LWT - Food Science and Technology 133 (2020) 109875

Contents lists available at ScienceDirect

LWT

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

Data fusion of UPLC data, NIR spectra and physicochemical parameters with chemometrics as an alternative to evaluating kombucha fermentation

Cosme Damião Barbosa [a], Michel Rocha Baqueta [b,d], Wildon César Rodrigues Santos [a], Dhionne Gomes [a], Verônica O. Alvarenga [a], Paula Teixeira [c], Helena Albano [c], Carlos Augusto Rosa [a], Patrícia Valderrama [b], Inayara C.A. Lacerda [a,*]

[a] Federal University of Minas Gerais – UFMG, Belo Horizonte, Minas Gerais, Brazil
[b] Federal University of Technology – Paraná - UTFPR, Campo Mourão, Paraná, Brazil
[c] Universidade Católica Portuguesa, CBQF - Biotechnology and Fine Chemistry – Laboratório Associado, Escola Superior de Biotecnologia, Rua Diogo Botelho 1327, 4169-005, Porto, Portugal
[d] Departament of Food Science, University of Campinas– UNICAMP, São Paulo, Brazil

ARTICLE INFO

Keywords:
Fermented beverage
Bioactive compounds
PCA analysis
Acetic acid bacteria

ABSTRACT

Kombucha consumption has become popular due to health benefits and sensorial properties. Different analytical techniques were associated with unsupervised chemometrics to evaluate kombucha fermentation using a low-level data fusion strategy. Kombucha was prepared from green and black teas (*Camellia sinensis*). The samples were analyzed by ultra-performance liquid chromatography (UPLC), portable near-infrared spectroscopy (NIR), and physicochemical analyses (ethanol, pH, total reducing sugars, and total titratable acidity). Also, the bioactive phenolic compounds were evaluated in the fermented samples. The merged results were analyzed by principal component analysis (PCA). The PCA was applied to discriminate substrate for kombucha production and the fermentation time. Although the fermentation behavior was similar for both substrates, the kombucha showed quantitative differences in physicochemical parameters. They also showed differences in bioactive compounds for each kombucha. Data fusion strategy was more effective to differentiate the two types of kombucha than single analysis. The portable NIR can be a reliable and robust analysis for fermentation monitoring. Moreover, the results can be used as a base to further studies and mainly to help in which substrate composition is better to be produced on an industrial scale.

1. Introduction

Kombucha is an Asiatic beverage obtained through the fermentation of sugared tea infusion, usually prepared with *Camellia sinensis*. The characteristics flavor and aroma of kombucha are sweet, slightly acidic, and naturally sparkling (Jayabalan et al., 2011; Jayabalan, Malbaša, Lončar, Vitas, & Sathishkumar, 2014). The substrate composition, e.g., black or green tea, can provide some biologically active substances, including polyphenols, flavonoids, and phenolic acids. These substances are known to be antioxidant, antimicrobial, anti-inflammatory, and anti-carcinogenic activities. Therefore, health benefits may be associated with kombucha consumption (Banerjee et al., 2010; Bhattacharya et al., 2016; Jayabalan et al., 2011, 2014; Shahidi & Ambigaipalan, 2015; Sreeramulu, Zhun, & Knol, 2000).

Several factors affect kombucha composition and sensorial characteristics such as the substrate, source, inoculum viability, temperature, and cell growth (De Filippis, Troise, Vitaglione, & Ercolini, 2018; Jayabalan et al., 2008, 2011, 2014; Sreeramulu et al., 2000). During the fermentation, the combined effects of microbial growth and substrate are among the main factors to influence the production of different metabolite profiles. Variation in substrate composition may lead to different pathways during fermentation. To several biochemical reactions occur in formation ethanol, bioactive substances, and volatile organic compounds (Battikh, Bakhrouf, & Ammar, 2012; Neffe-Skocińska, Sionek, Ścibisz, & Kołożyn-Krajewska, 2017).

The chemical composition encompasses organic acids, sugars, vitamins, biogenic amines, pigments, lipids, proteins, some hydrolytic enzymes, ethanol, antimicrobial compounds, carbon dioxide, and some tea

* Corresponding author.
E-mail addresses: barbosacosme@yahoo.com.br (C.D. Barbosa), vealvarenga@ufmg.br (V.O. Alvarenga), pcteixeira@porto.ucp.pt (P. Teixeira), microhel@gmail.com (H. Albano), carlrosa@icb.ufmg.br (C.A. Rosa), pativalderrama@gmail.com (P. Valderrama), inayarac@farmacia.ufmg.br (I.C.A. Lacerda).

https://doi.org/10.1016/j.lwt.2020.109875
Received 31 January 2020; Received in revised form 9 July 2020; Accepted 10 July 2020
Available online 26 July 2020
0023-6438/

polyphenols – in green tea: catechin and epicatechin; in black tea: quercetin (Jayabalan et al., 2014; Malbaša, Lončar, & Kolarov, 2004).

The kombucha is a complex food matrix in which the determination of its quality requires a holistic characterization. Thus, a single parameter or analytical technique may not be sufficient for a comprehensive evaluation of fermentation. In this case, a combination of different analytical methods may be interesting to study the relationship of distinct chemical information on the same samples, aiming to evaluate the stages of kombucha fermentation objectively. In the field of food and beverage analysis, ultra-performance liquid chromatography (UPLC) is a well-established technique widely applied for dealing with the determination of specific bioactive substances in a sample (Essawet et al., 2015; Jayabalan, Marimuthu, & Swaminathan, 2007). On the other hand, other analytical approaches such as vibrational spectroscopy have been proposed for a simpler, faster and relatively less expensive analysis compared with chromatographic techniques (Baqueta, Coqueiro, Março, & Valderrama, 2019; Correia et al., 2018; Lobato, Alamar, Caramês, & Pallone, 2018). Near-infrared spectroscopy (NIR) has emerged as a non-target technology for direct food analysis. The advantage of NIR spectroscopy over chromatographic techniques, e.g., UPLC, is that it performs non-destructive analysis and does not require extensive sample preparation (Monteiro et al., 2018).

Moreover, in this study, a portable NIR spectrometer (microNIR) was used. It has the same applications as conventional NIR, with the advantages that it is compact, low-cost, quick, and sensitive (Correia et al., 2018). In particular, the UPLC complements the molecular information from NIR with more specific composition information, and for this reason, these techniques were used in this study.

The use of data fusion may be considered as a strategy to combine data from distinct instrumental techniques (Assis et al., 2019; Li, Xie, Ning, Chen, & Zhang, 2019; Ríos-Reina, Callejón, Savorani, Amigo, & Cocchi, 2019). The advantage of data fusion is merging relevant chemical information from various equipment or experiments, resulting in more valuable information extraction from a single sample set (Banerjee, Roy, Tudu, Bandyopadhyay, & Bjhattacharyya, 2018). There are three principal approaches in data fusion: low, mid, and high-level. More information about data fusion strategies can be found in the literature (Cuevas, Pereira-Caro, Moreno-Rojas, Muñoz-Redondo, & Ruiz-Moreno, 2017; Godinho et al., 2014; Ríos-Reina et al., 2019). Here, low-level approach fusion was used because it is the only approach that fully exploits the multivariate advantage. In this approach, the data from different analytical sources are concatenated into a common data matrix after suitable pre-processing and weighting (Schwolow, Gerhardt, Rohn, & Weller, 2019). Then, some chemometric tools are applied in the data fusion matrix to obtain relevant information about the sample set analyzed under different techniques. In particular, principal component analysis (PCA) has been proposed with encouraging results as an unsupervised method for exploratory purposes (Gonçalves et al., 2020). So far up to the knowledge of the authors, no studies have been carried out using the data fusion approach associated with chemometrics for kombucha fermentation.

This study aims to assess differences in kombucha composition using UPLC, NIR, and physicochemical analyses merged in a low-level data fusion approach. Despite the limitations, this approach can provide qualitative differentiation of complex food matrices such as kombucha. Moreover, it allows the description of biochemical changes in kombucha fermentation (Biancolillo, Boqué, Cocchi, & Marini, 2019).

2. Material and methods

2.1. Reagent, substrate and culture

All reagents and the UPLC standards (chlorogenic acid, gallic acid, caffeine, catechin, quercetin, and rutin) used in this study were of analytical grade and were obtained from Sigma–Aldrich. Three batches of black and green tea samples (*Camellia sinensis*) were purchased in the local market at Belo Horizonte, Brazil. After that, the samples were brought to the laboratory where they were randomly sorted before the experiments were carried. An artisanal producer provided the kombucha starter culture (fermented broth and cellulosic pellicle). The located of an artisanal producer was Uberlândia, Minas Gerais-Brazil with the following geographical coordinates: 18° 55′ 07″ S; 48° 16′ 38″ W.

2.2. Inoculum preparation

The beverages were individually prepared by infusion of 22.5 g of green or black tea leaves in 1.5 L of boiling mineral water for 15 min; then, the infusions were filtered through a filter membrane followed by sucrose addition (120 g). After cooling (at 25 °C) of both teas, the kombuchas were produced by inoculating of the starter culture (150 mL of fermented broth and 75 g cellulosic pellicle) from our supplier and incubating for 15 days at 28 ± 2 °C in a bioreactor.

2.3. Sampling

The fermentation process was carried out for 15 days, and samples were collected at different times: 0, 3, 7, 10, and 15 days. A total of 6 fermentations were performed for green tea (n = 3) and black tea (n = 3). All fermentation processes were done in triplicate.

All samples were analyzed to determine bioactive substances (chlorogenic acid, gallic acid, caffeine, catechin, quercetin, and rutin), physicochemical parameters (pH, total reducing sugars, total titratable acidity, and ethanol) and NIR absorbance from kombucha beverages. The analyses are described below.

2.4. Identification of bioactive compounds by UPLC

Identification of bioactive compounds was carried out according to previous works (Chisté, Freitas, Mercadante, & Fernandes, 2012; Eça, Machado, Hubinger, & Menegalli, 2015). It was used as a UPLC system (Acquity ™, Waters) with a diode array detector. An Aquacity UPLC BEH C18 column (100 mm × 2.1 mm) with a 1.7 μm particle size was used for chromatographic separations. The samples were filtered through a membrane filter (KASVI, 0.45 μm) before injection. The mobile phase components were acetonitrile (A) and ultrapure water containing 0.5% formic acid (B) at a flow rate of 0.3 mL min^{-1}. Aliquots of 10 μL of samples were injected under the linear gradient starting at 5% A (0–3 min); 8% A (3–10 min); 19% A (10–14 min); 27% A (14–20 min). Bioactive compounds monitored were detected at 271 nm (gallic acid, catechin, and caffeine), 320 nm (chlorogenic acids), 354 nm (rutin), and 371 nm (quercetin).

2.5. Near-infrared analysis and spectra preprocessing

A NIR spectrum was obtained from all kombucha samples, where each replicate was considered as one sample (in total 90 samples). The absorbance was recorded by a portable microNIR (MicroNIR™ 1700, JDSU Uniphase Corporation) at room temperature (22 ± 2 °C) using a glass cuvette. The spectral profile of each sample was acquired as the mean of 32 scans and in the spectral range of 900 to 1.650 nm. The blank was measured using a NIR reflectance standard (Spectralon™) with a diffuse reflection coefficient of 99%, while a dark reference (zero - to simulate non-reflection) was obtained with the lamp off. No sample preparation was made. In the present study, pre-treatments on microNIR spectrum were: multiplicative scatter correction (Geladi, MacDougall, & Martens, 1985) and Savitzky–Golay smoothing with a window size of five points and first derivative with first-order polynomial (Savitzky & Golay, 1964) using the Matlab software version R2019a.

2.6. Determination of physicochemical parameters

Ethanol, pH, total reducing sugars, and total titratable acidity were analyzed for all samples. The ethanol was determined using a Thermo Plate TP Reader (600 nm) spectrophotometry based on the method described by Salik and Povoh (1993). The pH was measured using a pH meter with a combined electrode (MS Tecnopon MPA 210), according to AOAC (2007). For the evaluation of total reducing sugars, a spectrophotometry technique (Thermo Plate TP Reader) with 3,5-dinitrosalisylic acid (DNS) at 540 nm was used (Miller, 1959). Finally, total titratable acidity was determined by titration with 0.1 N NaOH, according to Instituto Adolfo Lutz (2008).

2.7. Data fusion approach

In this study, a low-level data fusion approach was implemented, in which a previous preprocessing was independently performed over each dataset. To applied data fusion, all variables studied were organized in matrices, where the lines represented the samples and the columns the variables.

Here, each replicate was considered as one sample, resulting in 90 samples studied. Samples were numbered from 1 to 90, comprising kombucha prepared from black (1–45) and green (46–90) teas. Low-level data fusion was applied to a matrix composed of 90 samples and 131 variables). The variables that form the matrix were bioactive compounds chlorogenic acid, gallic acid, caffeine, catechin, quercetin, and rutin - 06 variables), physicochemical parameters total reducing sugars, ethanol, pH, total titratable acidity - 04 variables) and NIR absorbance (121 variables). In the development of our data fusion, each dataset was previously pre-processed before combining the fusion matrix. Bioactive substances and physicochemical parameters were autoscaled, while NIR spectra were pre-treated by multiplicative scatter correction and Savitzky–Golay smoothing as previously described. After individual preprocessing, both datasets were individually normalized and joined in a fusion matrix with all variables (Gonçalves et al., 2020).

2.8. Multivariate analysis

The results obtained in this study were merged in a data fusion approach with a subsequent evaluation by classical PCA. Several multivariate tools have been used to collect valuable information regarding data fusion matrices (Gonçalves et al., 2020; Schwolow et al., 2019). Here, however, we are specifically concerned with the potential of PCA for exploring kombucha fermentation. PCA was performed according to established recommendations and more information on the unsupervised pattern recognition technique can be found in the literature (da Silva Sauthier et al., 2019; Penttilä, Martikainen, Gritsevich, & Muinonen, 2018; Santos et al., 2018). The model was built with a mean center preprocess.

3. Results and discussion

3.1. Statistics on chemical values

Due to the dimensionality of the table, the results for each sample are presented in Table S1 as supplementary material. The kombucha samples were analyzed by UPLC, NIR, and physicochemical analysis. Regarding UPLC analysis, the bioactive compounds chlorogenic acids, gallic acid, caffeine, catechin, quercetin, and rutin were identified in

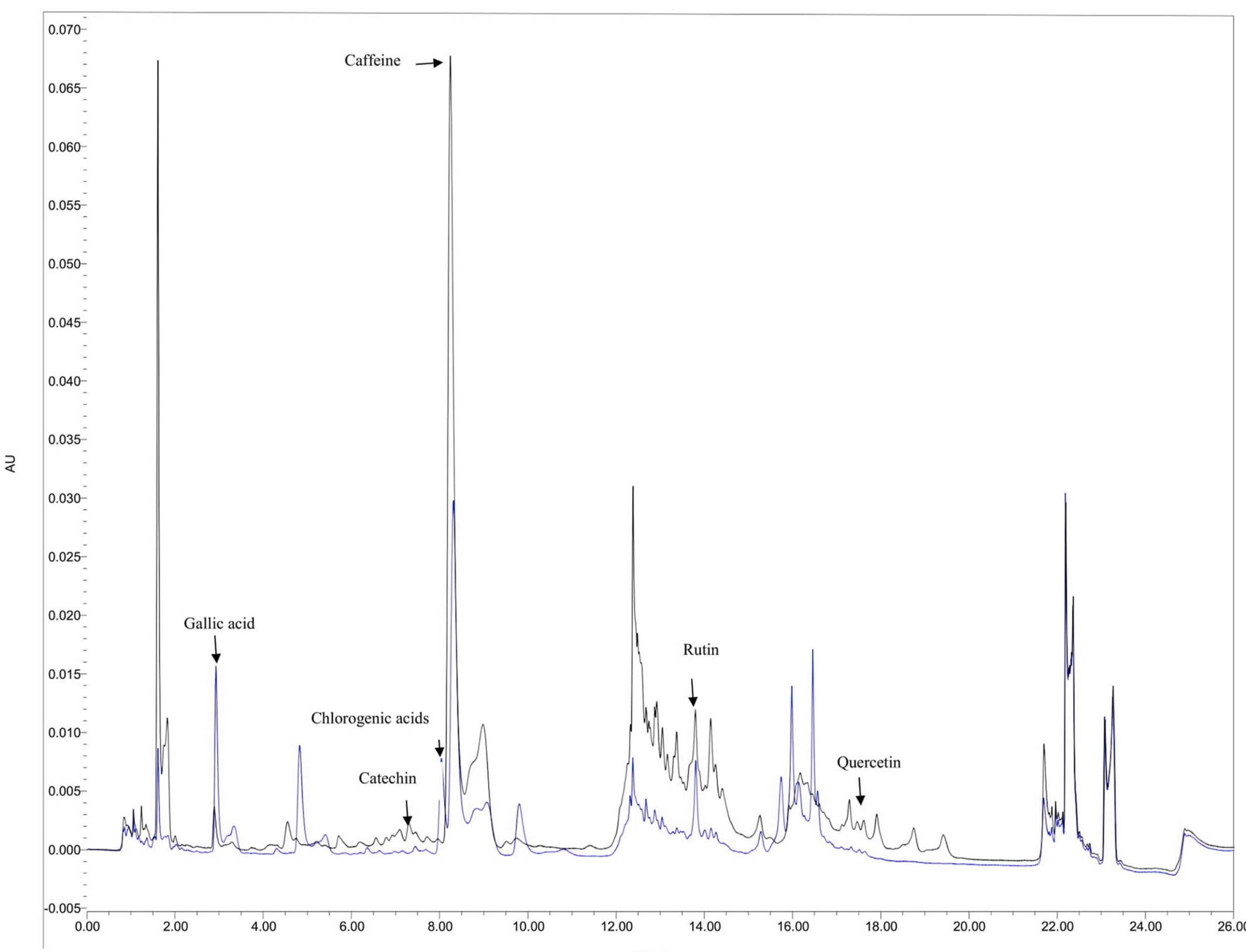

Fig. 1. Bioactive compounds identification of the kombucha prepared with green (blue line) and black tea (black line).

both kombucha (Fig. 1). The concentration of gallic acid (71.04 ± 2.59 mg L^{-1}), caffeine (177.37 ± 1.09 mg L^{-1}), rutin (30.19 ± 0.31 mg L^{-1}), quercetin (1.22 ± 0.01 mg L^{-1}) and catechin (8.00 ± 1.40 mg L^{-1}) in black tea kombucha (KB) is higher green tea kombucha (KG). While KG showed higher chlorogenic acid concentration (65.42 ± 0.63 mg L^{-1}).

Many of the protective effects of bioactive substances present in green and black teas are attributed to phenolic compounds such as phenolic acids, except rutin and quercetin, which are flavonoids. Phenolic acids occur in the form of hydroxybenzoic acids and hydroxycinnamic acids in vegetal fonts as in tea (Shahidi & Ambigaipalan, 2015). In general, the results obtained in this work indicated the presence of these biologically active compounds in both kombuchas produced.

Concerning to physicochemical parameters, at the end of fermentation, the pH was 3.05 ± 0.03 and 3.09 ± 0.01 for green tea and black tea kombucha, respectively, the total titratable acidity was of 27.44 ± 0.01 g L^{-1} for green tea and 24.17 ± 6.05 g L^{-1} for black tea. The final content of ethanol was less than 1 g L^{-1} (1%) for both kombuchas, which characterizes the kombuchas as non-alcoholic beverages. The total reducing sugars decreased during the fermentation process. This fact may be inferred from the good viability of the inoculum. The parameters showed that both kombuchas fermentation carried off a satisfactory way until 15 days. In this process, the sucrose was converted to ethanol for yeast, followed by acetylation to acetic acid. The pH and titratable acidity showed changes during the fermentation process due to the formation of organic acids.

3.2. NIR analysis

The raw microNIR spectra during the fermentation time of all samples are shown in Fig. 1S as supplementary material. The microNIR preprocessed spectra for the kombucha samples exhibited absorption bands in the regions of 906–1050 nm, 1150–1250 nm, and 1300–1500 nm, corresponding to the third, second, and first overtones, respectively (Fig. 2) (MetrohmNIR Systems, 2013; Osborne, 2000). Absorptions in the microNIR spectrum refer to the presented functional groups, such as OH, CH, and NH (Correia et al., 2018). However, how NIR spectroscopy is not selective, it is difficult to conclude only by observing the spectra of both kombuchas. There is no evident pattern in the spectroscopic profile of kombucha prepared from black tea and green tea. For this reason, a chemometric treatment is necessary to extract valuable information on this data.

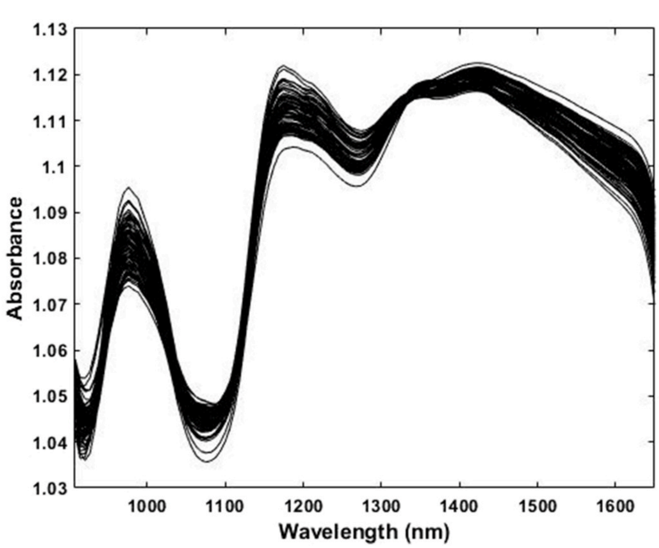

Fig. 2. Preprocessed NIR spectra from all kombucha samples.

3.3. Data fusion approach with chemometrics

For the data fusion approach applied in this study, all results from UPLC, NIR, and physicochemical analyses were used. After low-level data fusion applications on our datasets, classical PCA was used to provide informative plots through scores and loadings. Also, the data fusion combined with PCA proposed allows the assessment of which portion of each variable or analytical technique has a greater influence under the dispersion presented in the scores.

The first two PCA dimensions were sufficient to explain 80.01% of the variance in the data fusion matrix (56.62% in principal component (PC) 1 and 23.39% in PC2). Both dimensions present valuable information regarding the chemical composition and fermentation process of both kombuchas. The first PCA dimension mainly differentiated between the kombucha produced with different substrates (black or green tea) (Fig. 3A). The kombucha prepared with black tea presented positive scores, while kombucha made with green tea presented a negative score. It was possible to verify that the samples are separated along PC1 into two clusters that show a score profile of each kombucha.

Assessing NIR spectroscopy contributions for sample distribution (Fig. 3B), all spectral region (906–1650 nm) has importance for clusters observed in scores. The NIR spectroscopy influences can be assigned to a shift in the absorption bands in the regions of the first, second, and third overtones, probably overdue to the differences in the amount of the compounds that present these bonds in both kombuchas. Thus, it can be suggested that the kombucha prepared using different substrates had differences in chemical composition that the NIR spectroscopy detected and illustrated by the first PCA dimension.

The kombucha samples prepared with black tea were discriminated by the first model dimension, which mostly described variation in the gallic acid, catechin, caffeine, rutin, and quercetin bioactive compounds (Fig. 3C). Kombucha produced from black tea shows higher differences of these compounds compared to kombucha prepared from green tea. In opposite, kombucha prepared with green tea were better discriminated by the variations if total reducing sugars, ethanol, pH, total titratable acidity, and mainly chlorogenic acids, which varies largely in comparison to kombucha produced with green tea as can see in Table S1.

The results showed similar behavior for kombucha fermentation. In PCA second dimension (Fig. 4A) could be observed in the sample dispersion by fermentation time. The scores profiles in PC2 showed fermentation evolution along the time. The total period of fermentation (15 days) was divided into three main phases: start, middle, and end. Thus, a trend visual separation of clusters can be noted, where the behavior of both kombuchas samples (prepared with green or black tea) along fermentation seem similar. The samples at the starting stage of fermentation (zero-day) are distributed on the superior side (most positive scores) of PC2. The samples at the end of fermentation (fifteen days) are dispersed in a lower area (from negative scores), and the samples at the middle of fermentation (three, seven and ten days) are distributed in an intermediate zone, showing positive and negative scores along second PCA dimension. These results indicate that kombucha fermentation occurs in a similar way using different substrates. This finding can be useful in both quality control of the food industry and future applications.

Regarding the NIR analysis, all spectral region again has importance for clusters observed in second PCA dimension scores (Fig. 4B). However, this dimension could verify the differences and similarities of both kombuchas focusing on the fermentative process. Therefore, it is possible to deduce that despite qualitative differences in the chemical composition of the kombucha, the NIR spectroscopy associated with the PCA also can extract information beyond that already obtained in lower projections.

Considering the distribution from the samples in the second dimension, the total reducing sugars, pH, and total titratable acidity were the main variables associated with the observations found (Fig. 4C). The total reducing sugars and the pH were the most critical variables for

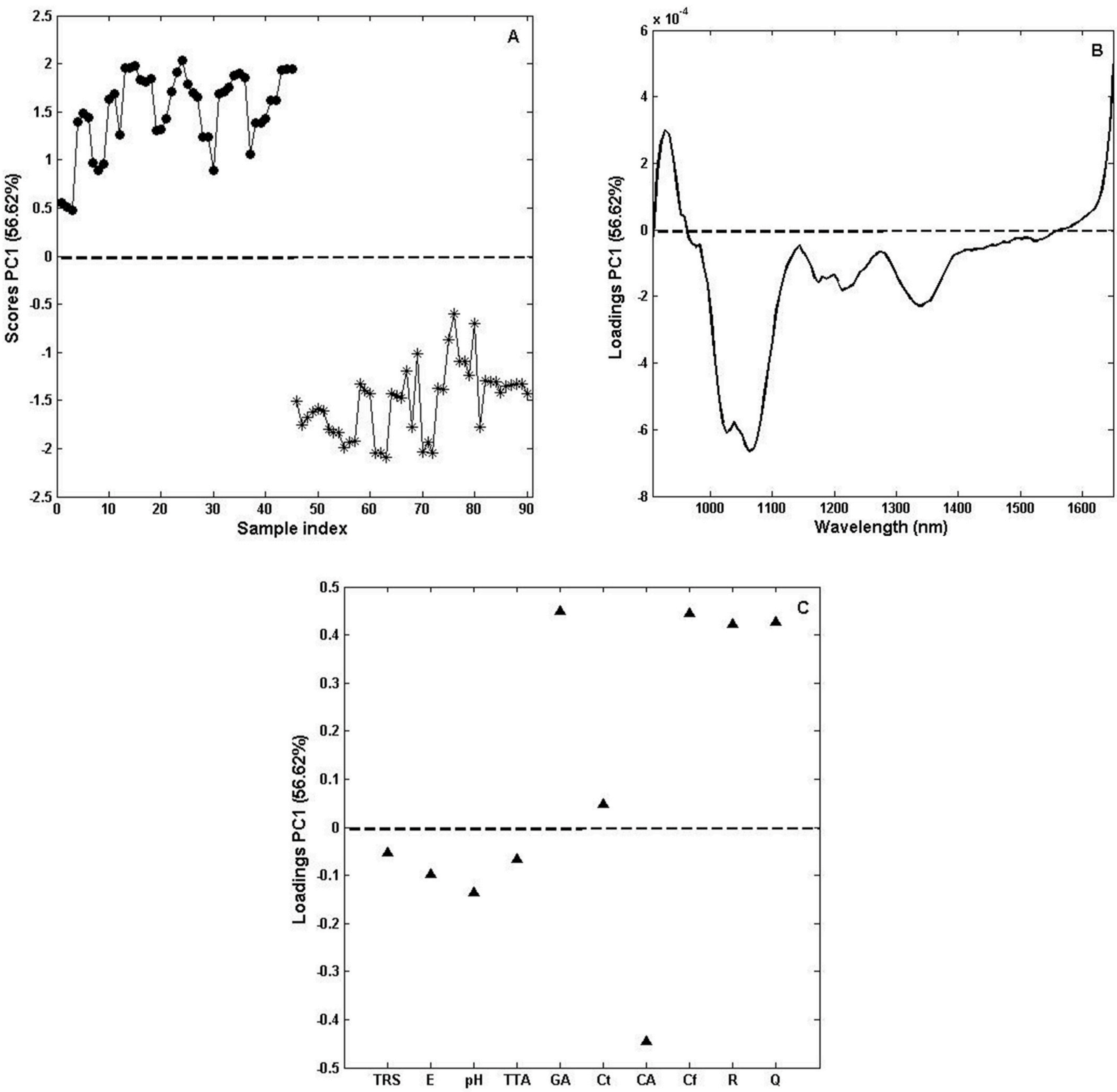

Fig. 3. PCA maps obtained from PC1. (A) Scores, (B) NIR loadings, and (C) loadings of the physicochemical parameters.

discriminating the fermentation starts (at day zero). In contrast, the total titratable acidity was more associated with the fermentation end (at fifteen days). These differences in acidity could be attributed to the decrease in total reducing sugars along the fermentative process, which decreases the pH and consequently increase the total titratable acidity as expected. In the middle stage of the fermentation (at three, five, and ten days), the samples were better discriminated by the variations in catechin, chlorogenic acids, caffeine, rutin, and quercetin bioactive compounds. Ethanol and gallic acid differences were not statistically significant in this dimension.

Additionally, the results gather evidence to show the significant differences between green and black kombucha – the green kombucha has higher concentrations of chlorogenic acids, and black has higher concentrations of caffeine, rutin, and quercetin. The key factors involved in these differences may be useful information to be used in the industrial fermentation to produce the highest quality and quantity kombucha. Furthermore, the results suggest that the use of a portable NIR is a reliable tool for on-line monitoring fermentation, especially when different substrates are compared.

4. Conclusions

In this study, kombucha fermentation was investigated by different analytical techniques, including UPLC, portable NIR spectroscopy, and physicochemical analyses. The results were merged in a low-level data fusion approach coupled with unsupervised chemometrics, which showed informative plots and an understanding of kombucha fermentation, mainly when different substrates are used in its production. Despite their quantitative differences, concerning bioactive compounds and physicochemical properties, the results show that both kombuchas,

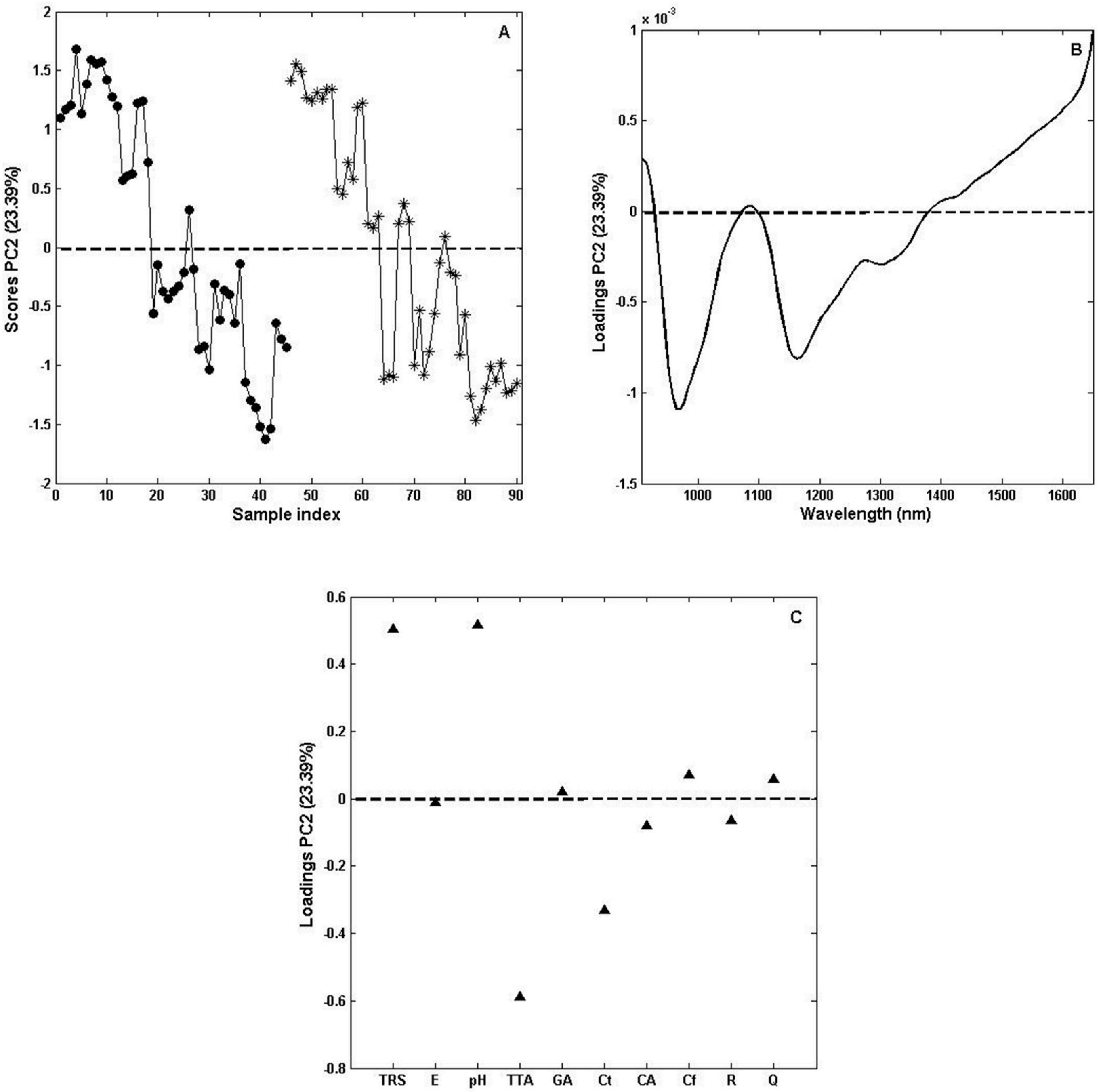

Fig. 4. PCA maps obtained from PC2. (A) Scores, (B) NIR loadings, and (C) loadings of the physicochemical parameters.

prepared with green or black tea, behaved similarly during fermentation. The achieved results allowed to conclude that the data fusion of UPLC, NIR, and physicochemical parameters at low-level combined with unsupervised chemometrics can be used as an alternative method to evaluate kombucha fermentation. Moreover, the results can be used as a base to further studies and mainly to help in which substrate composition is better to be produced in an industrial scale. Furthermore, portable NIR can be a reliable and robust analysis for fermentation monitoring.

CRediT authorship contribution statement

Cosme Damião Barbosa: Conceptualization, Methodology, Formal analysis, Writing - original draft. **Michel Rocha Baqueta:** Methodology, Writing - original draft, Software. **Wildon César Rodrigues Santos:** Methodology. **Dhionne Gomes:** Methodology. **Verônica O. Alvarenga:** Writing - review & editing. **Paula Teixeira:** Funding acquisition, Writing - review & editing. **Helena Albano:** Writing - review & editing, Supervision. **Carlos Augusto Rosa:** Writing - review & editing. **Patrícia Valderrama:** Methodology, Writing - original draft, Software. **Inayara C.A. Lacerda:** Conceptualization, Methodology, Formal analysis, Writing - review & editing, Supervision.

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. Cosme D. Barbosa.

Acknowledgments

The authors thank the CAPES (Coordenação de Aperfeiçoamento de Pessoal de Nível Superior) for the Doctoral Program Sandwich Abroad (Cosme D. Barbosa) [88881190024/2018–1, 2018] and the scientific collaboration under the Fundação para a Ciência e a Tecnologia (FCT, Portugal), project UID/Multi/50016/2019. Michel R. Baqueta thanks CAPES for MSc scholarship. Patrícia Valderrama thanks Fundação Araucária (process 033/2019).

Appendix ASupplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.lwt.2020.109875.

References

Assis, C., Pereira, H. V., Amador, V. S., Augusti, R., de Oliveira, L. S., & de Sena, M. M. (2019). Combining mid-infrared spectroscopy and paper spray mass spectrometry in a data fusion model to predict the composition of coffee blends. *Food Chemistry, 281*, 71–77. https://doi.org/10.1016/j.foodchem.2018.12.044.

Association of Official Analytical Chemists – AOAC. (2007). *Official methods of analysis* (18th ed.) (Gaithersburg, M.D, USA).

Banerjee, D., Hassarajani, S. A., Maity, B., Narayan, G., Bandyopadhyay, S. K., & Chattopadhyay, S. (2010). Comparative healing property of kombucha and black tea against indomethacin induced gastric ulceration in mice: Possible mechanism of action. *Food & Function, 1*(3), 284–293. https://doi.org/10.1039/c0fo00025f.

Banerjee, M. B., Roy, R. B., Tudu, B., Bandyopadhyay, R., & Bhattacharya, N. (2018). Black tea classification employing feature fusion of E-Nose and E-Tongue responses. *Journal of Food Engineering, 244*, 55–63. https://doi.org/10.1016/j.jfoodeng.2018.09.022.

Baqueta, M. R., Coqueiro, A., Março, P. H., & Valderrama, P. (2019). Quality control parameters in the roasted coffee industry: A proposal by using microNir spectroscopy and multivariate calibration. *Food Analytical Methods*, 1–11. https://doi.org/10.1007/s12161–019–01503–w (in press).

Battikh, H., Bakhrouf, A., & Ammar, E. (2012). Antimicrobial effect of Kombucha analogues. *Lebensmittel-Wissenschaft und -Technologie- Food Science and Technology, 47*(1), 71–77. https://doi.org/10.1016/j.lwt.2011.12.033.

Bhattacharya, D., Bhattacharya, S., Patra, M. M., Chakravorty, S., Sarkar, S., Chakraborty, W., et al. (2016). Antibacterial activity of polyphenolic fraction of kombucha against enteric bacterial pathogens. *Current Microbiology, 73*(6), 885–896. https://doi.org/10.1007/s00284-016-1136-3.

Biancolillo, A., Boqué, R., Cocchi, M., & Marini, F. (2019). Data fusion strategies in food analysis. In *Data handling in science and technology* (Vol. 31). https://doi.org/10.1016/B978-0-444-63984-4.00010-7.

Chisté, R., Freitas, M., Mercadante, A., & Fernandes, E. (2012). The potential of extracts of *Caryocar villosum* pulp to scavenge reactive oxygen and nitrogen species. *Food Chemistry, 135*(3), 1740–1749. https://doi.org/10.1016/j.foodchem.2012.06.027.

Correia, R. M., Tosato, F., Domingos, E., Rodrigues, R. R. T., Aquino, L. F. M., Filgueiras, P. R., et al. (2018). Portable near infrared spectroscopy applied to quality control of Brazilian coffee. *Talanta, 176*, 59–68. https://doi.org/10.1016/j.talanta.2017.08.009.

Cuevas, F. J., Pereira-Caro, G., Moreno-Rojas, J. M., Muñoz-Redondo, J. M., & Ruiz-Moreno, M. J. (2017). Assessment of premium organic orange juices authenticity using HPLC-HR-MS and HS-SPME-GC-MS combining data fusion and chemometrics. *Food Control, 82*, 203–211. https://doi.org/10.1016/j.foodcont.2017.06.031.

De Filippis, F., Troise, A. D., Vitaglione, P., Vitaglione, P., & Ercolini, D. (2018). Different temperatures select distinctive acetic acid bacteria species and promotes organic acids production during Kombucha tea fermentation. *Food Microbiology, 73*, 11–16. https://doi.org/10.1016/j.fm.2018.01.008.

Essawet, N. A., Cvetkovic, D., Velićanski, A., Čanadanović-Brunet, J., Vulić, J., Maksimović, V., et al. (2015). Polyphenols and antioxidant activities of Kombucha beverage enriched with Coffeeberry® extract. *Chemical Industry and Chemical Engineering Quarterly, 21*, 399–409. https://doi.org/10.2298/CICEQ140528042E.

Eça, K. S., Machado, M. T. C., Hubinger, M. D., & Menegalli, F. C. (2015). Development of active films from pectin and fruit extracts: Light protection, antioxidant capacity, and compounds stability. *Journal of Food Science, 80*(11), 2389–2396. https://doi.org/10.1111/1750-3841.13074.

Geladi, P., MacDougall, D., & Martens, H. (1985). Linearization and scatter-correction for near-infrared reflectance spectra of meat. *Applied Spectroscopy, 39*(3), 491–500. https://doi.org/10.1366/0003702854248656.

Godinho, M. S., Blanco, M. R., Neto, F. F. G., Lião, L. M., Sena, M. M., Tauler, R., et al. (2014). Evaluation of transformer insulating oil quality using NIR, fluorescence and NMR spectroscopic data fusion. *Talanta, 129*, 143–149. https://doi.org/10.1016/j.talanta.2014.05.021.

Gonçalves, T. R., Rosa, L. N., Torquato, A. S., da Silva, L. F. O., Março, P. H., Gomes, S. T. M., et al. (2020). Assessment of Brazilian monovarietal olive oil in two different package systems by using data fusion and chemometrics. *Food Analytical Methods, 13*, 86–96. https://doi.org/10.1007/s12161-019-01511-w.

Instituto Adolfo Lutz - IAL. (2008). *Normas analíticas: Métodos químicos e físicos para alimentos* (4 ed). São Paulo. http://www.ial.sp.gov.br/ial/publicacoes/livros/metodos-fisico-quimicos-para-analise-de-alimentos/. (Accessed 11 June 2020).

Jayabalan, R., Chen, P., Hsieh, Y., Prabhakaran, K., Pitcha, P., Marimuthu, S., et al. (2011). Effect of solvent fractions of Kombucha tea on viability and invasiveness of cancer cells- Characterization of dimethyl 2-(2- hydroxy-2-methoxypropylidine) malonate and vitexin. *Indian Journal of Biotechnology, 10*, 75–82.

Jayabalan, R., Malbaša, R. V., Lončar, E. S., Vitas, J. S., & Sathishkumar, M. (2014). A review on kombucha tea-microbiology, composition, fermentation, beneficial effects, toxicity, and tea fungus. *Comprehensive Reviews in Food Science and Food Safety, 13*(4), 538–550. https://doi.org/10.1111/1541-4337.12073.

Jayabalan, R., Marimuthu, S., & Swaminathan, K. (2007). Changes in content of organic acids and tea polyphenols during Kombucha tea fermentation. *Food Chemistry, 102*(1), 392–398. https://doi.org/10.1016/j.foodchem.2006.05.032.

Jayabalan, R., Marimuthu, S., Thangaraj, P., Sathishkumar, M., Binupriya, A., Swaminathan, K., et al. (2008). Preservation of kombucha tea -effect of temperature on tea components and free radical scavenging properties. *Journal of Agricultural and Food Chemistry, 56*, 9064–9071. https://doi.org/10.1021/jf8020893.

Li, X., Ning, Chen, Q., & Zhang, Z. (2019). Evaluating green tea quality based on multisensor data fusion combining hyperspectral imaging and olfactory visualization systems. *Journal of the Science of Food and Agriculture, 99*, 1787–1794. https://doi.org/10.1002/jsfa.9371.

Lobato, K. B. de S., Alamar, P. D., Caramês, E. T., dos, S., & Pallone, J. A. L. (2018). Authenticity of freeze-dried açai pulp by near-infrared spectroscopy. *Journal of Food Engineering, 224*, 105–111. https://doi.org/10.1016/j.jfoodeng.2017.12.019.

Malbaša, R., Lončar, S., & Kolarov, A. (2004). TLC analysis of some phenolic compounds in Kombucha beverage. *Acta Periodica Technologica, 35*. https://doi.org/10.2298/APT0435199M.

Metrohm Nir Systems. (2013). *A guide to near-infrared spectroscopic analysis of industrial manufacturing processes* (pp. 1–46). Herisau, Switzerland: Metrohm AG.

Miller, G. L. (1959). Use of dinitrosalicylic acid reagent for determination of reducing sugar. *Analytical Chemistry, 31*(3), 426–428. https://doi.org/10.1021/ac60147a030.

Monteiro, P. I., Santos, J. S., Alvarenga Brizola, V. R., Pasini Deolindo, C. T., Koot, A., Boerrigter-Eenling, R., et al. (2018). Comparison between proton transfer reaction mass spectrometry and near infrared spectroscopy for the authentication of Brazilian coffee: A preliminary chemometric study. *Food Control, 91*, 276–283. https://doi.org/10.1016/j.foodcont.2018.04.009.

Neffe-Skocińska, K., Sionek, B., Ścibisz, I., & Kołożyn-Krajewska, D. (2017). Acid contents and the effect of fermentation condition of Kombucha tea beverages on physicochemical, microbiological and sensory properties. *CyTA - Journal of Food, 15*(4), 601–607. https://doi.org/10.1080/19476337.2017.1321588.

Osborne, B. G. (2000). Near-infrared spectroscopy in food analysis. *Encyclopedia of Analytical Chemistry, 1–14*. https://doi.org/10.1002/9780470027318.a1.

Penttilä, A., Martikainen, J., Gritsevich, M., & Muinonen, K. (2018). Laboratory spectroscopy of meteorite samples at UV-VIS-NIR wavelengths: Analysis and discrimination by principal components analysis. *Journal of Quantitative Spectroscopy and Radiative Transfer, 206*, 189–197. https://doi.org/10.1016/j.jqsrt.2017.11.011.

Ríos-Reina, R., Callejón, R. M., Savorani, F., Amigo, J. M., & Cocchi, M. (2019). Data fusion approaches in spectroscopic characterization and classification of PDO wine vinegars. *Talanta, 198*, 560–572. https://doi.org/10.1016/j.talanta.2019.01.100.

Salik, F. L. M., & Povoh, N. P. (1993). Método espectrofotométrico para determinação de teores alcoólicos em misturas hidroalcoólicas. In *Congresso Nacional da Sociedade dos Técnicos Açucareiros e Alcooleiros do Brasil, Águas de São Pedro*. SP.

Santos, C. H. K., Baqueta, M. R., Coqueiro, A., Dias, M. I., Barros, L., Barreiro, M. F., et al. (2018). Systematic study on the extraction of antioxidants from pinhão (*Araucaria angustifolia* (bertol.) Kuntze) coat. *Food Chemistry, 261*, 216–223. https://doi.org/10.1016/j.foodchem.2018.04.057.

Savitzky, A., & Golay, M. J. E. (1964). Smoothing and differentiation of data by dimplified least squares procedures. *Analytical Chemistry, 36*(8), 1627–1639. https://doi.org/10.1021/ac60214a047.

Schwolow, S., Gerhardt, N., Rohn, S., & Weller, P. (2019). Data fusion of GC-IMS data and FT-MIR spectra for the authentication of olive oils and honeys—is it worth to go the extra mile? *Analytical and Bioanalytical Chemistry, 411*, 6005–6019. https://doi.org/10.1007/s00216-019-01978-w.

Shahidi, F., & Ambigaipalan, P. (2015). Phenolics and polyphenolics in foods, beverages and spices: Antioxidant activity and health effects–a review. *Journal of Functional Foods, 18*, 820–897. https://doi.org/10.1016/j.jff.2015.06.018.

da Silva Sauthier, M. C., da Silva, E. G. P., da Silva Santos, B. R., Silva, E. F. R., da Cruz Caldas, J., Minho, L. A. C., et al. (2019). Screening of *Mangifera indica* L. functional content using PCA and neural networks (ANN). *Food Chemistry, 273*, 115–123. https://doi.org/10.1016/j.foodchem.2018.01.129.

Sreeramulu, G., Zhun, Y., & Knol, W. (2000). Kombucha fermentation and its antimicrobial activity. *Journal of Agricultural and Food Chemistry, 48*, 2589–2594. https://doi.org/10.1021/jf991333m.