Journal of Food Composition and Analysis 145 (2025) 107786

Contents lists available at ScienceDirect

Journal of Food Composition and Analysis

journal homepage: www.elsevier.com/locate/jfca

Analysis of plant-based commercial milk substitutes using ATR-FTIR spectroscopy

Anna Luiza B. Brito [a,*], Catarina Duarte [a], Rui Fausto [a,b]

[a] CQC-IMS, Department of Chemistry, University of Coimbra, Coimbra 3004-535, Portugal
[b] Department of Physics, Faculty of Sciences and Letters, Istanbul Kultur University, Ataköy Campus, Bakırköy, Istanbul, Türkiye

ARTICLE INFO

Keywords:
Plant-based milk substitutes
Infrared spectroscopy
Chemometrics
PCA

ABSTRACT

Plant-based beverages have emerged as substitutes for cow's milk, and their consumption has been steadily increasing in recent years, largely due to health-related reasons, such as milk protein allergies or lactose intolerance. This raises the need for development of analytical approaches for these products that can capable of accurately identifying and classifying these products. This study focused on almond, rice, oat, and soy plant-based milk substitute drinks, which are the most popular among this type of beverages. Infrared spectroscopy data have been used to develop a fast, cost-effective and easy to implement in different settings chemometrics model for these beverages, which allows their classification according to their nature and compositional variability. It was found that the use of the spectral region of the characteristic Amide I and II bands of the proteins led to an optimal description of the data by the first two principal components in the developed Principal Component Analysis (PCA) model. For oat, rice, and soy beverages, distinct characteristic spectroscopic features allowed their successful clustering using the chemometric approach, while the results obtained for the studied almond beverages evidenced their significant compositional variability, resulting in a less defined clustering. These results are consistent with the known nutritional information for the different types of beverages.

1. Introduction

This study focused on plant-based beverages commonly used as milk substitutes (specifically, almond, rice, oat, and soy drinks), utilizing attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) together with principal component analysis (PCA) and hierarchical cluster analysis (HCA) to develop classification models for these beverages.

Cow's milk is one of the most widely consumed foods globally, across all age groups, and plays a crucial role in a balanced diet, serving as a significant source of energy. According to the Portuguese Institute of Statistics (Instituto Nacional de Estatítica, INE; Statistics Portugal), the annual average milk consumption per person in Portugal in the period 2020–2023 stayed in the 62–72 kg range (Instituto Nacional de Estatística (Statistics Portugal), 2024).

Nutritionally, milk is rich in proteins (around 3 % by weight), carbohydrates (4–5 %), lipids (3–4 %), vitamins (0.1 %), and minerals (0.8 %), with water making up approximately 87 % of its composition (Vašková et al., 2016). Among these, lipids are particularly important as they are the primary source of energy in milk and contribute to the desirable properties of dairy products.

Currently, a variety of milks with specific nutritional properties, such as low-fat, lactose-free, flavored, or vitamin D-fortified options, are available on the market to meet consumer demands (Vašková et al., 2016). Additionally, there is a growing trend toward the consumption of plant-based beverages, which are now widely marketed and have become an important part of many people's diets. The growing demand for alternative milk beverages is largely driven by health concerns, such as allergies to cow's milk proteins and lactose intolerance, or simply by nutritional options (e.g., vegan) (Berardy et al., 2022; Taeger and Thiele, 2024; Álvarez-Álvarez et al., 2024; Walther et al., 2022; Burciu Tuhut, 2023). Although there is a large variation in the protein values of drinks due to the different types available, they can match the protein values of cow's milk with soy drinks, approximately 3.4 g in a 100 mL serving (Berardy et al., 2022; Burciu Tuhut, 2023). Plant-based beverages are made from cereals like oats and rice, legumes like soy, or nuts like almonds and coconuts, with almond, soy, rice, and oat beverages being the most favored choices (Berardy et al., 2022; Taeger and Thiele, 2024; Álvarez-Álvarez et al., 2024; Walther et al., 2022; Burciu Tuhut, 2023).

Efficient regulation of plant-based beverages on the market is

* Corresponding author.
E-mail address: anna.brito@qui.uc.pt (A.L.B. Brito).

https://doi.org/10.1016/j.jfca.2025.107786
Received 27 February 2025; Received in revised form 26 April 2025; Accepted 15 May 2025
Available online 15 May 2025

essential to meet consumer needs. Such regulation depends on thorough studies of the products' composition and stability. Additionally, it is essential to conduct detailed analyses of milk composition also to detect adulteration processes and ensure the quality and authenticity of the products being sold (Mendes et al., 2016).

Nowadays, the analysis of milk can be undertaken using a plethora of techniques, which includes chromatographic [e.g., high-performance liquid chromatography (HPLC), gas chromatography (GC)], spectroscopic/spectrometric [infrared (IR), Raman and nuclear magnetic resonance (NMR) spectroscopies, mass spectrometry (MS)], refractometric, electrophoretic, cryoscopic, chemical (e.g., Kjedahl method for determination of the total protein contents), and enzymatic (enzyme-linked immunosorbent assay (ELISA)) methods. These methods are often used in combination to provide a comprehensive analysis of milk, ensuring its quality, safety, and authenticity in the marketplace. Among those techniques, infrared spectroscopy has the advantage of being inexpensive, easy to implement in different settings, cost-effective, fast, and essentially non-destructive, being a suitable technique to quantify major components of beverages, like fat, protein, and total solids. It has been used as an effective way to conduct exploratory compositional analysis, as well as a classification method for different types of milk (Mendes et al., 2016; Mazurek et al., 2015; El-Abassy et al., 2011; Balan et al., 2020a, 2020b; Mendes et al., 2020; Cuong et al., 2021; Reiner et al., 2020; Júnior et al., 2016; Silva et al., 2021; Thomas, 2008; Solís-Oba et al., 2011; Etzion et al., 2004; Li et al., 2015; Nieuwoudt et al., 2016; Gómez-Mascaraque et al., 2020; Xiao et al., 2022; Brandão et al., 2010).

Infrared spectroscopy is an extensively used method in many areas that is particularly powerful in providing detailed information on the constituents of a given sample, through analysis of their vibrational signatures. Because of its easy sampling, attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) has gained popularity among the existing variants of IR spectroscopy for application in quantitative and qualitative analyses, including those of milk, in particular due to its simplicity to apply (sample preparation is minimal), high reproducibility, and portability (Balan et al., 2020a; Thomas, 2008; Solís-Oba et al., 2011; Etzion et al., 2004).

ATR-FTIR spectroscopy has its analytical power amplified when used together with chemometric methods, because the information contained in vibrational spectra is generally extensive. Chemometrics allows for the efficient organization, classification, and quantification of the spectroscopic results. Among these methods, principal component analysis (PCA) appears as a simple, yet highly useful statistical method for analyzing large quantities of data, like these contained in vibrational spectra, and identifying patterns, recognizing differences, and extracting relevant information that may not be perceptible otherwise (Vašková et al., 2016). PCA is a widely used unsupervised linear projection method in exploratory data analysis. It allows for reduction of the dimensionality of the data, by creating new uncorrelated variables – the principal components – using the variance information defined in terms of the original set of variables (the frequencies, in the case of spectroscopic information) (Balan et al., 2020a; Ildiz et al., 2021; Brito et al., 2025). The method can also be used for classification, when coupled with an *a posteriori* criterion for sample grouping (Ildiz et al., 2021). Another popular chemometric method commonly used together with spectroscopic data is the hierarchical cluster analysis (HCA), which is applied to group the samples by their similarity using a specific metrics, usually the Euclidean distance between the points that define the samples in a specific vector space related to the variables, and a clustering criterion (Biancolillo and Marini, 2018; Shenbagalakshmi et al., 2023). Both PCA and HCA are unsupervised methods, so that no previous information is required for classification.

As mentioned before, this study focused on plant-based beverages commonly used as milk substitutes (specifically, almond, rice, oat, and soy drinks), utilizing ATR-FTIR spectroscopy together with PCA and HCA to develop classification models for these beverages.

2. Experimental methods

2.1. Samples

Forty samples of four different types of commercial brands of plant-based milk substituting beverages [almond (A), rice (R), oat (O), and soy (S); 10 samples of each)] were considered for analysis in this investigation (see Supplementary Material Table S1 for details). All samples were acquired from shops in Coimbra, Portugal. Before acquisition of the infrared spectra, the samples were subjected to lyophilization, which was carried out in a FreeZone 4.5 freeze dryer (Labconco, USA), at a pressure of 0.060 Torr and using a condenser temperature of –52 °C (Santos et al., 2018).

2.2. Infrared spectroscopy

Infrared spectra were obtained in the ATR-FTIR mode in a Nicolet iS5 FT-IR spectrometer (Thermo Fisher Scientific), using an iD7 ATR Accessory (Thermo Fisher Scientific) with a diamond crystal as the main component, and a deuterated triglycine sulfate detector (DTGS). Each spectrum was acquired in the range of 4000–400 cm^{-1}, with a resolution of 1 cm^{-1}, averaging 32 scans, and with data spacing of 0.120, resulting in a matrix of 29,869 variables. For each sample, measurements were taken in triplicate and averaged, and the order of the experiments was randomized.

2.3. Data analysis

The data pre-processing was conducted using Unscrambler® X.10.5.1 (Aspen UnscramblerTM, 2018). The spectra were area normalization and baseline corrected (liner correction). Scores, residuals and leverage plots were employed in the detection and elimination of outliers from the dataset. In the PCA analysis, the data were mean-centered, and equal weights were assigned to the variables (frequencies). In the HCA analysis, the Method of Hierarchical Complete-linkage with Squared Euclidean distance was used.

3. Results and discussion

The ATR-FTIR spectra of the 40 studied samples, in the range of 4000–400 cm^{-1}, was acquired, the spectral profile of all samples showing many similarities. The spectral range of 1780–680 cm^{-1} was initially chosen for the study (Fig. 1). After the preliminary data analysis for identification of outliers, a sub-range of the initially used spectral range was selected (1720.6–1371.1 cm^{-1}) for the analytical studies, as this sub-range shows more significant differences between the spectra. This sub-range comprehends essentially bands attributable to the amide groups of the proteins present in the various analyzed beverages (Amide I and II bands).

In the selected spectral region, the spectra of rice and oat beverage samples exhibit rather similar profiles, notably distinct from the spectra of soy beverage samples. On the other hand, the spectra of almond beverages show significant diversity, with some being more similar to those of soy beverages and others to the spectra of rice/oat beverages. In the characteristic region of lipids (1780.0–1720.6 cm^{-1}), all spectra are similar, indicating that the lipid content does not differ much in the samples, regardless of the type of plant-based beverage. It is important to mention that the spectra of different plant-based beverages differ significantly also in the 1146.1–880.1 cm^{-1} spectral region, which is associated with various distinct chemical species. In particular, the rice/oat group exhibits intense bands in this region and soy shows less intense bands, while almond displays a spectral variability, paralleling what is observed in the amide protein characteristic spectral region discussed above.

The composition of plant-based beverages directly impacts their FTIR spectra. The presence of emulsifiers and thickeners can modify the

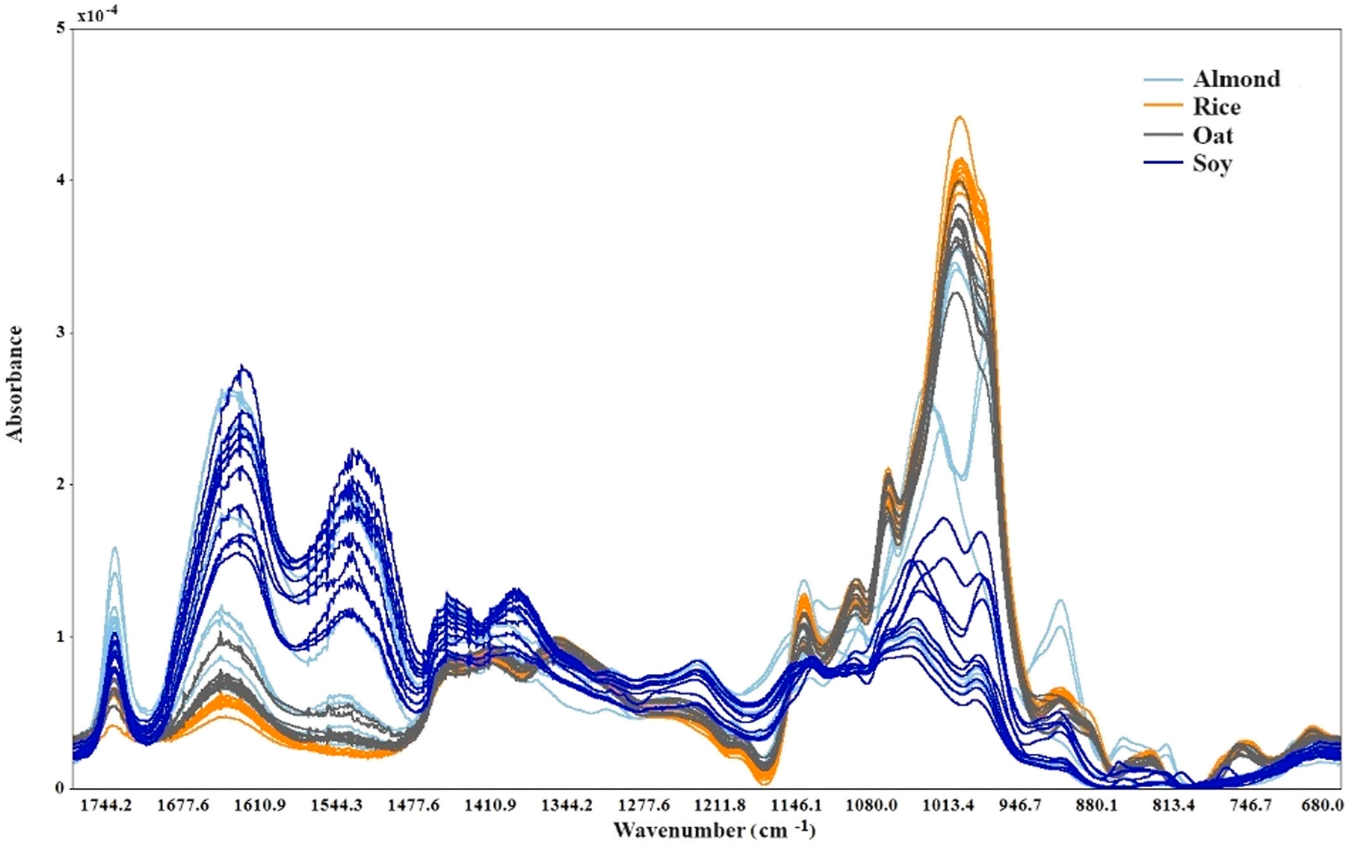

Fig. 1. 1780–680 cm^{-1} spectral region of the spectra of the studied lyophilized beverages, after area normalization and baseline correction.

spectral region associated with carbohydrates, while the addition of vegetable oils influences the bands related to lipids (~1740 cm^{-1}). In addition, thermal processing can affect the protein structure of the beverages, resulting in subtle changes in the intensity and shift of the Amide I and II bands (Khongphakdee et al., 2025). Different enzymatic hydrolysis methods used in the production of rice and oat beverages can alter the proportion of simple sugars and starches, reflected in the FTIR spectrum (Shahbal et al., 2023).

Fig. 2 presents the PCA results, performed using spectral information in the 1720.6–1371.1 cm^{-1} range, specifically the PC2 *vs* PC1 scores plot. The plot shows the high explicability in PC1, which accounts for 99 % variance in the data, PC2 accounting for the remaining 1 % variance.

In the plot, it can be seen that both the rice (R) and oat (O) samples

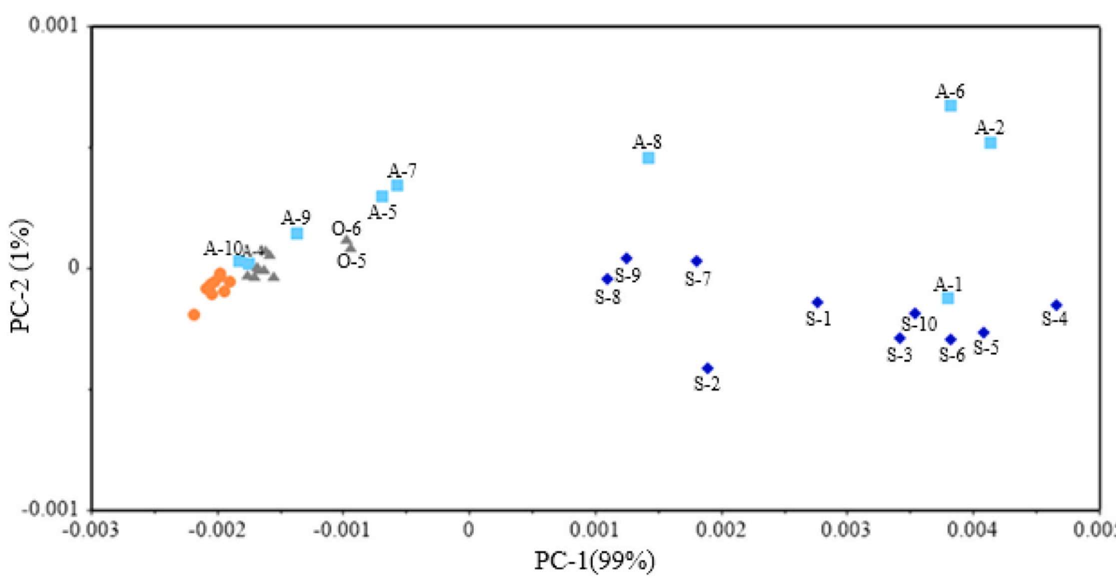

Fig. 2. Scores plot (PC1 *vs.* PC2) of plant-based beverage samples (amide vibrations region) (● - Rice, ▲ - Oat, ■ - Almond, and ◆ - Soy).

are closely clustered, while the soy (S) samples cluster exhibits a considerable larger dispersion. The rice and oat clusters stay close to each other but separated, being well-separated from the soy cluster. As anticipated considering the initial analysis of the spectra of the different types of samples, the almond (A) samples appear scattered in the scores plot. The explanation for these observations is simple: by looking to the compositions specified by the manufacturers in the labels of the different products (see Supplementary Material, Table S1) it can be seen that, whereas the different samples of each one of the rice, oat and soy beverages have similar compositions, those labeled as "almond beverage" have in fact very diverse compositions, in some cases almond contents being even smaller than their contents on soy or rice.

In the scores plot it is possible to observe that samples A-10, A-4 and A-9 are very close to the rice and oat groups. This can be explained by the fact that these samples, in spite of being designated commercially as "almond beverages" have high levels of rice in their composition (17 %, 15.2 % and 10 % respectively). The percentages of almond in these samples are in fact smaller than those of rice (1 %, 1.5 %, 2.5 %), and they should be labelled as rice beverages instead of almond drinks. In turn, sample A-1 is well included in the group of soy drinks due to its dominant content of soy in its composition (5.8 %, vs. 2.5 % of almond). The information provided in the label of the remaining samples (A-2, A-5, A-6, A-7 and A-8) indicates that they actually contained only almond. without the addition of other oilseeds. They appear scattered in the scores plot and, like for the case of the soy beverages, the scattering about the PC1 axis appears to be related with the different content of these samples in carbohydrates. For example, A-5 and A-7 have relatively large and similar carbohydrates contents and sit together for negative PC1 values (the A-samples having the most negative PC1 scores are those with the highest carbohydrates contents: A-10, A-4 and A-9), while A-2 and A-6 are carbohydrates-free samples and appear closely located to each other and in the most positive PC1 values in the plot; A8 is intermediate in this regard and occupies a location in the plot compatible with it. In the case of the soy samples, S-2, S-7, S-8 and S-9, which have the largest contents of carbohydrates (see Table S1), are located in the scores plot for the smallest positive values of PC1, while S-4 and S-5 are the soy samples with the smallest contents of carbohydrates and have the largest positive PC1 scores. The remaining samples appear have intermediate carbohydrate contents and, correspondingly, are located in the scores plot for intermediate PC1 scores values.

The results of the performed HCA are presented in Fig. 3. It can be seen that the algorithm divides the samples into two main groups, one composed by soy samples and other by oak and rice samples, while the almond samples, as expected, appear distributed by the two groups. The soy group exhibit two subgroups accounting for the intragroup dispersion already noticed in the PCA scores plot. On the other hand, the oat/rice group exhibits three subgroups: the first comprehends the rice samples, which are the most similar ones, as also evidenced in the PCA scores plot shown in Fig. 2; and the other two subgroups comprehend the oat samples, reflecting the difference between two of the samples (O-5 and O-6) and the remaining ones that can also be noticed in the PCA scores plot shown in Fig. 2. Samples O-5 and O-6 are very similar to each other in compositional terms (see Table S1) but their relative position in the PCA scores plot and in the HCA dendrogram cannot be attributed to a single compositional factor. Almond samples are present in the two subgroups associated with the oat samples, also following the pattern observed in the PCA scores plot.

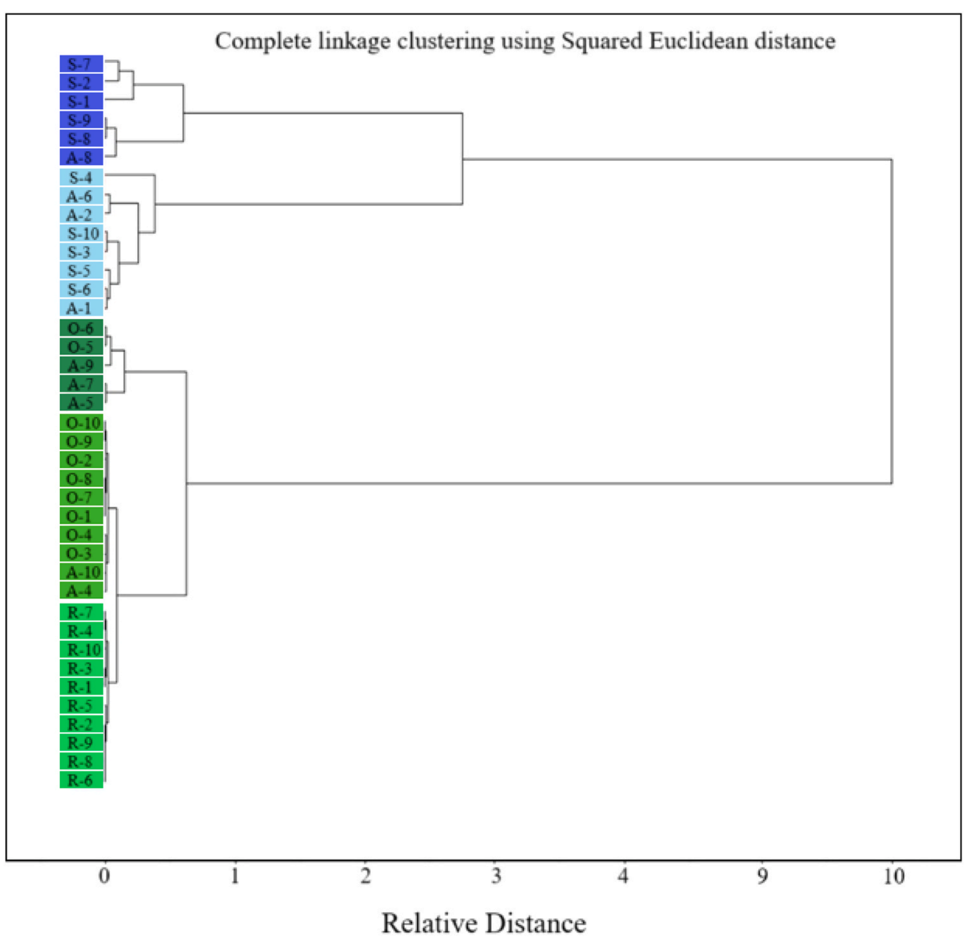

Fig. 3. HCA dendrogram for sample classification of the studied plant-based beverages, based on squared Euclidean distances (1720.6–1371.1 cm^{-1} region).

4. Conclusion

The ATR-FTIR spectral data obtained for the investigated plant-based beverages clearly distinguished all but the almond drinks based on their contents. ATR-FTIR spectroscopy is appropriate for this study, highlighting its speed, reproducibility and ability to provide compositional information without extensive sample preparation. The obtained results are in accordance with the label information on the packaging of the beverages. Both PCA and HCA analyses performed using the IR data successfully discriminated oat, rice and soy beverages, and allowed to identify major constituents in the designated "almond drinks" which have high percentages of other (rice, soy) than almond ingredients. In relation to this last point, we have to highlight that the models were shown to be able to recognize this compositional variability which appears as a characteristic of the "almond" beverage category available in the market. The followed method has the enormous advantage over the most commonly used analytical techniques for milk and milk substitutes of requiring minimum sample preparation, avoiding the requirement to separate the sample into its components for analysis. This approach demonstrates potential for qualitative analysis and classification of milk and milk substitute beverages, reducing both cost and time compared to traditional methods.

The present investigation also opens the gate for future extension of the used methodology to address other, more demanding problems. For example, the behavior of the developed models in presence of falsified beverages can be investigated in order to use them (or some more elaborated version of them) to identify possible fraud. Two main approaches can be foreseen for future studies: use the model (or an improved version of it) to perform qualitative fraud detection, or use the fundamentals of the method we developed for sugars evaluation (Brito et al., 2025) and attempt a semi-quantitative analysis. The first goal appears very much achievable, considering that, with all probability, most of the false materials added to the beverages will change the compositional profile of the falsified sample in a manner that it will not group together with the non-falsified ones. The second objective would be considerably more relevant in practical terms, but it is also much more demanding to achieve and difficult to apply in different settings. Another possible development of the strategy presented in this article is to address specific quality parameters of the beverages. However, for this to be possible, at least semi-quantitative evaluation of the compositional characteristics of the beverages has to be achieved.

CRediT authorship contribution statement

Rui Fausto: Supervision, Funding acquisition, Conceptualization, Validation, Writing – review & editing. **Catarina Duarte:** Investigation. **Anna Luiza B. Brito:** Writing – original draft, Validation, Investigation, Conceptualization, Writing – review & editing.

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 CQC-IMS is supported by FCT through projects UI0313B/QUI/2025, UI0313P/QUI/2025 and LA/P/0056/2020 (national funds). This study has also been supported by the European research Agency through the Horizon-Widera-2023-Talents-01 ERA-Chair 1011848998: Spectroscopy@IKU "*Manipulating and Characterizing Molecular Architectures: From Isolated Molecules to Molecular Crystals*". The authors also acknowledge the Laboratory for Advanced Computing at University of Coimbra (LCA-UC; https://www.uc.pt/lca) for providing computing resources, and Coimbra LaserLab (CLL) for experimental facilities.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.jfca.2025.107786.

Data availability

Data will be made available on request.

References

Álvarez-Álvarez, L., Vitelli-Storelli, F., Rubín-García, M., Martín-Sánchez, V., Fernández, C.G., Carvalho, C., Araújo, J., Ramos, E., 2024. Environmental impact of the diet of young Portuguese and its relationship with adherence to the Mediterranean diet. Eur. J. Nutr. 63, 2307–2315. https://doi.org/10.1007/s00394-024-03396-w.

Aspen UnscramblerTM(version X.5.1), AspenTech, Bedford, MA (USA), 2018.

Balan, B., Dhaulaniya, A.S., Jamwal, R., Amit, Sodhi, K.K., Kelly, S., Cannavan, A., Singh, D.K., 2020a. Application of Attenuated Total Reflectance-Fourier Transform Infrared (ATR-FTIR) spectroscopy coupled with chemometrics for detection and quantification of formalin in cow milk. Vib. Spectrosc. 107, 103033. https://doi.org/10.1016/j.vibspec.2020.103033.

Balan, B., Dhaulaniya, A.S., Jamwal, R., Yadav, A., Kelly, S., Cannavan, A., Singh, D.K., 2020b. Rapid detection and quantification of sucrose adulteration in cow milk using attenuated total reflectance-Fourier transform infrared spectroscopy coupled with multivariate analysis. Spectrochim. Acta Part A: Mol. Biomol. Spectrosc. 240, 118628. https://doi.org/10.1016/j.saa.2020.118628.

Berardy, A.J., Rubín-García, M., Sabaté, J., 2022. A scoping review of the environmental impacts and nutrient composition of plant-based milks. Adv. Nutr. 13, 2559–2572. https://doi.org/10.1093/advances/nmac098.

Biancolillo, A., Marini, F., 2018. Chemometric methods for spectroscopy-based pharmaceutical analysis. Front. Chem. 6, 576. https://doi.org/10.3389/fchem.2018.00576.

Brandão, P.M.C.A., Carmo, P.A., Bell, V.J.M., Anjos, C.V., 2010. Characterization of milk by infrared spectroscopy. Revista do Instituto de Laticínios Cândido Tostes 373, 30–33. Retrieved from Accessed March 26, 2025. http://www.researchgate.net/publication/222716940_CHARACTERIZATION_OF_MILK _BY_INFRARED_SPECTROSCOPY.

Brito, A.L.B., Cardoso, I.F., Viegas, L.P., Fausto, R., 2025. Semi-quantitative chemometric models for characterization of mixtures of sugars using infrared spectral data. Spectrochim. Acta Part A: Mol. Biomol. Spectrosc. 326, 125225. https://doi.org/10.1016/j.saa.2024.125225.

Burciu Tuhut, A.C. (2023). Análisis comparativo entre la leche, productos lácteos y bebidas vegetales. Retrieved from ⟨https://uvadoc.uva.es/bitstream/handle/10324/59968/TFG-H2765.pdf?sequence= 1&isAllowed=y⟩ Accessed March 26, 2025.

Cuong, N.M., Cao, D.T., Thu, V.T., Ngan, L.T.-Q., 2021. Direct detection of melamine in liquid milk and infant formula using surface-enhanced Raman scattering combined with silver nanodendrites. Optik 243, 167504. https://doi.org/10.1016/j.ijleo.2021.167504.

El-Abassy, R.M., Eravuchira, P.J., Donfack, P., von der Kammer, B., Materny, A., 2011. Fast determination of milk fat content using Raman spectroscopy. Vib. Spectrosc. 56, 3–8. https://doi.org/10.1016/j.vibspec.2010.07.001.

Etzion, Y., Linker, R., Cogan, U., Shmulevich, I., 2004. Determination of protein concentration in raw milk by mid-infrared fourier transform infrared/attenuated total reflectance spectroscopy. J. Dairy Sci. 87, 2779–2788. https://doi.org/10.3168/jds.S0022-0302(04)73405-0.

Gómez-Mascaraque, L.G., Kilcawley, K., Hennessy, D., Tobin, J.T., O'Callaghan, T.F., 2020. Raman spectroscopy: a rapid method to assess the effects of pasture feeding on the nutritional quality of butter. J. Dairy Sci. 103, 8721–8731. https://doi.org/10.3168/jds.2020-18716.

Ildiz, G.O., Bayari, S., Yorguner, N., Fausto, R., 2021. Chapter 10 - blood serum–infrared spectra-based chemometric models for auxiliary diagnosis of autism spectrum disorder. Neural Eng. Tech. Autism Spectr. Disord. 1, 185–213. https://doi.org/10.1016/B978-0-12-822822-7.00010-7.

Instituto Nacional de Estatística (Statistics Portugal). (2024). Human consumption of milk and dairy products per capita (kg/ inhab.) by type of milk and dairy products; Annual. [database]. Retrieved from http://www.ine.pt/xportal/xmain?xpid=INE&xpgid=ine_indicadores&indOcorrCod=0000214&selTab=table0&xlang=en. Accessed January 28, 2025.

Júnior, P.H.R., Oliveira, K.S., Almeida, C.E.R. de, Oliveira, L.F.C., Stephani, R., Pinto, M.S., Carvalho, A.F., Perrone, I.T., 2016. FT-Raman and chemometric tools for rapid determination of quality parameters in milk powder: classification of samples for the presence of lactose and fraud detection by addition of maltodextrin. Food Chem. 196, 584–588. https://doi.org/10.1016/j.foodchem.2015.09.055.

Khongphakdee, P., Peanparkdee, M., Sae-tan, S., 2025. Dual effects of thermal processing and polyphenol incorporation on bioaccessibility and functionality of soy and whey proteins. Food Chem. Adv. 6, 100905. https://doi.org/10.1016/j.focha.2025.100905.

Li, M., Chen, J., Xu, J., Fu, S., Gong, H., 2015. Determination of lactose in milk by Raman spectroscopy. Anal. Lett. 48, 1333–1340. https://doi.org/10.1080/00032719.2014.979358.

Mazurek, S., Szostak, R., Czaja, T., Zachwieja, A., 2015. Analysis of milk by FT-Raman spectroscopy. Talanta 138, 285–289. https://doi.org/10.1016/j.talanta.2015.03.024.

Mendes, T.O., Junqueira, G.M.A., Porto, B.L.S., Brito, C.D., Sato, F., Oliveira, M.A.L., Anjos, V., Bell, M.J.V., 2016. Vibrational spectroscopy for milk fat quantification: line shape analysis of the Raman and infrared spectra: vibrational spectroscopy for milk fat quantification. J. Raman Spectrosc. 47, 692–698. https://doi.org/10.1002/jrs.4878.

Mendes, T.O., Rodrigues, B.V.M., Porto, B.L.S., Rocha, R.A., Oliveira, M.A.L., Castro, F. K., Anjos, V.C., Bell, M.J.V., 2020. Raman spectroscopy as a fast tool for whey quantification in raw milk. Vib. Spectrosc. 111, 103150. https://doi.org/10.1016/j.vibspec.2020.103150.

Nieuwoudt, M.K., Holroyd, S.E., McGoverin, C.M., Simpson, M.C., Williams, D.E., 2016. Screening for adulterants in liquid milk using a portable Raman miniature spectrometer with immersion probe. Appl. Spectrosc. 71, 308–312. https://doi.org/10.1177/0003702816653130.

Reiner, J., Protte, K., Hinrichs, J., 2020. Investigation of the applicability of Raman spectroscopy as online process control during consumer milk production. ChemEngineering 4, 45. https://doi.org/10.3390/chemengineering4030045.

Santos, G., Nogueira, R.I., Rosenthal, A., 2018. Powdered yoghurt produced by spray drying and freeze drying: a review. Braz. J. Food Technol. 21, e2016127. https://doi.org/10.1590/1981-6723.12716.

Shahbal, N., Jing, X., Bhandari, B., Dayananda, B., Prakash, S., 2023. Effect of enzymatic hydrolysis on solubility and surface properties of pea, rice, hemp, and oat proteins: implication on high protein concentrations. Food Biosci. 53, 102515. https://doi.org/10.1016/j.fbio.2023.102515.

Shenbagalakshmi, G., Shenbagarajan, A., Thavasi, S., Gomathy Nayagam, M., Venkatesh, R., 2023. Determination of water quality indicator using deep hierarchical cluster analysis. Urban Clim. 49, 101468. https://doi.org/10.1016/j.uclim.2023.101468.

Silva, M.G., Paula, I.L., Stephani, R., Edwards, H.G.M., Oliveira, L.F.C., 2021. Raman spectroscopy in the quality analysis of dairy products: a literature review. J. Raman Spectrosc. 52, 2444–2478. https://doi.org/10.1002/jrs.6214.

Solís-Oba, M., Teniza-García, O., Rojas-López, M., Delgado-Macuil, R., Díaz-Reyes, J., Ruiz, R., 2011. Application of infrared spectroscopy to the monitoring of lactose and protein from whey after ultra and nano filtration process. J. Mex. Chem. Soc. 55, 190–193. Retrieved from. ⟨https://www.scielo.org.mx/pdf/jmcs/v55n3/v55n3a11.pdf⟩.

Taeger, M., Thiele, S., 2024. Replacement of milk and dairy products with soy-based alternatives–how to avoid nutrient deficiencies in a milk-free diet? J. Nutr. 154, 163–173. https://doi.org/10.1016/j.tjnut.2023.11.003.

Thomas, W.L. (2008). Use of Fourier Transform Infrared (FTIR) Spectroscopy to Determine the Health-Promoting Index (HPI) of Cow's Milk. Master of Science, Iowa State University, Digital Repository, 7019471. https://doi.org/10.31274/rtd-180813-16548. Retrieved from http://dr.lib.iastate.edu/handle/20.500.12876/68937. Accessed March 26, 2025.

Vašková, H., Bučková, M., Zálešáková, L., 2016. Spectroscopic analysis of milk fat and its mathematical evaluation. Int. J. Biol. Biomed. Eng. 10, 168–175. Retrieved from. ⟨http://www.naun.org/main/NAUN/bio/2016/a382001-452.pdf⟩.

Walther, B., Guggisberg, D., Badertscher, R., Egger, L., Portmann, R., Dubois, S., Haldimann, M., Kopf-Bolanz, K., Rhyn, P., Zoller, O., Veraguth, R., Rezzi, S., 2022. Comparison of nutritional composition between plant-based drinks and cow's milk. Front. Nutr. 9, 988707. https://doi.org/10.3389/fnut.2022.988707.

Xiao, S., Wang, Q., Li, C., Liu, W., Zhang, J., Fan, Y., Su, J., Wang, H., Luo, X., Zhang, S., 2022. Rapid identification of A1 and A2 milk based on the combination of mid-infrared spectroscopy and chemometrics. Food Control 134, 108659. https://doi.org/10.1016/j.foodcont.2021.108659.