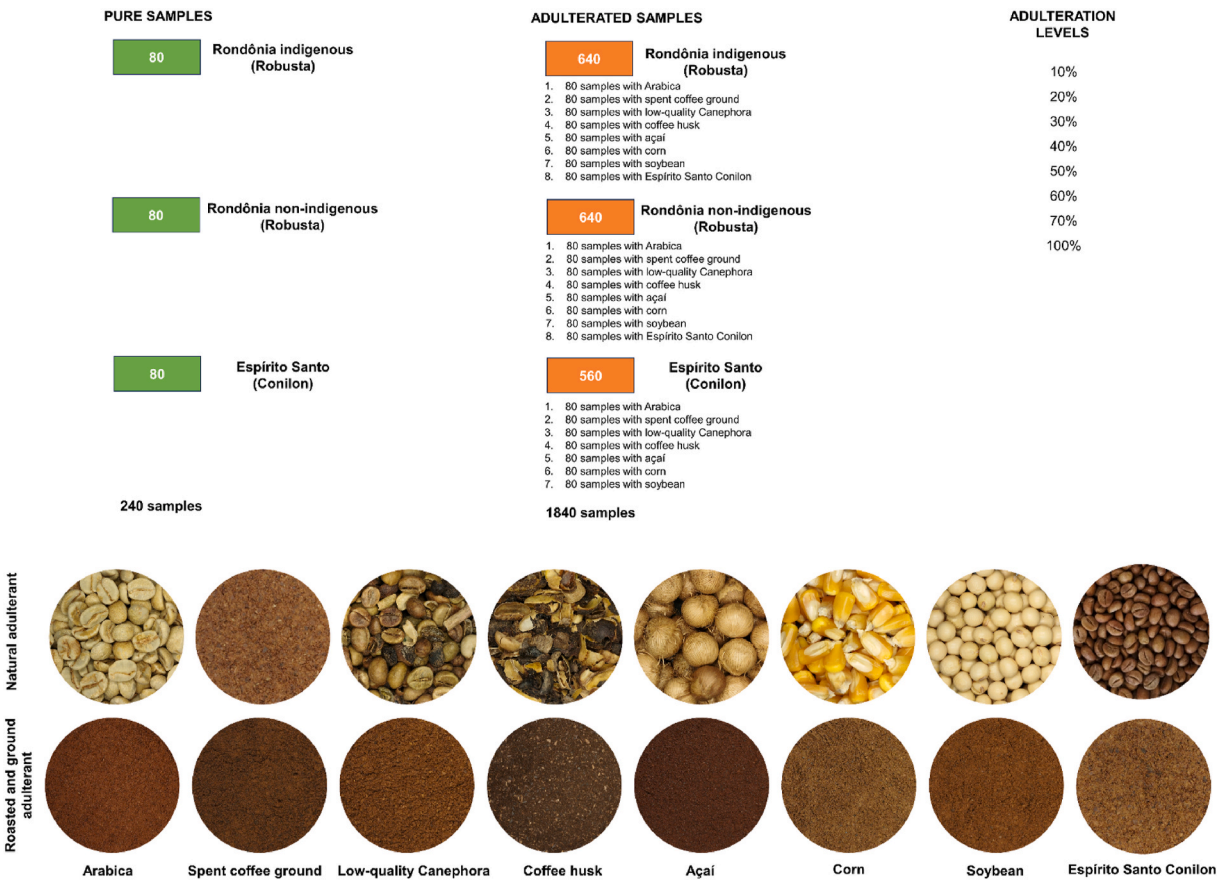

Fig. 1. Schematic representation of the samples.

scans accumulated per sample at a nominal resolution of 4 cm^{-1}. The powder samples (2 g) were placed in glass vial holder with 12.5 mm diameter. Measurements were carried out at 22 °C, with the samples presenting a moisture content of 12 % on average. Spectra were obtained in triplicate and subsequently averaged prior to constructing the chemometric models. A NIR reflectance standard was used to assess the blank.

2.4. Chemometric procedures

Initially, various pre-processing techniques were employed on the NIR spectra to address baseline shifts and scattering issues. These techniques encompassed offset correction (OFF), multiplicative scattering correction (MSC), standard normal variation (SNV), and first derivative Savitzky-Golay with a second-order polynomial and a 15-point window (SGD). Subsequently, an exploratory analysis was conducted using Principal Component Analysis (PCA) to examine sample groupings based on geographical origins. Following this, new PCA models were constructed to visualize the presence of multiple adulterants in each individual pure coffee group from the three studied geographical origins.

For the construction of the DD-SIMCA and PLS-DA models, the Kennard-Stone (KS) uniform sampling algorithm (Kennard & Stone, 1969) was always used to divide each target class into training (75 %) and test (25 %) samples.

To authenticate the geographical origins of Brazilian specialty Canephora coffees, DD-SIMCA models were developed using two approaches. The first approach focused solely on the 240 pure samples from indigenous Rondônia ($n = 80$), non-indigenous Rondônia ($n = 80$), and Espírito Santo ($n = 80$). In this scenario, DD-SIMCA models were constructed using a training set comprising 60 samples from each target class, while the test set included 20 target samples and 160 samples from different geographical origins. In the second approach, the same target classes were authenticated against adulteration with açaí, corn, soybean, Arabica coffee, low-quality Canephora coffee, coffee husks, and spent coffee grounds, with the addition of Conilon coffees in the case of adulteration of Amazonian coffees. Once again, exclusively training samples ($n = 60$) from each target class were used in model construction, while the test samples comprised 20 target samples along with 560 adulterated samples from Espírito Santo, 640 adulterated samples from indigenous Rondônia, or 640 adulterated samples from non-indigenous Rondônia. Target samples were always utilized to evaluate the sensitivity of the models, whereas non-target samples were employed to assess specificity. For DD-SIMCA model construction, the acceptance area was determined based on the chi-square distribution in the robust mode, considering a significance level of 0.01 for type I and II errors, as well as outlier significance. The optimal number of principal components (PCs) was determined by outstanding the best balance between the number of true positive (TP) cases in both the training and test sets (Zontov et al., 2017).

Once the pure specialty Canephora coffee samples were authenticated, PLS-DA models were employed to discriminate the type of adulterant, regardless the geographical origin of the pure samples. To guarantee the class balance across all adulterants, 80 synthetic samples were generated from Rondônia samples adulterated with Espírito Santo coffee (Folli et al., 2024), thereby balancing the training dataset. As a result, each adulterant class was composed of 180 training samples and 60 test samples. Thus, a total of 1440 and 480 adulterated samples composed the training and test sets, respectively. PLS-DA models were constructed using the training set and validated through Monte Carlo cross-validation with 20 % data hold-out. Model selection was based on the lowest root mean square error of cross-validation (RMSECV). The

independent test set was subsequently employed solely to evaluate and compare the predictive performance of the final discriminant models.

The performance of the DD-SIMCA and PLS-DA models was evaluated in terms of sensitivity and specificity for each target class, and overall accuracy considering both the training and test sets. Sensitivity is calculated as the number of true positive (TP) decisions divided by the total number of positive cases, while specificity is calculated as the number of true negative (TN) decisions divided by the total number of negative cases. Also, accuracy is calculated as the number of true classifications divided by the total number of samples (Gomes et al., 2022).

A lab-made routine was run for KS, while PCA and Classification Toolboxes were downloaded from https://michem.unimib.it/download/matlab-toolboxes/. DD-SIMCA interface is available at https://github.com/yzontov/dd-simca. All chemometric procedures were performed using Matlab® 2018b (Mathworks Inc.).

3. Results and discussion

3.1. Exploratory analysis

The average raw NIR spectra of the pure samples from the three geographical origins (Espírito Santo, indigenous Rondônia, and non-indigenous Rondônia) displayed a remarkably similar profile across almost the entire range, as illustrated in Fig. 2a. Notably, the average spectra of the Rondônia coffees, whether indigenous or non-indigenous, exhibited more comparable intensities, whereas the spectrum of the Espírito Santo coffee appeared more distinct from them. In essence, discernible patterns in the spectral data of authentic coffees emerged, reflecting both their geographical origin and variety. Despite all being Canephora coffees, their distinct botanical varieties—Robusta and Conilon—further influenced by their terroir, contributed to variations in their NIR spectra. These chemical distinctions among the NIR spectra of pure coffees often correlate with absorption regions of aroma and flavor precursors, including chlorogenic acids, carbohydrates, proteins, trigonelline, caffeine, and lipids (Barbin et al., 2014; Ribeiro et al., 2011).

The NIR spectra of coffee samples exhibit complex signals resulting from combination bands and overtones of fundamental vibrations, making interpretation challenging yet highly informative. The region from 4200 to 4040 cm^{-1} is associated with the combination band of C−H vibrations and C−C vibrations (Santos et al., 2016). Intense signals in the 5200–5000 cm^{-1} and 7200–6800 cm^{-1} regions are associated with water O−H absorption, reflecting its presence even in the roasted coffee matrices. The 5300–5200 cm^{-1} region, indicative of C=O and O−H vibrations, provides insights into compounds such as chlorogenic acids, carbohydrates, and organic acids. Signals within 6100–4965 cm^{-1}, attributed to the first overtone of aliphatic and aromatic C−H bonds, relate to lipids and volatile aroma compounds. The region between 9800 and 9000 cm^{-1} highlights second overtones of C−H and N−H vibrations, pointing to proteins, alkaloids (e.g., caffeine), and certain lipids, while peaks near 7000 cm^{-1} emphasize structural features of hydrocarbons, aiding in the identification of fatty acid profiles. Specific lipid-associated peaks at 5797 and 5666 cm^{-1} are particularly informative for distinguishing *Coffea canephora* and *Coffea arabica* coffees, as canephora generally contains lower levels of fatty acids. The overlapping nature of carbonyl (C=O), CH, and CH_2 group vibrations, spanning multiple constituents such as proteins, chlorogenic acids, volatile and non-volatile acids, lipids, and alkaloids, underscores the complexity of peak assignments and highlights the need for advanced analytical approaches to fully leverage the information provided by NIR spectra (Assis et al., 2020; Barbin et al., 2014; Ribeiro et al., 2011).

Conversely, Fig. 2b shows the average raw NIR spectrum of the three genuine coffees diverging from those of the pure adulterants. Analysis of the spectral fingerprints reveals significant differences in absorption bands between authentic Canephora samples and their adulterants. Notably, disparities between the spectra become apparent from 6000 cm^{-1} onwards, particularly in the region of combination bands associated with carbohydrates (Barbin et al., 2014), owing to the distinct chemical compositions of the materials. The most distinguishable spectrum belongs to coffee husks, which, being a thin layer, undergo carbonization during roasting (Correia et al., 2018). Both portable NIR (Boadu et al., 2023; Correia et al., 2018, 2022) and benchtop NIR (Couto et al., 2022; Araújo et al., 2021) instruments have demonstrated clear distinctions in spectral profiles between pure coffees, pure adulterants, and coffee-adulterant mixtures.

To visualize the trends of grouping among the samples, Fig. 3 presents the PCA score plots considering the explained variance in the first and second principal components with NIR spectra pre-processed with the Savitzky-Golay first derivative using a second-order polynomial and a 15-point window. This pre-processing showed a better initial distinction between the three pure sample groups individually (Fig. 3a) and between pure and adulterated samples (Fig. 3c and d) compared to other pre-processing methods available in Fig. S1 in the supplementary material, which resulted in significant overlap between the classes under study. In all PCA models, coffee husks (depicted in dark green) were frequently distinguishable among the coffee samples and adulterated samples, suggesting that its composition was the most distinctive. Preliminary spectral analysis using PCA has also shown promising results in detecting coffee fraud through adulteration with rice, corn, soy, barley, and coffee husks (Couto et al., 2022) as well as with peels/sticks and corn (Correia et al., 2018).

3.2. Geographical origin authentication

As expected from PCA exploratory analysis, the best classification

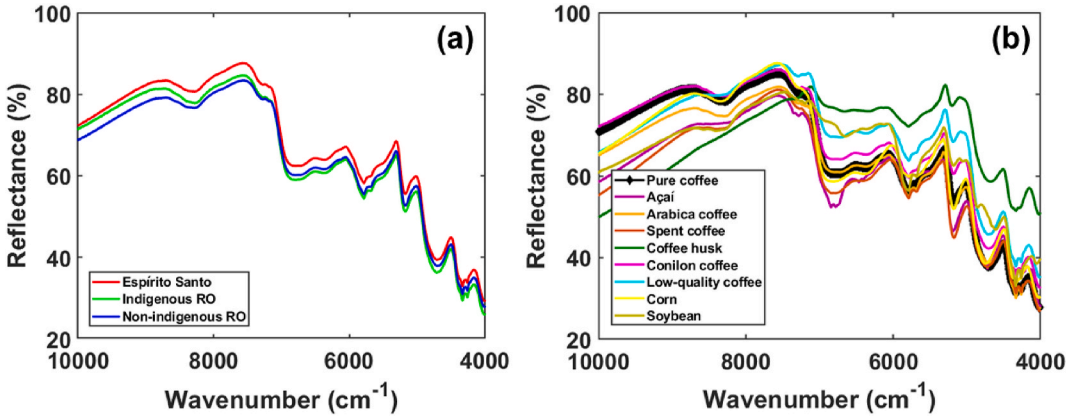

Fig. 2. (a) Average raw NIR spectra of the pure samples from Espírito Santo, indigenous Rondônia, and non-indigenous Rondônia, and **(b)** the eight different adulterants.

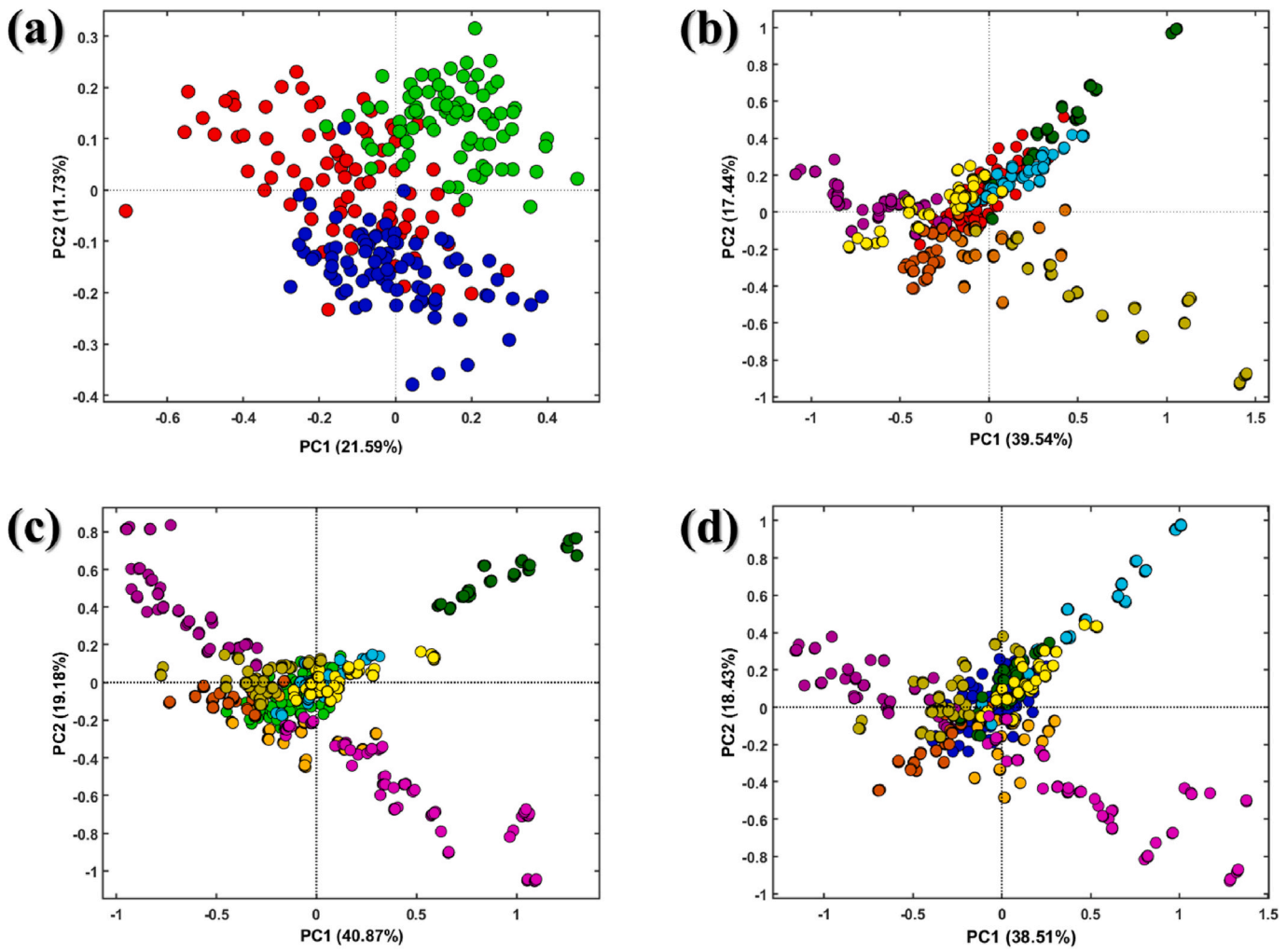

Fig. 3. Score plots (PC1 vs PC2) obtained in PCA to visualize the distinction between the three pure Espírito Santo (in red), indigenous Rondônia (in green), and non-indigenous Rondônia (in blue) sample groups individually **(a)**, between Espírito Santo adulterated and pure samples **(b)**, between indigenous Rondônia adulterated and pure samples **(c)**, and between non-indigenous Rondônia adulterated and pure samples **(d)** using the NIR spectra pre-processed with first derivative Savitzky-Golay with a second-order polynomial and a 15-point window (SGD). Canephora coffees adulterated with açaí (in purple), Arabica coffee (in orange), spent coffee grounds (in brown), coffee husks (in dark green), low-quality Canephora coffee (in cyan), corn (in yellow), soybean (in gold), and Conilon coffees (in magenta). (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

results obtained by DD-SIMCA ($\alpha = 0.01$) for the geographical origin authentication of specialty Canephora coffees was achieved using the Savitzky-Golay first derivative with second-order polynomial and 15-point window (SGD), as summarized in Table 1. For a comprehensive overview of the results with all pre-processing techniques, please refer to Table S1 (for Espírito Santo), **S2** (for indigenous Rondônia), and **S3** (for non-indigenous Rondônia) in the Supplementary material.

Indeed, DD-SIMCA holds appeal for authentication purposes, demonstrating perfect classification between pure coffee samples based on geographical origin and between pure and adulterated coffee samples. Since the optimal number of principal components (PCs) was consistent for both authentication approaches, Fig. 4a, b, and 4c depict the acceptance areas obtained by the DD-SIMCA/SGD models for the pure Espírito Santo, indigenous Rondônia, and non-indigenous Rondônia training samples, respectively. As illustrated, all pure samples were accurately projected into their respective acceptance areas delineated by solid lines matching the color of the training samples (red, green, and blue, respectively). Dashed lines denote outlier detection thresholds; however, no samples were assigned as extreme or outliers by the DD-SIMCA/SGD models. When each pure target class was confronted against non-target pure samples (gray circles) (Fig. 4d, e, and 4f) and non-target adulterated samples (bronze circles) (Fig. 4g, h, and 4i), all target samples were precisely projected within their respective acceptance areas, while non-target samples did not breach these boundaries, providing 100 % sensitivity and 100 % specificity in both the approaches. It is important to note that the geographical origin of each coffee, including those from Rondônia, cultivated in the same region referred to as "Matas de Rondônia" by both indigenous and non-indigenous producers, could be authenticated as unique products. This underscores the social diversity inherent in the production of distinct Amazonian coffees by various coffee growers in the Amazon region. When considering adulterated versions of coffee, even with the inclusion of various food materials, DD-SIMCA models based on NIR spectra preprocessed with SGD accurately identified all pure and adulterated samples, consistently achieving 100 % overall accuracy.

Compared to the results obtained in this study, DD-SIMCA or even original SIMCA demonstrated comparable or even superior classification results to previous works using NIR or other spectral techniques (Agnoletti et al., 2023; Santos et al., 2023; Manuel et al., 2022; Araújo et al., 2021; Luna et al., 2019). However, the issue of authenticating coffee produced by indigenous and non-indigenous groups is being reported for the first time, and therefore, no comparisons can be made. Nonetheless, it is feasible to authenticate their origins as well as those of Espírito Santo with 100 % correct classifications.

Table 1
Best results (confusion matrix, with the sensitivity, specificity, and overall accuracy) obtained by DD-SIMCA (α = 0.01) for the authentication of specialty Canephora coffees using NIR spectra pre-processed with Savitzky-Golay first derivative with second-order polynomial and 15-point window.

Sample set	Target *vs* Other pure coffees				Target *vs* Adulterated coffees			
	PCs	Training	Test		PCs	Training	Test	
		Target	Target	Non-target		Target	Target	Non-target
Espírito Santo								
Target	3	60	20	0	3	60	20	0
Non-target		0	0	160		0	0	480
Sensitivity (%)		100	100			100	100	
Specificity (%)		–	100			–	100	
Accuracy (%)		100				100		
Indigenous (Rondônia)								
Target	3	60	20	0	3	60	20	0
Non-target		0	0	160		0	0	480
Sensitivity (%)		100	100			100	100	
Specificity (%)		–	100			–	100	
Accuracy (%)		100				100		
Non-indigenous (Rondônia)								
Target	6	60	20	0	6	60	20	0
Non-target		0	0	160		0	0	480
Sensitivity (%)		100	100			100	100	
Specificity (%)		–	100			–	100	
Accuracy (%)		100				100		

3.3. Discrimination of adulterants

Since all pure samples were correctly authenticated, PLS-DA was assessed as a discriminant method to differentiate between various types of adulterants in the Espírito Santo, indigenous Rondônia, and non-indigenous Rondônia coffees simultaneously. Once again, SGD emerged as the optimal pre-processing method for discriminating between eight common adulterants found in Brazilian specialty Canephora coffees using NIR spectroscopy. Table 2 displays the confusion matrix, along with the sensitivity, specificity, and overall accuracy obtained by the PLS-DA/SGD model. Complete results for all pre-processing techniques were provided in Table S4 in the Supplementary material.

The PLS-DA/SGD models performed exceptionally well in discriminating coffee samples adulterated with açaí, arabica, spent coffee, low quality Canephora coffee, corn, and soybean in both the training and test sets. In terms of misclassifications, only one sample of coffee husk and two samples of Espírito Santo were erroneously classified as spent coffee, coffee husk, and low-quality Canephora coffee, respectively, in the training set. However, all coffee husk and low-quality Canephora coffee test samples were accurately classified. Moreover, even in cases where pure Conilon Espírito Santo samples were used as a form of sophisticated adulteration for Rondônia (both indigenous and non-indigenous) samples, few misclassifications were observed, demonstrating the robustness of the model in distinguishing them from those produced in the Amazonian terroirs of Rondônia. Only three Conilon samples were incorrectly classified as coffee husk and low-quality Canephora coffee in the test set. Nevertheless, the overall accuracy of the PLS-DA/SGD model was 99.8 % and 99.4 % in the training and test sets, respectively.

For visualization, Fig. 5 depicts the differentiation of Brazilian specialty Canephora coffees adulterated with various substances: açaí (in purple; Fig. 5a), Arabica coffee (in orange; Fig. 5b), spent coffee grounds (in brown; Fig. 5c), coffee husks (in dark green; Fig. 5d), low-quality Canephora coffee (in cyan; Fig. 5e), corn (in yellow; Fig. 5f), soybean (in gold; Fig. 5g), and Conilon coffees (in magenta; Fig. 5h). Filled circles represent training samples, while empty circles represent test samples. The horizontal dotted red line signifies the threshold of the responses calculated for each target class. As evident from the data, there is significant discrimination, with only 6 out of 1920 samples misclassified. Therefore, the results can be deemed excellent, particularly considering the evaluation involved a substantial number of genuine and complex adulterated samples.

Table 3 compares key studies from the past decade on coffee adulteration detection utilizing NIR classification (Boadu et al., 2023; Correia et al., 2022) and other analytical techniques, including digital images (Baqueta, Postigo, et al., 2024; Souto et al., 2015), high performance liquid chromatography (Núñez et al., 2021; Tavares et al., 2016), mid-infrared spectroscopy (Reis et al., 2017), laser-induced breakdown spectroscopy (Sezer et al., 2018), voltammetry (de Morais et al., 2019), and proton nuclear magnetic resonance (Milani et al., 2020). As observed, the proposed study achieved classification results that were comparable to or exceeded those reported in previous studies. Notably, this study demonstrates a significant advancement by modeling a total of eight different classes comprising 1840 samples. This represents a considerable challenge for multi-class PLS-DA, as the method requires extensive and detailed information from each class to develop representative and reliable models capable of delineating distinct boundaries among the studied classes (Pomerantsev & Rodionova, 2018).

4. Conclusions

In this study, we addressed the critical issue of authenticity in high-value Brazilian *Coffea Canephora* (Conilon and Robusta) coffees, which are increasingly sought after for their sensory qualities but have become susceptible to fraud and adulteration. Our research provides a non-destructive and highly accurate analytical approach for both the authentication of these coffees and the detection of common adulterants. Considering the advanced analytical methods and their applications in food chemistry, this study represents an innovative use of NIR spectroscopy and chemometrics to significantly enhance food authenticity and quality control.

NIR spectroscopy coupled with chemometric modeling has proved to be an effective tool for ensuring the quality of Brazilian specialty Canephora coffees, with proving particularly useful in distinguishing their geographical origins and adulterations with açaí, corn, soybean, arabica coffee, coffee husks, and spent coffee grounds, along with Conilon coffee from Espírito Santo in the case of adulteration of the Rondônia samples. PCA provided initial insights indicating the Savitzky-Golay first derivative with second-order polynomial and 15-point window (SGD) as a promise pre-processing to aim the aims of proposed study. In the following, DD-SIMCA/SGD models achieved an overall accuracy of 100 % to authenticate pure Espírito Santo, indigenous Rondônia, and non-indigenous Rondônia in terms of their geographical origins and adulterations. Additionally, PLS-DA/SGD model reached 99.8 % and 99.4 % in the training and test sets, respectively, to discriminate the eight

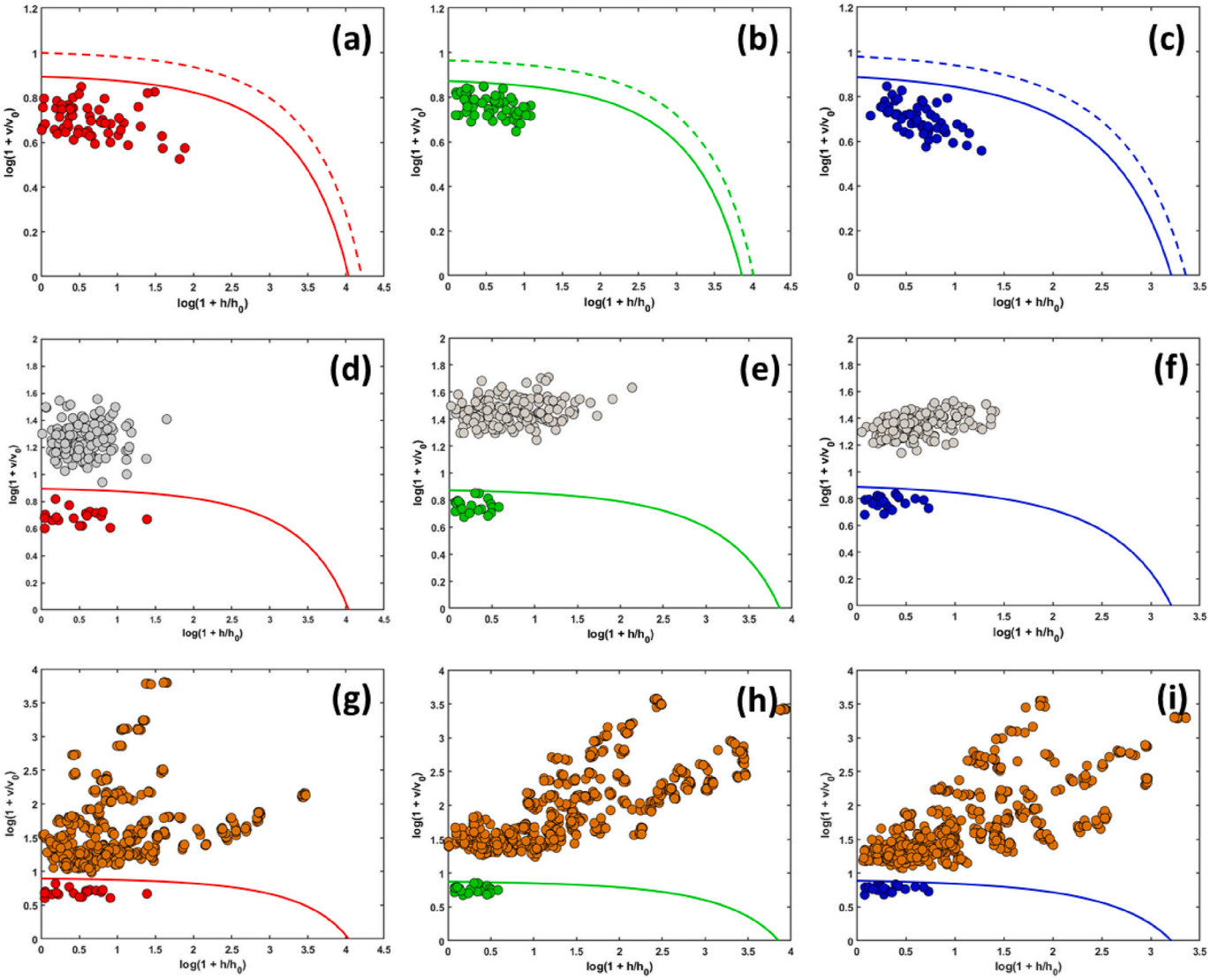

Fig. 4. Acceptance areas obtained by the DD-SIMCA (α = 0.01) using the NIR spectra pre-processed with the first derivative Savitzky-Golay with a second-order polynomial and a 15-point window (SGD) for the training samples of the pure Espírito Santo **(a)**, indigenous Rondônia **(b)**, and non-indigenous Rondônia **(c)**, and the test samples regarding their authentication in terms of geographical origins **(d–f)** and adulterations **(g–i)**, respectively.

Table 2
Best result (confusion matrix, with the sensitivity, specificity, and overall accuracy) obtained by PLS-DA for the discrimination of eight typical adulterants in Brazilian specialty *Canephora* coffees using NIR spectra pre-processed with the Savitzsky-Golay first derivative with a second-order polynomial and 15-point window.

SGD/PLS-DA model (10 LVs)		Training set							Test set								
		AC	AR	SP	HU	LQ	CO	SO	ES	AC	AR	SP	HU	LQ	CO	SO	ES
Matrix confusion	**AC**	180	–	–	–	–	–	–	–	60	–	–	–	–	–	–	–
	AR	–	180	–	–	–	–	–	–	–	60	–	–	–	–	–	–
	SP	–	–	180	–	–	–	–	–	–	–	60	–	–	–	–	–
	HU	–	–	1	179	–	–	–	–	–	–	–	60	–	–	–	–
	LQ	–	–	–	–	180	–	–	–	–	–	–	–	60	–	–	–
	CO	–	–	–	–	–	180	–	–	–	–	–	–	–	60	–	–
	SO	–	–	–	–	–	–	180	–	–	–	–	–	–	–	60	–
	ES	–	–	–	1	1	–	–	178	–	–	–	–	2	1	–	57
Sensitivity		100 %	100 %	100 %	99.4 %	100 %	100 %	100 %	98.9 %	100 %	100 %	100 %	100 %	100 %	100 %	100 %	95.0 %
Specificity		100 %	100 %	99.7 %	100 %	99.7 %	100 %	100 %	100 %	100 %	100 %	100 %	100 %	99.7 %	99.8 %	100 %	100 %
Accuracy					99.8 %									99.4 %			
Overall accuracy									99.6 %								

AC: açaí; AR: *Arabica* coffee; SP: spent coffee; HU: coffee husk; LQ: low-quality *Canephora* coffee; CO: corn; SO: soybean; ES: Espírito Santo Conilon coffee.

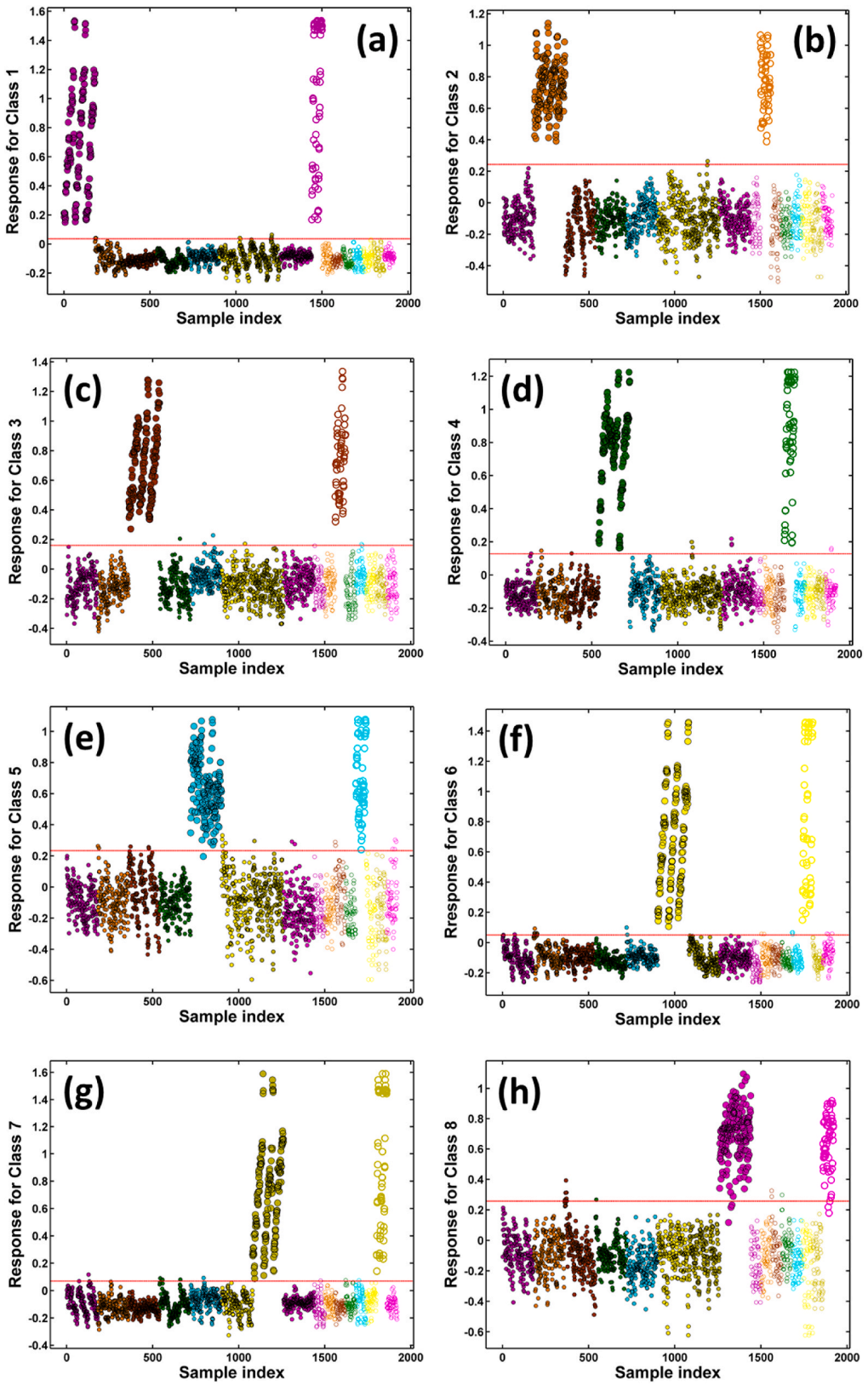

Fig. 5. Plots of the calculated responses obtained by PLS-DA using the NIR spectra pre-processed with the first derivative Savitzky-Golay with a second-order polynomial and a 15-point window (SGD) to discriminate Brazilian specialty Canephora coffees adulterated with **(a)** açaí (in purple), **(b)** Arabica coffee (in orange), **(c)** spent coffee grounds (in brown), **(d)** coffee husks (in dark green), **(e)** low-quality Canephora coffee (in cyan), **(f)** corn (in yellow), **(g)** soybean (in gold), and **(h)** Conilon coffees (in magenta). Filled circles represent training samples, while empty circles represent test samples. The horizontal dotted red line signifies the threshold of the responses calculated for each target class. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

Table 3
Comparison of key studies from the past decade on coffee adulteration detection.

Analytical technique	Adulterants	Sample preparation	Number of modeled samples	Accuracy	Reference
Digital images	coffee husks and sticks	no	103	92.5 %	Souto et al. (2015)
High performance liquid chromatography	maize, husks and cleaned husks	extraction with organic solvents	60	77.8 %	Tavares et al. (2016)
Mid-infrared spectroscopy	spent coffee ground, coffee husks, corn, and barley	no	310	96.5 %	Reis et al. (2017)
Laser-induced breakdown spectroscopy	corn, wheat and chickpea	no	58	Not provided	Sezer et al. (2018)
Voltammetry	husks and sticks	extraction with deionized water	90	98.9 %	de Morais et al. (2019)
Proton nuclear magnetic resonance	barley, corn, coffee huss, soybean, rice, and wheat	extraction with deuterated water	75	100 %	Milani et al. (2020)
High performance liquid chromatography	chicory, barley, and different flours (wheat, rice, cornmeal, rye, and oatmeal)	extraction with methanol:water	123	100 %	Núñez et al. (2021)
Portable near-infrared spectroscopy	spent coffee ground	no	212	92 %	Correia et al. (2022)
Portable near-infrared spectroscopy	coffee husk	no	170	98.9 %	Boadu et al. (2023)
Digital images	Arabica coffee, low-quality Canephora coffee, coffee huss, spent coffee ground, açaí, corn, and soybean	no	300	95.0 %	Baqueta, Postigo, et al. (2024)
Near-infrared spectroscopy	Arabica coffee, Conilon coffee, coffee huss, and spent coffee ground, açaí, corn, and soybean	no	1840	99.6 %	This work

different classes of adulterants, detecting adulteration levels as low as 10 % w/w. These methods offer comprehensive solutions for ensuring the authenticity and quality of Brazilian specialty Canephora coffees amidst growing concerns over adulteration in the coffee industry.

CRediT authorship contribution statement

Michel Rocha Baqueta: Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Paulo Henrique Gonçalves Dias Diniz:** Writing – original draft, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Venancio Ferreira de Moraes Neto:** Methodology, Investigation, Formal analysis, Conceptualization. **Enrique Anastácio Alves:** Resources, Methodology, Conceptualization. **Patrícia Valderrama:** Writing – review & editing, Supervision, Conceptualization. **Juliana Azevedo Lima Pallone:** Writing – review & editing, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization.

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.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.foodcont.2025.111750.

Data availability

Data will be made available on request.

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