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Assessment of Brazilian Monovarietal Olive Oil in Two Different Package Systems by Using Data Fusion and Chemometrics

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Abstract
The olive oil consumption has spread worldwide, increasing the necessity of quality assessment, and so forth, the search for new, alternative, and rapid data interpretation has started, boosting the interest and the use of data fusion that seek for an integration of results from different techniques or methodologies for the same data set. To better understand the storage effects on the Brazilian monovarietal extra virgin olive oil, data fusion was applied in the classical and alternative analysis, highlighting the similarities and differences between the techniques, assisting in the result interpretation. This perspective and strategy bring development to food chemistry analysis.

Keywords Spectroscopy · Data fusion · Chemometrics · Brazilian monovarietal olive oil

Introduction

Consumer's demand for high-quality food products has steadily increased, especially for agricultural products, specified in terms of traceable origin, known chemical composition, adequate physical properties, safety, and health safeguards (Borràs et al. 2015). Extra virgin olive oil (EVOO) is characterized by their importance to health benefits. This oil, which is obtained only by mechanical and physical means of unique or different olive varieties, provide a singular composition of unsaturated fatty acids, polyphenols, vitamin E, carotenoids, sterols, and chlorophylls (Merás et al. 2018). Consequently, EVOO is economically important, so there are control measures to establish its quality and authenticity, proofing that is an important topic for food safety, food quality, and consumer's protection (Danezis et al. 2016).

Quality can be defined as the combination of attributes or characteristics of a product that has significance in determining the degree of acceptability of the product by a user (Brody and Lord 2007). EVOO can suffer lipid oxidation, which is one of the major factors that causes deterioration, modifying major quality control parameters, such as color, flavor, aroma, and nutritive value (Keramat et al. 2016). Moreover, quality is influenced by olive variety, edaphoclimatic conditions, harvesting, and technological procedures of olive oil extraction. Another factors that influence EVOO quality are the storage time and conditions, temperature, type of packing materials, and exposition to air and/or to the light (Rodrigues et al. 2016).

The olive oil package allows its worldwide distribution and retention of quality for an extended period of time. The type of material and the storage conditions (light, temperature), besides the storage period, can significantly influence the quality of olive oil (Kanavouras and Coutelieris 2006), since the containers protect the product from both oxygen and light (Piscopo and Poiana 2012). For the light exposure, it is usually the high-energy UV part of the light spectrum with which concerns around 290–400 nm. For fatty products, the effect

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of exposure to light becomes more complex and critical, since light accelerates the oxidation process and therefore the rate at which rancidity develops (Emblem 2000). In this sense, a wide variety of materials have been used like olive oil packaged, i.e., plastic and coated paperboard; however, the most used remain to be glass and tin. Glass is one of the most inert materials; colored glass bottles prevent or slow down the oxidation process, and dark green bottles protect the oil from light rays with a wavelength of 300–500 nm (Kiritsakis et al. 2002). Tinplates have long been used to package oils; they offer total protection against light, oxygen, and water vapor. The inside of the can is coated with resins, which protect the metal surface against corrosion (Piergiovanni and Limbo 2010).

International Olive Council (COI/T.15/No 3/Rev. 11 July 2016), in order to estimate and guarantee the EVOO's quality, established the quality based on physicochemical parameters (free acidity, peroxide value, iodine value, moisture, smoke point, etc.) determined by reference methodologies (Borràs et al. 2016). In addition to the physicochemical parameters, other classic analysis can give useful information on EVOO quality, as the chromatographic analysis of fatty acid methyl esters (Longobardi et al. 2012). Although the methods mentioned are used worldwide as the quality indicators, some alternative methods, such as spectroscopic techniques, can also be used for this propose, e.g., the spectroscopies in the regions of ultraviolet and visible—UV-Vis (Vieira and D'Arce 1998; Gonçalves et al. 2014; Forina et al. 2015; Milanez et al. 2015; Aroca-Santos et al. 2016; Ferreiro-González et al. 2017) and near-infrared—NIR (Inarejos-García et al. 2013; Forina et al. 2015; Wójcicki et al. 2015; Cayuela and García 2017; Pizzi et al. 2018).

The amount of data provided by conventional and alternative methods is massive. And sometimes, it can overwhelm the scientists, demonstrating a necessity of advanced data interpretation tools to better identify and distinguish significant trends and to achieve proper interpretation (Bevilacqua et al. 2017). Considering the complexity of the foodstuff matrices, food quality derives a complex combination of characteristics. Therefore, analytical methods for a single analyte can rarely be correlated with fulfilling (Borràs et al. 2015). The use of multivariate analysis tools can provide a multivariate understanding by elucidating relationships in data sets (Hada et al. 2017). In this sense, chemometrics has become a crucial and dedicated tool for extracting valuable information (Yi et al. 2016). Here, the fusion of results from different analysis and techniques in order to evaluate the feasibility of combining physicochemical parameters, gas chromatography (GC), UV-Vis, and NIR spectroscopy, to explain the effect of storage time in two packaging systems, dark glass bottles and tinplate cans, during 1 year is proposed. Besides in assisting in the decision-making of which technique provides a better response for the Brazilian monovarietal EVOO quality characterization, the principal component analysis (PCA) was employed as a tool to assist in the evaluation of the data fusion.

Material and Methods

Monovarietal Extra Virgin Olive Oils Samples

The samples of the Brazilian monovarietal EVOO were obtained from the *Empresa de Pesquisa Agropecuária de Minas Gerais – Epamig*, *Mari da Fé – Minas Gerais – Brazil*; the harvest time was from February to March of 2015. A total of 24 samples from six different varietals: *Arbequina*, *Empeltre*, *Coratina*, *Grappolo*, *Koroneiki*, and *Maria da Fé*, were analyzed.

Brazilian Monovarietal EVOO Storage

The Brazilian monovarietal EVOO have conditioned in two different systems: 18 samples remained in the original package, dark green glass bottles of 500 mL, and the other six were manually placed in tinplate cans of 500 mL. The samples were stored for 12 months, to study the effect on the stability and the oil's quality. The storage conditions were room temperature and without light incidence. The samples were analyzed right after the opening of the glass bottles and after 1, 3, 6, and 12 months of storage. They were evaluated by physicochemical parameters (peroxide value, iodine value, free acidity, refraction index), chromatographic analysis of fatty acid methyl esters (codified as GC), UV-Vis and NIR spectroscopies.

Reagents

Ethanol P.A., sodium hydroxide P.A., potassium hydroxide P.A., glacial acetic acid P.A., and potassium iodine P.A. were purchased from *Alphatec*. Sodium thiosulfate P.A. and chloroform P.A. were purchased from (*Cinética*). Phenolphthalein P.A. and soluble starch P.A. (*Vetec*). Cyclohexane P.A., n-heptane P.A. and methanol P.A. (*Synth*). Wij's solution (*Dinâmica*).

Analysis

Physicochemical Parameters

Peroxide value (PV, expressed as milliequivalents of active oxygen per kilogram of oil (mEq O_2 kg^{-1})), iodine value (IV, measures the unsaturation of fatty acids, is expressed in grams of iodine absorbed by 100 g of sample (% iodine absorbed)), free acidity (FA, expressed as percentage of oleic acid), and refraction index (related to the degree of the saturation of the bonds, i.e., the number of single bonds present in the molecule) were determined according to the American Oil Chemists' Society (AOCS).

Instrumental Analysis

Fatty Acid Methyl Ester Fatty acid methyl esters (FAMEs) were analyzed by the gas chromatograph (GC) Claus 680 (Perkin Elmer) using Agilent CP-7420, a fused silica capillary column with 0.25 μm × 100 m × 0.25 mm, with helium as the carrier gas (flow rate, 1.1 mL/mi; split ratio, 1:1000, *v*/*v*) and with flame ionization detector (FID). Chromatographic parameters were as follows: injector temperature 240 °C; detector temperature 250 °C; column temperature programming 80 °C maintained for 1 min, with elevation to 160 °C; 20 °C/min temperature ramp; and final oven temperature 250 °C maintained for 58 min. The data obtained were analyzed using the Total Chrom (Perkin Elmer) software.

FAMEs were prepared according to ISO 5509 (ISO 2000). Approximately 50 mg of the grease matter were weighted and transferred to a test tube with a screw cap (capacity of 10 mL), then 2.0 mL of n-heptane and 2.0 mL of a methanolic solution of KOH (2 mol L^{-1}) were added to the undergo transmethylation. The mixture was stirred for 5 min with a test tube agitator. After the phase separation, the superior phase containing the FAMEs was carefully collected and transferred to an Eppendorf and kept in the freezer until analysis. The time of retention and area percentage were automatically computed by the software Total Chrom (Perkin Elmer).

UV-Vis Spectroscopy UV-Vis spectra of each sample were recorded with a portable UV-Vis spectrometer from Ocean Optics, interfaced to a personal computer using the software integration SpectraSuite. The spectra were collected with a 1-mm quartz cuvette, without any prior preparation, from 200 to 800 nm. The spectra were preprocessed with the savgol algorithm (Savitzky and Golay 1964) (7 points and first-order polynomial), and the baseline correction made by the algorithm was available on PLS-Toolbox 5.2 by Matlab software version R2007b.

NIR Spectroscopy The NIR spectra were obtained from a portable equipment microNIR spectrometer JDSU. The spectra were recorded with a glass cuvette from 950 to 1650 nm. No sample preparation was made. The spectra were transformed through the first derivative by the savgol algorithm (Savitzky and Golay 1964) (first-order polynomial and 7 points) by using the Matlab software version R2007b.

Data Fusion

Multivariate analysis tools can provide the extraction of more information about the quality state of food, facilitating the evaluation of authenticity. However, to improve the quality assessment of food, a further step is to combine—fuse—the outputs of multiple instrumental sources (Borràs et al. 2015). Data fusion involves using different instrumental techniques and combines its generated data (Cuevas et al. 2017). The data fusion is useful for a variety of applications such as object detection, recognition, identification, and classification, besides being useful for a decision-maker (Zhang 2010). Data fusion is emerging as a branch in chemometrics. In fact, the possibility to join results of different analytical methods (conventional and alternative) for a set of samples can enhance the quantity and quality of the information which can be extracted. Hence, the association of physicochemical parameters, fatty acid composition results, and the spectroscopies UV-Vis and NIR analysis can furnish a complete understanding about the most used techniques to assist the quality of EVOO through storage time.

Some data fusion approaches have been proposed to assess olive oil quality by data fusion from electronic nose and tongue (Haddi et al. 2013), spectroscopic measures, as MIR and NIR (Dupuy et al. 2010), fatty acid composition (Casale et al. 2012) and cultivar identification (Casale et al. 2010). However, to the best of our knowledge, there is no study that describes the application of data fusion from physicochemical parameters, gas chromatography, UV-Vis, and NIR for Brazilian monovarietal EVOO quality evaluation over the storage time. Data fusion merges the information from different analytical techniques and/or physicochemical information allowing a large number of information that can be assessed through chemometric tools. Data compilation from different techniques provides complementary interpretations and facilitates full sample description (Vera et al. 2011). The data fusion can provide more accurate knowledge about a system under study (Borràs et al. 2015).

There are three levels of data fusion, namely low, mid, and high levels. Data fusion from low- and mid-level approaches are the most commonly applied (Borràs et al. 2016). Low-level fusion consists of directly combining original signals after some preprocessing steps. Medium-level fusion involves the extraction of features or selection of variables before data fusion. Finally, in high-level fusion, a multivariate model is built separately for each technique and individual outputs are combined to produce a final result (Godinho et al. 2014). In this study, the low-level data fusion was applied.

Principal Component Analysis

Tools of pattern recognition are used to find tendencies or similarities in a data set. Based on the patterns obtained, it is possible to interpret results and, mainly, make more assertive decisions (Ferreira 2015). Principal component analysis (PCA) is an unsupervised pattern recognition method also known as the exploratory data analysis method. It is a statistical tool for analyzing large data sets with correlated variables and can be used to identify patterns in multidimensional data. PCA removes the correlations between different variables of the data set and transforms into a new coordinate system by using an orthogonal transformation. Then, the new coordinates in the data set have the largest variances (Penttilä et al. 2018).

The mathematical steps are described by Ferreira (2015). Basically, in a matrix **X**, each sample is represented by a row vector and each variable has a column vector. The PCA procedure can be described as the decomposition of the matrix **X** in two matrices, one of scores **T** and one of the loadings **P**:

$$\mathbf{X} = \mathbf{T}\mathbf{P}^{\mathbf{T}} \tag{1}$$

The scores express the relation between the samples, while the loadings indicate the relation between the variables. Therefore, with the low-level data fusion, all data of physicochemical analysis, GC, NIR, and UV-Vis were coupled in a new matrix where the PCA was applied by using the Matlab software version R2007b and the PLS-Toolbox 5.2, according to the schema shown in Fig. 1.

Results and Discussion

For the Brazilian monovarietal EVOO, all the physicochemical parameters had presented changes during the storage time (Table 1). Thus, as expected, the peroxide value (PV) was the index most affected by the storage conditions. In general, the variation of this level over time occurs in a Gaussian mode; however, low levels of peroxide value do not constitute generally low levels of oxidation (Jorge 2015). The free acidity (FA) and iodine value (IV) presented the main changes, respectively. The established limit for peroxide value for EVOO (PV ≤ 20 mEq O_2 kg^{-1} (COI 2015)) was exceeded for the varietal storage in tinplate cans *Empeltre*, *Coratina*, and *Maria da Fé*, after 12 months under storage condition. These results are in agreement with Laroussi-Mezghani et al. (2015) where the quality essentially depends on the olive varietal and storage conditions.

High free acidity is considered a problem, and it is essentially attributed to triglyceride degradation, resulting in the formation of free fatty acids (Korifi et al. 2016). The *Maria da Fé* varietal presented the highest acidity among the samples. The FA is less pronounced to the *Arbequina*, *Empeltre*, and *Coratina* samples, demonstrating higher stability. In agreement with the previous study where the oxidative stability of Brazilian monovarietal EVOO was evaluated (Gonçalves et al. 2018), these varietals demonstrated the higher tocopherol content, especially *Coratina*, that exhibited oxidation products only from the sixth month forward. Complementary, Table 2 shows the fatty acid content: oleic acid (C18:1), linoleic acid (C18:2), linolenic acid (C18:3), and the palmitic acid (C16:0), demonstrating the percentages of these fatty acids in the Brazilian monovarietal EVOO.

The UV-Vis and NIR spectra of the Brazilian monovarietal EVOO during storage time are shown in Fig. 2. Due to the lack of selectivity in the spectroscopies, NIR and UV-Vis, it is difficult to draw conclusions only by observing the spectra. Then, data fusion approach was used, in an attempt to improving the interpretability and the reliability of the results.

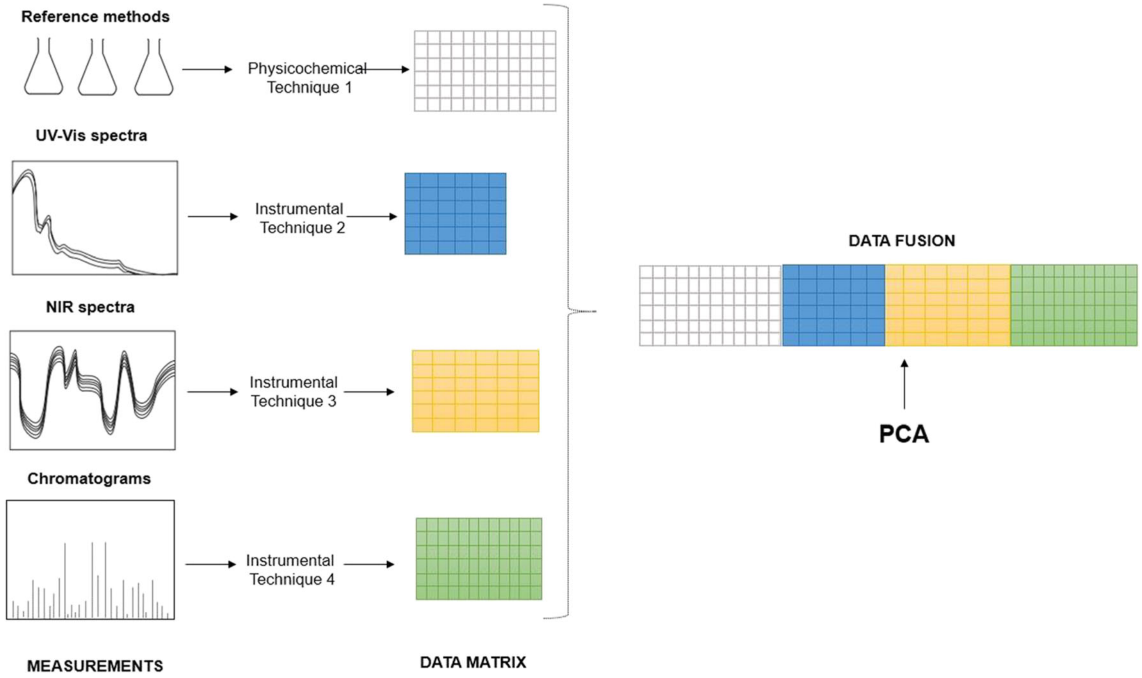


Fig. 1 Scheme of the procedure for the fusion matrix

Table 1 Physicochemical parameters

Samples	Free acidity (oleic ac. g 100 g^{-1})					Peroxide index (O_2 mEq kg^{-1})					Iodine value (%)					Refraction index				
	0 (Months)	1	3	6	12	0 (Months)	1	3	6	12	0 (Months)	1	3	6	12	0 (Months)	1	3	6	12
A1	0.22	0.23	0.29	0.22	0.26	4.75	6.77	8.47	11.57	15.37	84.37	88.09	93.19	87.44	82.50	1464	1464.5	1464	1464	1464
A2	0.20	0.24	0.26	0.24	0.32	5.71	6.77	10.01	12.03	15.78	82.20	85.68	92.96	88.82	79.26	1464.2	1465	1464.5	1464.5	1463.5
A3	0.21	0.22	0.28	0.22	0.26	5.69	4.41	8.31	10.70	14.22	82.64	84.15	94.92	86.49	84.79	1463.8	1465	1464	1464	1463.5
A4	–	0.21	0.29	0.22	0.28	–	6.11	9.11	15.56	22.43	–	88.54	91.74	86.52	84.80	–	1465	1464.3	1464.5	1463.5
E1	0.18	0.19	0.24	0.22	0.26	4.32	5.47	8.30	10.64	14.45	78.39	94.73	86.57	81.90	82.35	1464.6	1464.7	1463.5	1464	1464.4
E2	0.18	0.19	0.23	0.27	0.26	4.33	5.47	8.30	11.36	15.18	78.17	104.15	88.28	80.77	83.74	1463.6	1464	1464	1464	1463.9
E3	0.18	0.19	0.23	0.25	0.27	4.34	5.81	8.49	11.65	16.95	77.83	99.05	83.26	79.94	81.60	1463.4	1464	1463.5	1464	1464.2
E4	–	0.18	0.22	0.24	0.25	–	5.15	7.10	10.89	24.31	–	98.47	85.11	78.99	81.72	–	1464.7	1463.5	1463.5	1463.7
C1	0.25	0.28	0.28	0.28	0.28	3.81	3.96	5.38	4.97	9.73	97.01	92.28	78.72	85.11	78.32	1464	1464.2	1463.5	1464	1464.3
C2	0.25	0.28	0.29	0.28	0.28	3.23	5.48	5.47	4.87	9.10	91.98	96.20	81.19	88.09	81.62	1464	1464.2	1464.3	1464	1463.8
C3	0.21	0.27	0.29	0.27	0.29	3.42	5.10	5.74	4.88	8.88	92.23	98.54	86.54	86.53	79.57	1464	1464.3	1464	1464	1463.8
C4	–	0.25	0.28	0.27	0.27	–	4.21	5.48	7.72	22.22	–	93.64	84.74	86.11	84.04	–	1464.1	1464	1464	1463.7
G1	0.35	0.37	0.46	0.46	0.45	6.27	4.75	6.14	6.59	18.50	76.00	83.57	100.93	82.71	83.60	1464.3	1464.5	1464.9	1464	1464.5
G2	0.36	0.36	0.46	0.44	0.44	5.51	4.95	6.13	6.11	18.21	74.29	86.32	104.57	81.74	83.74	1463.5	1464.5	1465	1464	14,643.5
G3	0.31	0.35	0.45	0.49	0.45	4.76	6.48	7.74	6.78	18.00	75.89	81.58	99.60	79.79	84.80	1463.8	1464.5	1465.2	1464.5	1463.5
G4	–	0.35	0.45	0.43	0.42	–	6.83	7.27	6.02	18.62	–	84.38	91.47	82.39	86.45	–	1464.5	1465	1463.6	1464
K1	0.30	0.28	0.35	0.32	0.34	6.65	10.39	6.23	7.17	8.68	75.83	108.43	80.39	89.05	75.40	1461.3	1464.1	1463.5	1463.5	1463.3
K2	0.26	0.26	0.35	0.36	0.35	6.99	9.63	6.51	7.65	9.31	69.50	102.93	80.50	87.14	75.90	1461.3	1464.1	1463.5	1463.4	1463.5
K3	0.29	0.29	0.34	0.36	0.34	6.76	10.58	6.42	7.08	9.42	70.23	92.55	85.71	83.64	75.57	1461.5	1464	1463.5	1463.6	1463.5
K4	–	0.27	0.29	0.33	0.34	–	8.73	4.28	7.06	11.27	–	92.23	81.16	82.69	76.99	–	1463.3	1463.5	1463.4	1463.6
MF1	0.48	0.53	0.61	0.61	0.62	10.82	12.77	15.38	14.81	17.57	92.23	83.27	76.71	82.17	75.86	1464.3	1464	1464	1464.2	1463.7
MF2	0.47	0.49	0.62	0.62	0.63	10.85	13.22	15.58	14.89	17.90	83.17	89.69	77.46	84.15	71.80	1464.3	1464	1464.1	1464.1	1463.7
MF3	0.49	0.50	0.67	0.64	0.62	10.58	13.69	15.27	15.19	18.41	84.46	88.53	82.39	87.62	82.24	1464.5	1464	1464	1464.4	1463.6
MF4	–	0.45	0.58	0.60	0.62	–	13.23	15.92	14.70	21.29	–	87.88	80.69	91.36	79.13	–	1464.5	1464.5	1464	1463.5
EVOO[a]	≤0.8					≤20					75–94									

[a] Reference value of extra virgin olive oil formulated by International Olive Council (COI/T15.2015)

Samples stored in dark green bottles: A1, A2, A3—*Arbequina*; E1, E2, E3—*Empeltre*; C1, C2, C3—*Coratina*; G1, G2, G3—*Grappolo*; K1, K2, K3—*Koroneiki*; MF1, MF2, MF3—*Maria da Fé*. Samples stored in tinplate cans: A4—*Arbequina*; E4—*Empeltre*; C4—*Coratina*; G4—*Grappolo*; K4—*Koroneiki*; MF4—*Maria da Fé*

Table 2 Fatty acid composition (% *m*/*m* methyl esters)

Samples	Oleic acid ($C_{18:1}$)					Linoleic acid ($C_{18:2}$)					Linolenic acid ($C_{18:3}$)					Palmitic acid ($C_{16:0}$)				
	0 (Months)	1	3	6	12	0 (Months)	1	3	6	12	0 (Months)	1	3	6	12	0 (Months)	1	3	6	12
A1	69.17	66.93	69.24	68.61	67.28	10.24	9.29	10.28	10.49	10.02	0.70	0.70	0.68	0.70	0.36	14.96	14.65	14.78	15.08	14.25
A2	68.61	66.80	68.67	68.63	69.36	10.25	9.25	10.08	10.10	10.24	0.69	0.70	0.67	0.69	0.36	15.26	14.64	15.21	15.10	15.23
A3	69.13	66.88	69.24	69.21	67.20	10.30	9.26	10.30	10.34	10.05	0.70	0.70	0.69	0.69	0.36	14.92	14.61	14.78	14.69	14.25
A4	–	66.88	68.97	68.96	66.80	–	9.24	10.15	10.15	9.83	–	0.69	0.68	0.68	0.35	–	14.61	15.00	14.92	14.53
E1	68.15	66.05	68.27	68.39	66.43	10.28	10.05	10.31	10.29	10.01	0.75	0.75	0.74	0.75	0.36	15.81	15.12	15.63	15.43	15.08
E2	68.21	66.05	68.28	68.32	66.43	10.34	10.05	10.35	10.31	10.01	0.75	0.76	0.74	0.73	0.36	15.69	15.12	15.63	15.43	15.07
E3	68.20	66.11	67.62	68.30	66.37	10.31	10.13	10.50	10.26	10.01	0.75	0.76	0.75	0.73	0.35	15.70	15.20	15.94	15.56	15.10
E4	–	65.95	69.53	69.61	67.44	–	10.10	8.36	8.30	8.02	–	0.76	0.76	0.75	0.34	–	15.17	15.80	15.77	15.19
C1	78.72	77.16	78.83	78.74	77.89	6.27	6.45	6.20	6.25	6.28	0.60	0.63	0.58	0.58	0.36	10.06	10.29	10.04	10.01	10.00
C2	78.75	77.35	78.77	78.72	77.96	6.24	6.37	6.22	6.24	6.29	0.59	0.63	0.57	0.58	0.36	10.07	10.08	10.03	10.10	9.94
C3	78.69	78.18	78.77	78.76	77.86	6.25	6.44	6.21	6.24	6.27	0.60	0.64	0.59	0.58	0.37	10.12	10.27	10.05	10.04	9.95
C4	–	77.18	73.58	73.61	72.24	–	6.46	8.25	8.23	8.02	–	0.64	0.66	0.65	0.36	–	10.29	12.79	23.79	12.42
G1	82.01	80.63	81.69	82.23	81.37	4.32	4.41	4.36	4.25	4.26	0.74	0.78	0.73	0.70	0.47	9.13	9.20	9.23	9.04	8.93
G2	82.11	80.59	81.43	82.13	81.35	4.29	4.42	4.42	4.26	4.28	0.73	0.78	0.75	0.71	0.47	9.07	9.23	9.36	9.06	8.90
G3	82.10	81.44	81.74	82.19	81.22	4.28	4.45	4.34	4.23	4.33	0.74	0.78	0.74	0.69	0.48	9.08	9.32	9.23	9.01	8.94
G4	–	81.40	81.73	82.10	81.26	–	4.46	4.35	4.25	4.29	–	0.78	0.72	0.70	0.48	–	9.37	9.21	9.06	8.90
K1	77.68	75.68	77.75	77.80	76.13	4.28	4.48	4.30	4.34	4.35	0.64	0.69	0.68	0.61	0.30	12.30	12.42	12.34	12.30	12.05
K2	77.81	75.7	77.71	77.79	76.26	4.30	4.48	4.28	4.32	4.32	0.65	0.69	0.64	0.64	0.29	12.34	12.49	12.39	12.29	12.09
K3	77.79	75.79	77.79	77.79	76.26	4.37	4.43	4.29	4.32	4.32	0.65	0.68	0.63	0.64	0.29	12.28	12.28	12.31	12.29	12.09
K4	–	75.80	77.72	77.76	76.20	–	4.45	4.33	4.32	4.31	–	0.68	0.64	0.61	0.29	–	12.34	12.37	12.31	12.04
MF1	74.10	72.81	74.65	74.73	73.35	7.34	7.37	7.27	7.27	7.28	0.98	1.02	0.97	0.95	0.36	12.26	12.21	12.34	12.29	12.12
MF2	74.66	72.80	74.38	74.78	73.61	7.31	7.41	7.35	7.27	7.26	0.97	1.02	0.98	0.93	0.36	12.35	12.24	12.47	12.25	12.04
MF3	74.1	72.77	74.73	74.74	73.61	7.27	7.36	7.22	7.25	7.23	0.98	1.02	0.95	0.95	0.36	12.31	12.23	12.30	12.26	12.05
MF4	–	72.74	74.68	74.73	70.69	–	7.39	7.23	7.26	8.01	–	1.02	0.95	0.95	0.40	–	12.29	12.34	12.30	13.44
EVOO[a]	55–83					3.5–21					≤1					7.5–20				

[a] Reference value of extra virgin olive oil formulated by International Olive Council (COI/T15.2015)

Samples stored in dark green bottles: A1, A2, A3—*Arbequina*; E1, E2, E3—*Empeltre*; C1, C2, C3—*Coratina*; G1, G2, G3—*Grappolo*; K1, K2, K3—*Koroneiki*; MF1, MF2, MF3—*Maria da Fé*. Samples stored in tinplate cans: A4—*Arbequina*; E4—*Empeltre*; C4—*Coratina*; G4—*Grappolo*; K4—*Koroneiki*; MF4—*Maria da Fé*

For the data fusion approach, a fusion matrix (114 samples and 712 variables) composed of four datasets (UV-Vis + NIR + physicochemical + GC, respectively) was built using the low-level strategy. For the low-level data fusion, each data set was previously preprocessed before the combination of the fusion matrix. The physicochemical results were autoscaled; the UV-Vis spectra were smoothed; and the baseline was corrected. The first derivative was applied to the NIR spectra for the baseline correction. After these preprocesses, the UV-Vis, NIR, and GC data block each were individually normalized. As a general guideline, it would seem sensible to normalize the data sets first whenever the measured features show a difference in variances, or when are concerned with very different measured entities or units (Krazanowski 2000).

After the normalization of the fusion matrix, the interpretation was made through principal component analysis (PCA), without preprocessing. In this sense, the PCA results allowed us to obtain valuable information from the scores and loadings plots. And still, from this strategy of data fusion and PCA, it was possible to evaluate which portion of each block has a greater influence under the dispersion presented in the scores.

Two principal components (PCs) were able to explain more than 98% of the variance in the fusion matrix (97.03% in PC1 and 1.17% in PC2). Although the PC1 had higher variance, it does not present an interesting classification among the samples, making it impossible to interpret along with PC1 loadings, whose results are presented in the form of a supplementary material. However, PC2 brings the relevant information to explain the behavior of the Brazilian monovarietal EVOO during the storage time and the package effects. This result is not uncommon and had been reported before on genetically modified coffee discrimination (Moreira and Scarminio 2013).

During the storage period, autoxidation reactions happen, a series of compounds are formed that can cause rancidity and off flavors. Observing the scores plot of PC2, Fig. 3 is possible to verify that, at different packing systems, the Brazilian olive oils are affected differently by the storage conditions, as endorsed by Gutiérrez-Rosales et al. 1988 that affirm that headspace and oxygen permeability of the packaging material can influence in the oxidative stability. Figure 3 shows the scores obtained for PC2. The samples are clearly separated along PC2 into six clusters that show, in most cases, a scores profile that changes and evolve accordingly with the time of storage.

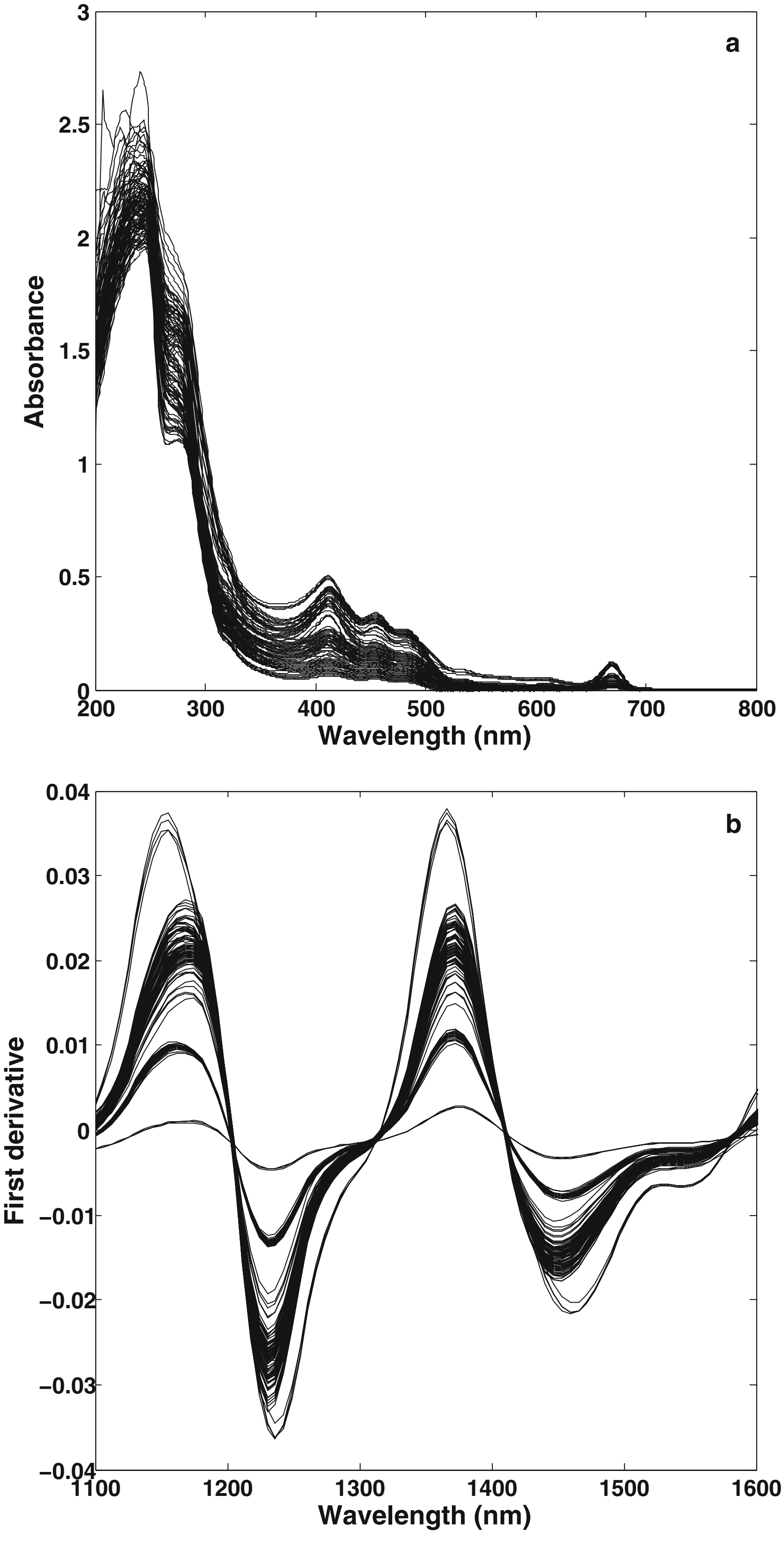
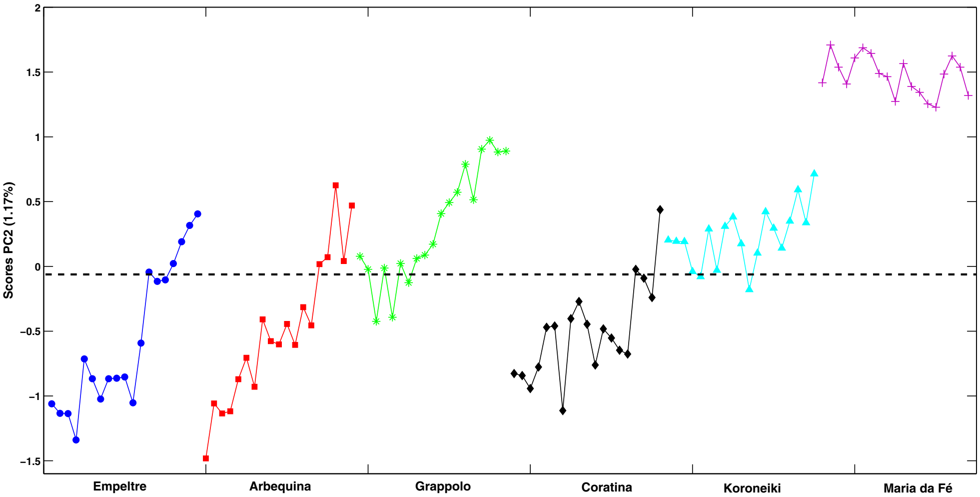


Fig. 2 **a** UV-Vis spectra for the BMEVOO. **b** NIR spectra for the BMEVOO

The Brazilian varietals *Empeltre* and *Arbequina* presented a similar behavior, in which the samples until the third month of storage are on the negative side of PC2. The samples of the *Coratina* cultivar are on the negative part of PC2, and only the sample stored in tinplate can reach the positive part of this PC after 12 months of storage. The samples from the varietals

Fig. 3 Time evolution for score values from PC2 for each varietal (●) Empeltre; (■) Arbequina; (*) Grappolo; (♦) Coratina; (▲) Koroneiki; (+) Maria da Fé



Grappolo, *Koroneiki*, and *Maria da Fé* are presented on the positive side of PC2.

Examination of the PC2 loadings (Fig. 4) suggests that scores separation is due to spectral domains situated around 200–230 nm, from 230 to 530 nm, and around 670 nm in the UV-Vis region. For NIR, all spectral region has importance for clusters observed in scores.

The absorption in the UV-Vis region around 200–230 nm can be attributed mainly to primary oxidation products that occur due to factors such as auto-oxidation. The main constituents of primary oxidation products are dienes, which have maximum absorption from 220 to 230 nm (Vieira and D'Arce 1998; Alves et al. 2018). Beyond the diene absorptions, it is also reported the tocopherol absorption from 220 to 300 nm (Craft 2016; Gonçalves et al. 2018).

UV-Vis absorptions in the regions from 230 to 530 nm can be assigned to phenolic compounds in 270 and 330 nm (Park et al. 1998; Alves et al. 2018). These compounds have an impact on the sensory aspects and in the olive oil quality (Dimitrios 2006). Tocopherol presents maximum absorption around 325 nm (Gonçalves et al. 2014), shows antioxidant properties, and is considered a criterion for purity (García-González et al. 2008). Among the chlorophylls, pheophytin is responsible for the greenish color, while compounds such as lutein and β-carotene are responsible for the yellowish coloring. The amount of these pigments depends on factors such as varietal type and storage conditions (García-González et al. 2008). The carotenoids present absorption in the visible region at 447 nm for the α-carotene, at 451 nm for the β-carotene, and at 462 nm for the γ-carotene (Koplík 2015). Chlorophylls show an intense band that is superimposed on the carotenoid

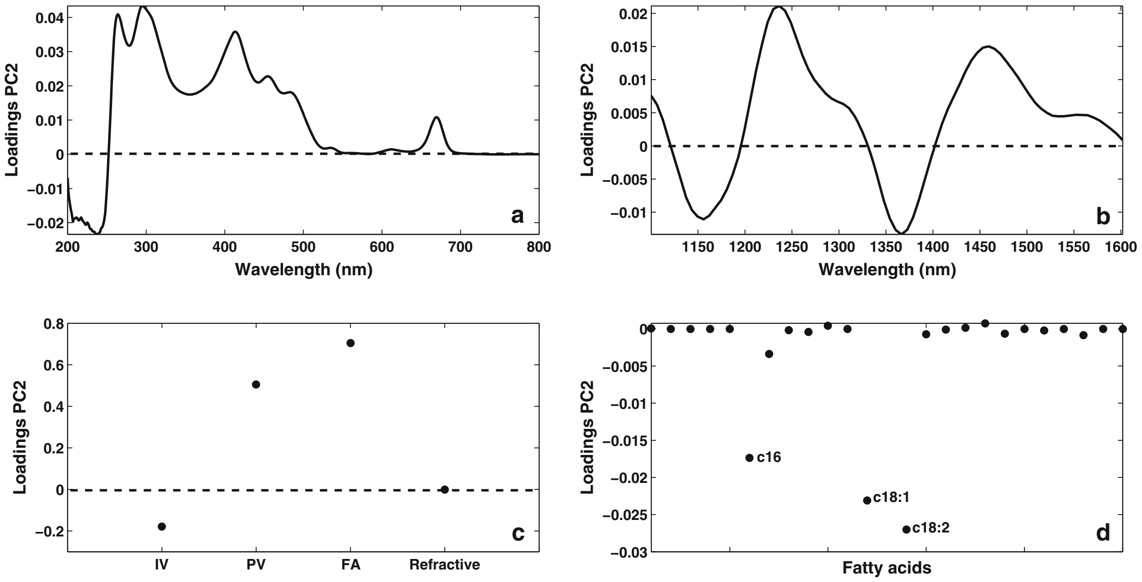


Fig. 4 Loadings from PC2. **a** UV-Vis; **b** NIR; **c** physicochemical parameters; **d** fatty acids. IV iodine value; PV peroxide value; FA free acidity

absorption around 420 nm, besides presenting absorption in 670 nm (Domenici et al. 2014; Giuffrida et al. 2007; Psomiadou and Tsimiodou 2002).

In the NIR region, the absorption from 1000 to 1200 nm corresponds to the C=O in the fourth overtone (1160 nm), C–H of the second overtone concerning the bonds HC=CH (1170 nm), and C–H of the second overtone regarding the bonds CH_3 (1195 nm) (Shenk et al. 2008; Rosa et al. 2017). In the NIR region, Rosa et al. (2017) described that the absorptions below 1000 nm, from 1200 to 1350 nm, and above 1400 nm have attributed to the samples of edible oils that demonstrated the lower amount of tocopherol and phenolic compounds. Rotondi et al. (2013) reported that the olive oil produced from the monovarietal *Coratina* presents higher phenolic compound content. In fact, the samples produced from this varietal are on the opposite side towards the varietals *Grappolo*, *Koroneiki*, and *Maria da Fé* in PC2. This result also agrees with a previous study (Gonçalves et al. 2018), where the olive oils produced from the varietals *Koroneiki* and *Maria da Fé* presented a higher formation of oxidation products and lower amounts of tocopherol.

Regarding the physicochemical parameters and fatty acid composition (Fig. 4c, d), the iodine value (IV), peroxide value (PV), free acidity (FA), and fatty acid composition of C16:0, C18:1, and, C18:2 are the variables with significant intensity in the PC2 loadings and have importance in the cluster separation observed in the scores. From these results, the samples of *Empeltre*, *Arbequina*, and *Coratina* exhibit similar behavior in relation to the composition of saturated and unsaturated fatty acids and, in iodine value, along the storage time. Correlation between the fatty acid composition and iodine value are reported by Rosa et al. (2017), in the evaluation of edible oils employing multi-block data analysis.

The samples from the cultivars *Grappolo*, *Koroneiki*, and *Maria da Fé* and also the samples from the varietals *Arbequina* and *Empeltre* from the sixth month of storage, and the *Coratina* sample, on the 12 months of storage conditioned in tinplate cans show similarities due to physicochemical parameters: free acidity and peroxide value. Regarding free acidity and peroxide indexes, indeed, the samples of the varietals *Grappolo*, *Koroneiki*, and *Maria da Fé* demonstrated the higher indexes (Table 1). The obtained results suggest that the higher indexes for acidity and peroxide are related to lower amounts of tocopherol and phenolic compounds. Consequently, with the achieved results, it is possible to affirm that the olive oils produced from the varietals *Maria da Fé*, *Koroneiki*, and *Grappolo* demonstrate less stability regarding olive oils produced from the other varietals used in this study, and through the storage time.

Conclusions

In this study, the storage time and the varietals were investigated by three different analytical techniques, and through physicochemical parameters, free acidity, iodine value, peroxide value, and refractive index. The PCA was applied in the low-level data fusion, showing informative plots, demonstrating the relationship between the samples by the scores plot, and a complete understanding when combining it with the loadings plot. The achieved results allowed to conclude that glass bottles are a package system that provides more protection for the Brazilian monovarietal olive oil. Furthermore, they demonstrate that the olive oils produced from the varietals *Empeltre*, *Arbequina*, and *Coratina* present similar characteristics on the storage and are more resistant to oxidation due to the unsaturated fatty acid content. On the other hand, the olive oils produced from the varietals *Grappolo*, *Koroneiki*, and *Maria da Fé* were similar during the storage time and showed less resistance to oxidation due to the lower amount of tocopherol and phenolic compounds.

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Compliance with Ethical Standards

Conflict of Interest Thays R. Gonçalves declares that she has no conflict of interest. Larissa N. Rosa declares that she has no conflict of interest. Alex S. Torquato declares that he has no conflict of interest. Luiz F. O. da Silva declares that he has no conflict of interest. Paulo Henrique Março declares that he has no conflict of interest. Sandra T. Marques Gomes declares that she has no conflict of interest. Makoto Matsushita declares that he has no conflict of interest. Patrícia Valderrama declares that she has no conflict of interest.

Ethical Approval This article does not contain any studies with human participants or animals performed by any of the authors.

Informed Consent Not applicable.

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