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Application of mid-infrared vibrational spectroscopy with Fourier transform (FTIR) in quality evaluation in commercial coffees

Aplicação da espectroscopia vibracional no infravermelho médio com transformada de Fourier (FTIR) na avaliação de qualidade em cafés comerciais

Aplicación de la espectroscopia vibracional del infrarrojo medio con transformada de Fourier (FTIR) en la evaluación de la calidad de los cafés comerciales

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Abstract

Currently, Brazil is the largest exporter and producer of coffee in the world, and it is the second most consumed beverage in the world, only behind water. In the years 2019 and 2020 it is estimated that the world consumption of coffee was 168.84 million bags of 60 kg, Brazil consumed 20 million bags of coffee, the second-largest consumer in the world, only behind the United States with 25 million bags. The techniques such as infrared spectroscopy has been applied in the food industry, as it is a fast, easy technique, without the need for reagents, free from polluting processes, and capable of analyzing the simultaneous composition of the constituents. The present study aims to analyze the changes in the chemical constituents of Brazilian commercial coffees as a function of shelf life through Fourier transformed infrared spectroscopy (FT-IR) associated with chemometric methods. The experiments were carried out within the expiration date, 6 months, and a year after the expiration date. Spectra were obtained in the range from 4000 to 500 cm-1. The studies of Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA) were made as discrimination methods. The areas in the region from 2970 to 2830 cm-1 and 1765 to 1720 cm-1 were calculated to analyze the alteration as a function over time. The results suggest that these bands in coffee are sensitive over time and to the storage conditions, promoting changes in aroma and flavor.

Keywords: Coffee; Infrared spectroscopy; Chemometric methods.

Resumo

Atualmente, o Brasil é o maior exportador e produtor de café do mundo, sendo o café a segunda bebida mais consumida no mundo, atrás apenas da água. Nos anos 2019 e 2020, estima-se que o consumo mundial de café foi de 168,84 milhões de sacas de 60 kg, sendo que, o Brasil consumiu 20 milhões, tornando-o o segundo maior consumidor do mundo, atrás apenas dos Estados Unidos com 25 milhões de sacas. Técnicas como a espectroscopia no infravermelho têm sido aplicadas na indústria alimentícia, por serem rápidas, fáceis, não necessitarem reagentes, não envolverem processos poluentes e serem capazes de analisar a composição simultânea dos constituintes. O presente estudo tem como objetivo analisar as alterações nos constituintes químicos de cafés comerciais brasileiros em função da vida de prateleira por meio de espectroscopia no infravermelho com transformada de Fourier (FT-IR) associada a métodos quimiométricos. Os experimentos foram realizados dentro do prazo de validade, 6 meses e um ano após o prazo de validade. Os espectros foram obtidos na faixa de 4000 a 500 cm-1. O estudo de Análise de Componentes Principais (PCA) e Análise de Agrupamentos Hierárquicos (HCA) foram realizados como métodos de discriminação. As áreas na região de 2970 a 2830 cm-1 e 1765 a 1720 cm-1 foram calculadas para analisar a alteração em função do tempo. Os resultados sugerem que essas bandas no café são sensíveis ao tempo e às condições de armazenamento, causando assim, alterações no aroma e sabor.

Palavras-chave: Café; Espectroscopia de infravermelho; Métodos quimiométricos.

Resumen

Brasil es hoy el mayor exportador y productor de café del mundo, siendo la segunda bebida más consumida en el mundo, después del agua. En 2019 y 2020 se estima que el consumo mundial de café fue de 168,84 millones de sacos de 60 kg, Brasil consumió 20 millones de sacos, siendo el segundo mayor consumidor del mundo, sólo detrás de Estados Unidos con 25 millones de sacos. Las técnicas como la espectroscopia infrarroja fueron aplicada en la industria alimentaria, ya que es una técnica rápida y fácil, sin necesidad de reactivos, libre de procesos contaminantes y capaz de analizar la composición simultánea de los constituyentes. El presente estudio tiene como objetivo analizar los cambios en los componentes químicos de los cafés comerciales brasileños en función de la vida útil mediante espectroscopia infrarroja con transformada de Fourier (FT-IR) asociada a métodos quimiométricos. Los experimentos fueron realizados en la fecha de caducidad, 6 meses y un año después de la fecha de vencimiento. Los espectros se obtuvieron en el rango de 4000 a 500 cm-1. El estudio del Análisis de Componente Principal (PCA) y del Análisis de Conglomerados Jerárquico (HCA) fueron realizados como métodos de discriminación. Se calcularon las áreas en la región de 2970 a 2830 cm-1 y 1765 a 1720 cm-1 para analizar la alteración en función del tiempo. Los resultados sugieren que estas bandas en el café son sensibles con el tiempo y a las condiciones de almacenamiento, promoviendo cambios en el aroma y el sabor.

Palabras clave: Café; Espectroscopia infrarroja; Métodos quimiométricos.

1. Introduction

Coffee is one of the most traded commodities (Munyendo et al, 2022) in the world besides being one of the world's most popular foods, according to the U.S. Department of Agriculture (USDA, 2021) and it is the second most consumed beverage in the world, only behind water. World coffee production in 2020/2021 season increased 4.15% compared to last year's harvest, which could reach 175.5 million bags of 60 kg. The main reason for the increase in coffee production this year was the record production of Brazilian Arabica coffee, which this year is expected to reach 47.8 million bags (USDA, 2021; Sezer et al, 2018).

Brazil is now the largest exporter and producer of coffee in the world (Mendes & Duarte, 2021), and quality is considered a major aspect of the industry because a high-quality product is associated with success in the market (Barrios-Rodrigues et al, 2021b). Many factors affect the quality of the product (Moreira et al, 2021). According to the Ministry of Agriculture, Livestock and Supply (MAPA, 2010), Normative Instruction No. 16, in force since 2010, establishes that 1% for every kilogram of roasted coffee ground there may be impurities such as shells, sediments (stones, lumps, and sand) and foreign matter (corn, sugar, barley, among others). Generally, Arabica coffee is considered superior to robusta and its price is higher. As the result, the identification of adulteration is very important for the consumer protection (Assis et al, 2018). Consequently, coffee beverage quality depends on the chemical constituents present in coffee beans, this composition is determinant for beverages' sensory characteristics, promoting the difference in aroma and flavor (Assis et al, 2019).

Analytical methods have been employed over the years to detect adulteration in food (Ferreira et al, 2021; Tavares et al, 2012), most of them based on destructive, time-consuming, and waste-producing techniques (Craig et al, 2018; Rubayiza et al, 2005). With its complex chemical composition, factors such as species, growing region, altitude, harvesting method, processing, and roasting degree influence the flavor and aroma of the drink. Thus, techniques such as infrared spectroscopy has been applied in the food industry, as it is a fast, easy technique, without the need for reagents, free from polluting processes, and capable of analyzing the simultaneous composition of the constituents (Mendes & Duarte, 2021).

Molecular vibrations involve energies that correspond to infrared photon energies. Such photons can be absorbed by the molecule under study by exciting vibrational modes of the molecule, resulting from this interaction, absorption spectra in the infrared region. Thus, it can be investigated the geometry and the forces of interaction between the atoms that make up the molecule, because infrared spectra depend on these factors (Barbosa, 2013; Smith, 2011).

The infrared spectrum of biological systems such as food, microorganisms, cells, and tissues is the result of the contribution of active infrared absorption bands of all biomolecules that make up biological tissue. Thus, the differentiation through direct visual inspection becomes often unfeasible, leading to the need to resort to mathematical methods to obtain more complex structural information (Stuart, 1997).

The present study aims to study the changes in the chemical constituents of Brazilian commercial coffees as a function of shelf life and the storage condition through mid-infrared spectroscopy (FTIR) associated with chemometric methods.

2. Methodology

Six samples of commercial coffees were purchased in two hypermarkets in the city of São José dos Campos on May 22, 2019, all samples are roasted and ground coffee, of Brazilian origin, industrialized, and from different producers. The samples were divided into six groups (A, B, C, D, E, F) according to each brand. Measurements were always performed within expiration, 6 months, and a year after the expiration date. The samples were stored at a temperature controlled at 20 °C.

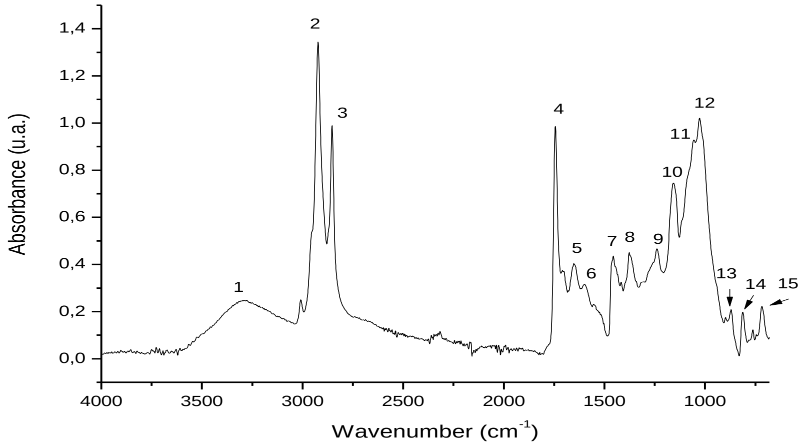
A total of 54 spectra (18 spectra within the expiration date, 18 spectra 6 months after expiration, and 18 a year after) were processed in this follow-up period, obtained in the medium infrared (MIR) region from 4000 to 500 cm^{-1} with a resolution of 4 cm^{-1}. Each spectrum was calculated as the average of 32 scans and submitted to background subtraction at the controlled temperature of 20 ˚C. A Spectrum Two spectrophotometer with Fourier Transform (FT-IR) and Attenuated reflectance technology (ATR) of PerkinElmer were used. The spectra obtained were processed with spectrum 5.3 and 10.5 (PerkinElmer) software, treatment consisted of baseline corrections, spectral smoothing with the Savitsky Golay algorithm (9 points), normalization, and absorbance plotting.

Spectra processed with Spectrum 5.3 and 10.3 software were plotted in graphics in Origin Pro 8.5 software. Subsequently, the data were submitted to principal component analysis (PCA) in the MiniTab 17 software to reduce the data set to the smallest orthogonal matrix through data covariance. The matrix obtained was then submitted to hierarchical cluster analysis (Hierarchical Cluster Analysis - HCA) to classify the variables into groups according to the statistical similarity of the evaluated components. For hierarchical cluster analysis, the following parameters were used: the Euclidean distance for the similarity measure as an algorithm for hierarchical grouping and the Ward known as the minimum variance that allows grouping clusters to produce the minimum increase in variance. (Craig et al, 2011; Bro & Smilde, 2014; Grasel et al, 2016). The results are shown through tree-shaped dendrograms.

3. Results and Discussion

The medium and normalized infrared spectrum of commercial brand C coffee and its vibrational modes are shown respectively in Figure 1 and Table 1.

Figure 1 - Infrared spectrum of commercial coffee brand C.



Source: Authors (2021).

Table 1 - Vibration modes and their approximate assignments of the medium spectrum of commercial coffee C following literature.

No.	Wavenumber (cm^{-1})	Vibrational mode
1	3288	O-H bond stretching of carboxylic acid and of hydroxyl group
2	2922	Asymmetric stretching of the C-H bond in $–CH_2$ mostly associated with lipids Asymmetric stretching of the C-H bond in $–CH_3$ in the caffeine molecule
3	2853	Symmetrical stretching of the C-H bond in $–CH_2$, mostly associated with lipids
4	1744	Stretching vibration of the carbonyl bonds, related to lipids or aliphatic ester present in coffee.
5	1651	C=O bond stretching in caffeine and chlorogenic acids
6	1598	stretch C=C in a nitrogen-based ring as caffeine and trigonelline
7	1455	Asymmetric angular deformation of the C-H bond O-H angular deformation
8	1376	Symmetrical angular deformation of the C-H bond O-H angular deformation
9	1239	C-N bond stretching in chlorogenic acid
10	1157	C-O bond stretch in carbohydrates
11	1055	C-O bond stretching in quinic acid
12	1027	C-O stretching, and C-C stretching of Arabinogalactans
13	870	Angular deformation of the C-H bond in carbohydrates
14	812	Angular deformation of the C-H bond in carbohydrates
15	717	Angular deformation of the C-H bond in carbohydrates

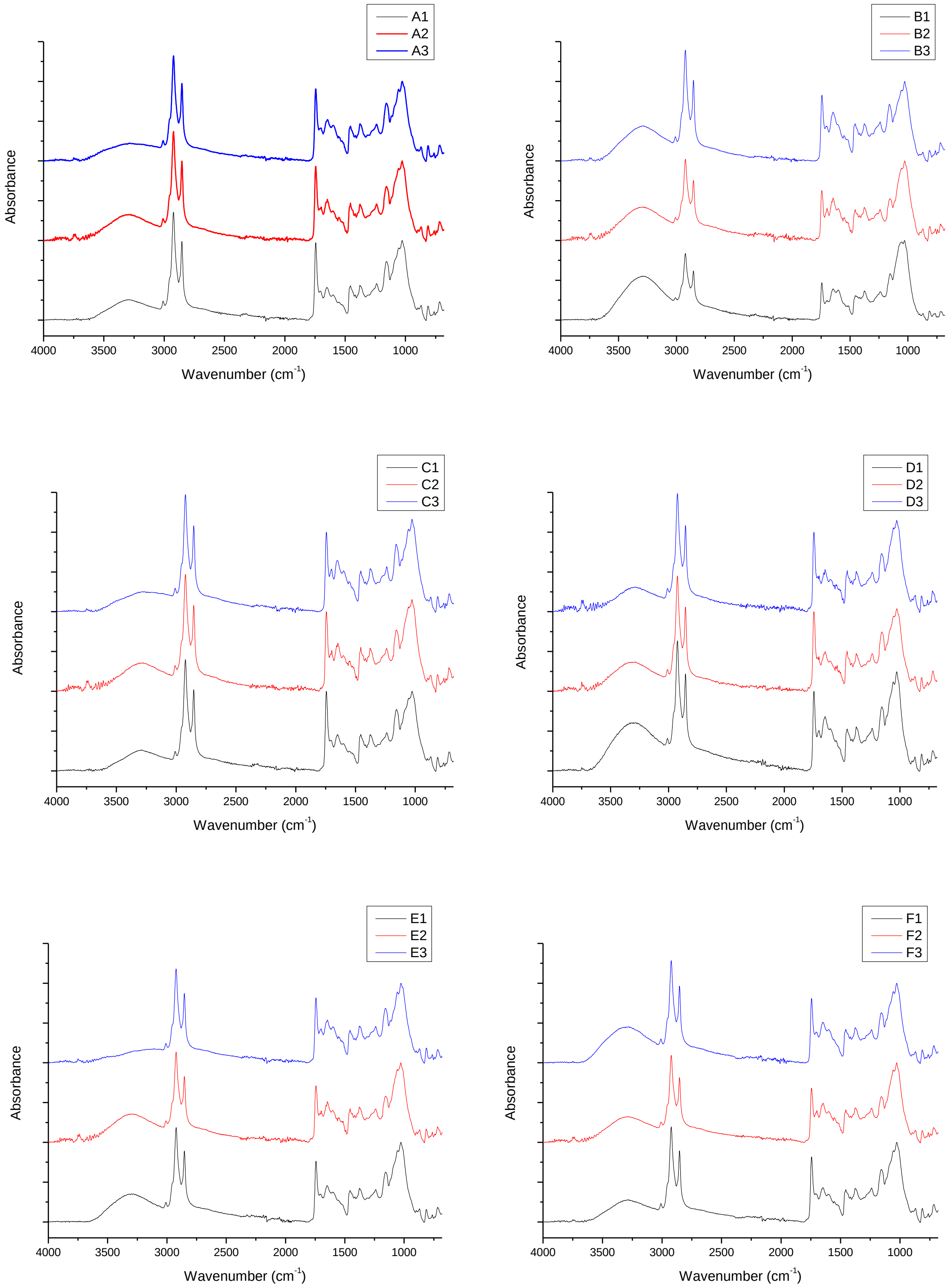
Source: Liu et al, 2021; Barrios-Rodrígues et al, 2021a; Assis et al, 2019; Assis et al.; 2018; Craig et al., 2018; Craig et al, 2015; Reis et al, 2013; Craig et al., 2012; Craig et al., 2011; Ribeiro et al., 2010; Paradkar & Irudayaraj, 2002.

According to the literature cited in Table 1, the peaks present in the region between 3300 and 2800 cm^{-1} correspond to stretching vibrations of bonds from multiple constituents of the coffee. These vibrations include O-H stretching of carboxylic acid in 3288 cm^{-1}, asymmetric stretching vibration of C-H bonds of methyl ($-CH_3-$) groups of caffeine, and/or asymmetric stretching vibration of C-H bonds of methylene ($-CH_2-$) groups of lipids in 2922 cm^{-1}. The peak at 2853 cm^{-1} corresponds to the symmetrical stretching of the C-H bond in $–CH_2$, mostly associated with lipids. The vibration of the O-H stretching of the hydroxyl bond is observed in this region.

The peak at 1742 cm^{-1} is attributed to the stretching vibration of the carbonyl bond, usually related to lipids or aliphatic esters present in coffee. The bond around 1543 cm^{-1} is related to C-C stretching from the nitrogenous ring, associated with molecules such as de caffeine and trigonelline, both present in significant amounts in coffees. The intense band between 1085 and 1050 cm^{-1} can be assigned to axial C-O deformation vibration of quinic acid, the band between 1420 and 1330 cm^{-1} is ascribed to O-H angular deformation, and the band in the range from 1300 to 1000 cm^{-1} is assigned to C-O-C ester bond vibration. In addition, the wavenumber range from 1400 to 900 cm^{-1} is characterized by vibrations of several types of bonds, such as C-H, C-O, and C-N. The principal compounds of coffee, carbohydrates, are absorbed in 1800-700 cm^{-1}. There are many types of carbohydrates in roasted and ground coffee, mainly galactomannans, arabinogalactans cellulose, and pectin. (Liu et al, 2021).

The average infrared spectra of the coffee samples within the expiration, 6 months, and 1 year after the expiration date are shown in Figure 2.

Figure 2 - Infrared spectra of commercial coffees A, B, C, D, E, F.



Note. Group 1 = Non-Expired samples; Group 2 = Expired for 6 months; Group 3 = Expired for 1 year. Source: Authors (2021).

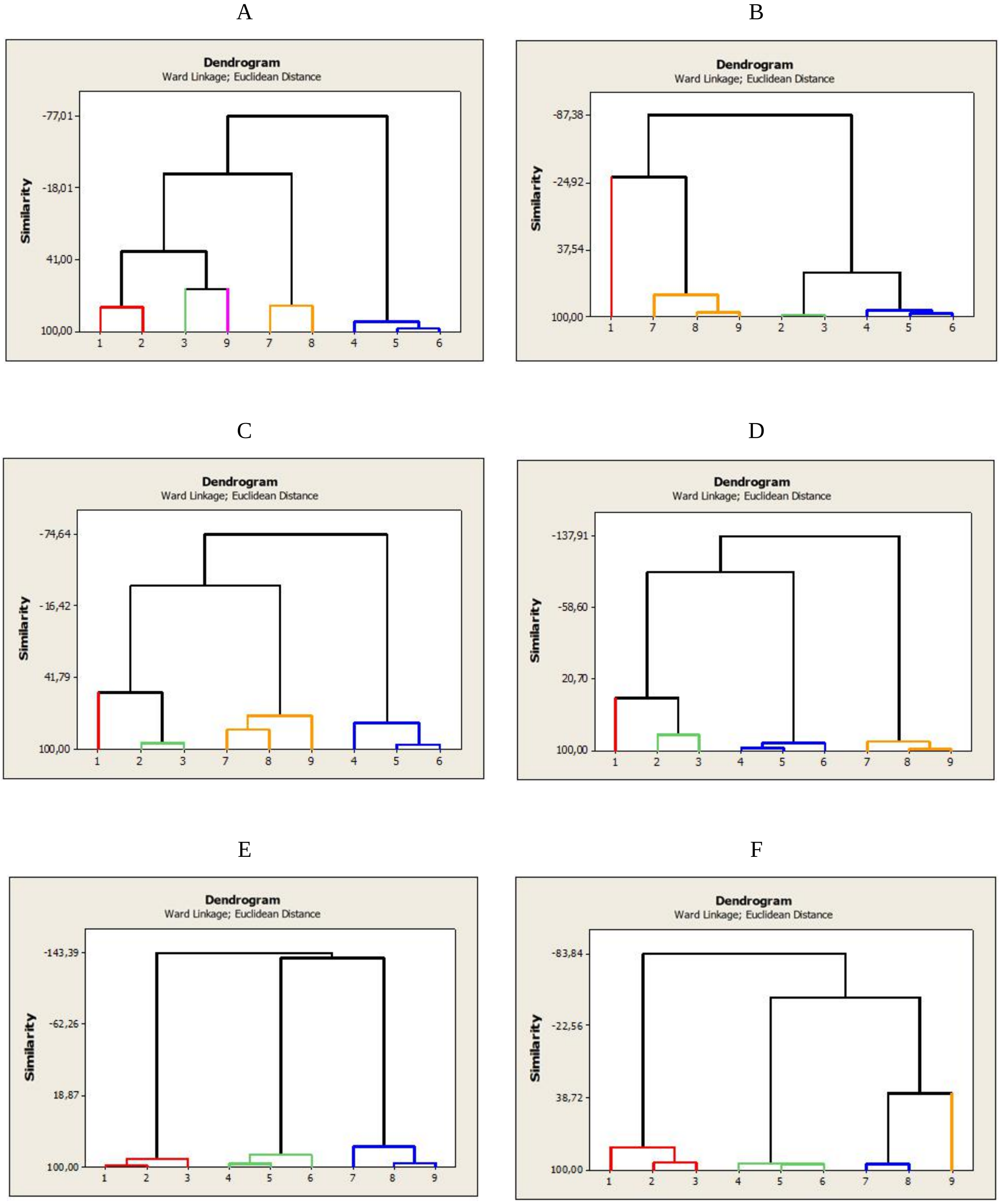
The visual analysis of IR spectra of samples A, B, C, D, E, and F in and out of the shelf life is rather difficult since all of them are very similar. The contours of bands and the number of peaks are similar, making it difficult to detect the spectral differences between the six samples in and out of the shelf life. In this way, it is necessary to resort to mathematical and statistical calculations to discuss the degree of similarity of the spectra. Therefore, the methods of Principal Component

Analysis (PCA) and Hierarchical Cluster Analysis (HCA) were used to discriminate the samples. According to Mendes and Duarte (2021), two regions were considered, 3030 to 2750 cm^{-1} and 1775 to 1500 cm^{-1} important for the discrimination of the chemical components of coffee. Thus, for the present work, the regions from 3000 to 2800 cm^{-1} and 1800 to 1500 cm^{-1} were chosen for the study of PCA and HCA, because these spectral regions contain the principal compounds of coffee, mainly lipids, caffeine, chlorogenic acids, and trigonelline, which are important in distinguishing the coffee samples. (Mendes & Duarte, 2021). Hierarchical cluster analysis was applied as a discrimination method to calculate the distance between samples using Ward´s clustering algorithm with Euclidean distance and HCA was applied to the set of variables employed for PCA.

Among the trademarks studied, samples C, D, E, and F showed clear discrimination in the region 3000 to 2800 cm^{-1}, indicating the alteration in chemical components of coffee, mainly caffeine and lipids, over the time. Samples A, B, C, D, and E discriminated in 1800 to 1500 cm^{-1}, indicating the alteration in chemical components of coffee as a function over time. Dendrograms in the region from 3000 to 2800 cm^{-1} and 1800 to 1500 cm^{-1} are shown in Figures 3 and 4 respectively.

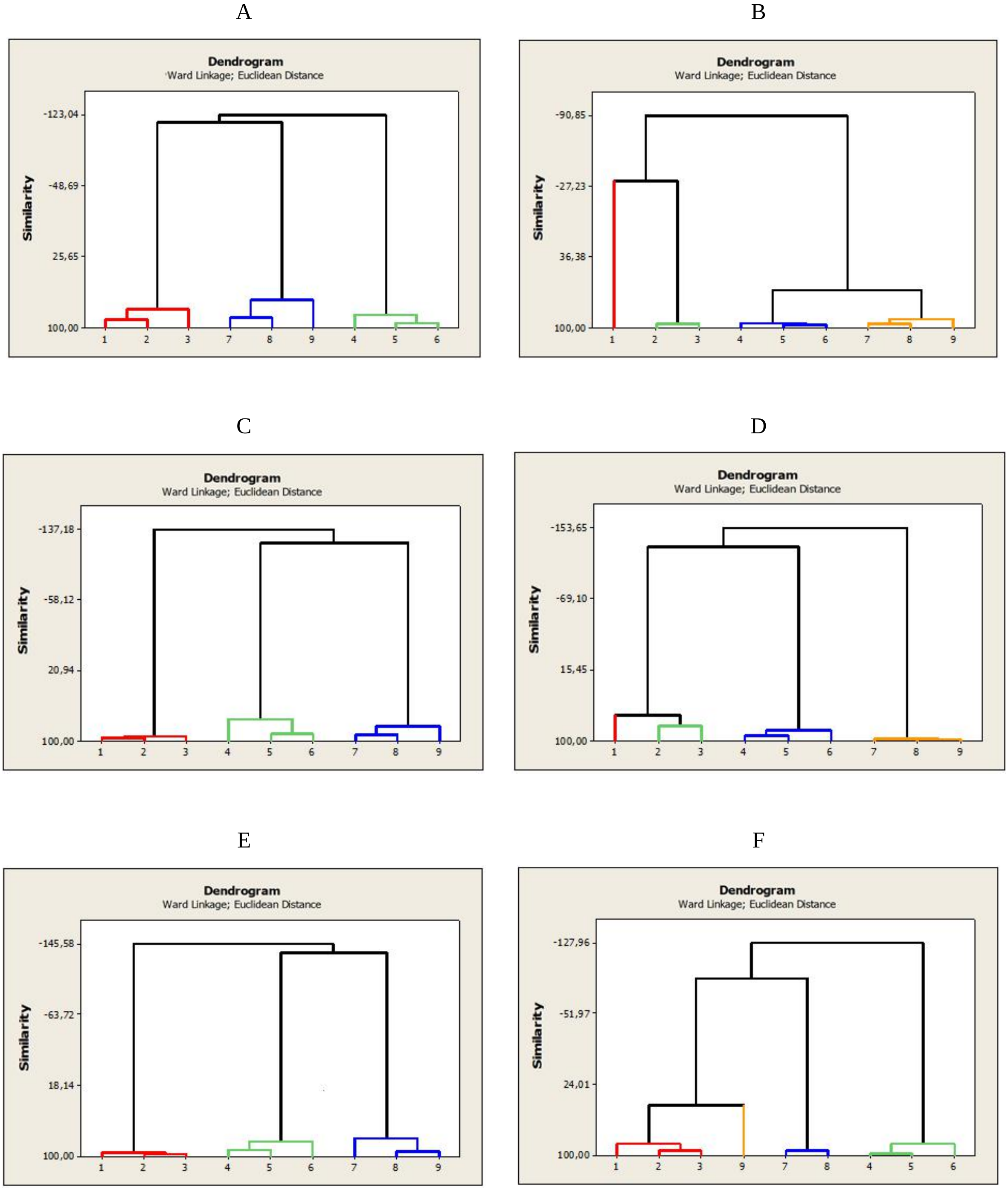
The interpretation of a tree-shaped dendrogram between samples is based on the discussion of the values of similarities: two close samples should have similar values for the measured variables. Therefore, the greater the proximity between the measurements related to the samples, the greater the similarity between them. The dendrogram hierarchizes this similarity.

Figure 3 – Dendrograms of commercial coffees A, B, C, D, E, and F in the region from 3000 to 2800 cm^{-1}.



Source: Authors (2021).

Figure 4 - Dendrograms of commercial coffees A, B, C, D, E, and F in the region from 1800 to1500 cm^{-1}.


A B C D E F

Source: Authors (2021).

Table 2 shows the HCA results of commercial coffee brands in both the region from 3000 to 2800 cm^{-1} and the region from 1800 to 1500 cm^{-1}.

Table 2 - HCA results in the regions from 3000 to 2800 cm^{-1} and 1800 to 1500 cm^{-1}.

Sample	Region 3000 to 2800 cm^{-1}		Region from 1800 to 1500 cm^{-1}	
	Spectra	Similarity	Spectra	Similarity
A - Non-Expired	1,2,3	X	1,2,3	80,12
A - Expired 6 months	4,5,6	91,56	4,5,6	86,32
A - Expired 1 year	7,8,9	X	7,8,9	70,71
B - Non-Expired	1,2,3	X	1,2,3	-31,62
B - Expired 6 months	4,5,6	92,99	4,5,6	95,40
B - Expired 1 year	7,8,9	X	7,8,9	91,64
C - Non-Expired	1,2,3	50,09	4,5,6	75,30
C - Expired 6 months	7,8,9	72,80	7,8,9	83,80
C - Expired 1 year	4,5,6	78,00	1,2,3	94,50
D - Non-Expired	1,2,3	41,70	1,2,3	60,40
D - Expired 6 months	4,5,6	91,30	4,5,6	88,00
D - Expired 1 year	7,8,9	88,50	7,8,9	76,70
E - Non-Expired	1,2,3	90,40	1,2,3	94,90
E - Expired 6 months	4,5,6	91,30	4,5,6	83,30
E - Expired 1 year	7,8,9	88,50	7,8,9	79,00
F - Non-Expired	1,2,3	80,66	1,2,3	X
F - Expired 6 months	4,5,6	87,87	4,5,6	90,00
F - Expired 1 year	7,8,9	34,80	7,8,9	X

Source: Authors (2021).

In the range of 3000 to 2800 cm^{-1} samples A and B were not able to discriminate between the groups within the period and one year expired, indicating that samples A and B showed similar spectra. In the region from 1800 to 1500 cm^{-1}, only sample F could not discriminate between groups within the expiration period and one year expired.

According to Craig et al. (2018), a study on the quality of Arabica coffee with different degrees of roasting showed that the regions around 2922, 2840, and 1740 cm^{-1} were important in the discrimination of coffee.

Assis et al. (2018) analyzed infrared spectra of commercial coffees with different levels of roasting: light, medium, and strong. Their spectra were similar, however, they showed significant differences in absorbance intensities. The two peaks at 3000 to 2800 cm^{-1} and a peak at 1742 cm^{-1} increase in intensity with the increase of the level of roasting. These peaks are in a region relatively free of the influence of other bands which allows the calculation of integrated intensities or areas.

In this work, the areas in the regions from 2970 to 2830 cm^{-1} and 1765 to 1720 cm^{-1} were calculated to quantify the alteration as a function of time. The important bands for the discrimination of coffee, 2922, 2840, and 1740 cm^{-1} are found in this region.

The results of the calculations of areas are found in Tables 3 and 4, respectively.

Table 3 - Result of the calculation of the area of the region from 2970 to 2830 cm^{-1} and the percentage of temporal fall.

Brand	Non-Expired (X) Area ± SD	Expired for 6 months (Y) Area ± SD	Reduction (%) (X ÷ Y)	Expired for 1 year (Z) Area ± SD	Reduction (%) (Y ÷ Z)
A	59,85 ± 2,35	53,78 ± 1,31	10	39,84 ± 1,81	26
B	39,23 ± 9,26	36,99 ± 4,00	5,7	30,32 ± 1,48	18,3
C	40,72 ± 1,98	38,92 ± 0,40	4,6	30,59 ± 1,92	27,2
D	53,67 ± 7,62	39,53 ± 1,93	35,7	37,67 ± 1,04	4,7
E	39,40 ± 0,54	34,19 ± 0,67	15,2	28,33 ± 1,04	20,6
F	40,19 ± 0,39	33,23 ± 0,38	20,9	26,44 ± 0,78	25,6

Note. SD = Standard deviation; (X ÷ Y) = Area reduction from Expired for 6 months compared to Non-Expired; (Y ÷ Z) = Area reduction from Expired for 1 year compared to Expired for 6 months. Source: Authors (2021).

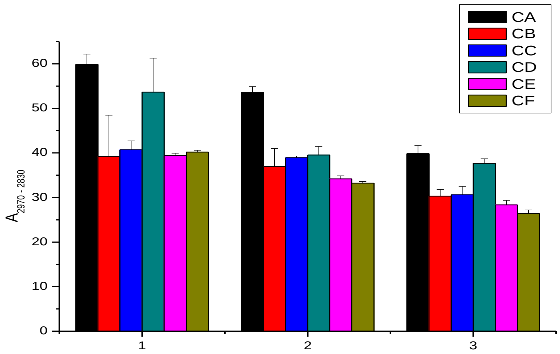
Table 4 - Result of the area calculation of the region 1765 at 1720 cm^{-1} and the percentage of temporal fall.

Brand	Non-Expired (X) Area ± SD	Expired for 6 months (Y) Area ± SD	Reduction (%) (X ÷ Y)	Expired for 1 year (Z) Area ± SD	Reduction (%) (Y ÷ Z)
A	14,34 ± 0,57	11,65 ± 0,33	18,7	5,33 ± 0,30	54,2
B	10,43 ± 3,83	9,51 ± 0,19	9,6	9,33 ± 2,50	5,3
C	11,37 ± 9,48	8,02 ± 0,14	41,7	6,33 ± 0,48	26,7
D	14,58 ± 2,16	10,43 ± 0,37	39,8	9,53 ± 0,11	9,4
E	10,66 ± 0,19	6,85 ± 0,18	55,6	6,85 ± 0,26	33,7
F	10,79 ± 0,20	7,10 ± 0,07	52	6,08 ± 0,18	16,7

Note. SD = Standard deviation; (X ÷ Y) = Area reduction from Expired for 6 months compared to Non-Expired; (Y ÷ Z) = Area reduction from Expired for 1 year compared to Expired for 6 months. Source: Authors (2021).

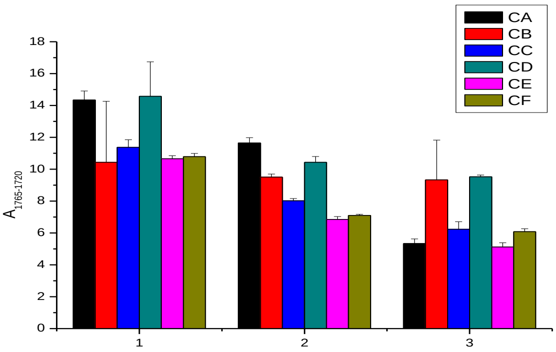
Figures 5 and 6 show the areas of the bands in the region from 2970 to 2830 cm^{-1} and 1765 to 1720 cm^{-1} of samples A, B, C, D, E and F, respectively.

Figure 5 - Areas of the bands in the region from 2970 to 2830 cm^{-1} in the infrared spectra of commercial coffees A, B, C, D, E and F in a function of the time.



Note. Group 1 = Non-Expired samples; Group 2 = Expired for 6 months; Group 3 = Expired for 1 year. Source: Authors (2021).

Figure 6 - Areas of the bands in the region from 1765 to 1720 cm^{-1} in the infrared spectra of commercial coffees A, B, C, D, E and F in function of the time.



Note. Group 1 = Non-Expired samples; Group 2 = Expired for 6 months; Group 3 = Expired for 1 year. Source: Authors (2021).

The results suggest that those spectral regions are chemically related to the alteration as a function over time. It is important to analyze how the samples are stored over time. If the package is opened, a sample is taken from it, and it is closed again to be reopened six months or a year later, an equilibrium condition is altered within the package. The original non-oxidative atmosphere within the package will be altered and, if oxygen is allowed to enter it, the product will be more susceptible to oxidation. Trigonelline derivatives can be easily oxidized, depending on the storage conditions.

Higher oxidation of triglycerides and volatile compounds could impact producing a decrease in the flavor of the beverage. (Craig et al, 2018). It is probable that the different chemical compounds react and interact among themselves during the time, resulting in the alteration of the products. This fact could produce a change in the aroma and flavor of commercial coffee. Consequently, the results reported in Tables 3 and 4 and Figures 5 and 6 could have a significant influence on oxidation. The 1800 - 1680 cm^{-1} carbonyl region provided information on the taste and aroma perceived by sensory analysis (Barbin et al, 2014; Lyman et al, 2003). Consequently, the results presented in tables 3 and 4 suggest the alteration of the taste and aroma of the products as a function over time. The FTIR technique allows rapid detection of the differences between the compounds of coffee over time as a function of shelf life and storage condition.

4. Conclusion

In this work, we presented an evaluation of the potential of the FTIR technique associated with chemometric methods for the quality assessment of commercial coffee as a function over time and the storage condition. The results suggest that the spectral regions facilitate quick identification of the chemical composition of commercial coffee in these conditions. The intensities of the bands in the regions of 2970 to 2830 cm^{-1} and of 1765 to 1720 cm^{-1} are decreased over time. It is important to emphasize how the samples are stored over time.

The HCA and PCA results of the data obtained from the spectrum showed that it is possible to discriminate the samples C, D, E, and F in the regions of 2970 to 2830 cm^{-1} and the samples A, B, C, D, and E in the region of 1800 to 1500 cm^{-1} according to shelf life.

Thus, the methodology proposed could be a useful and rapid tool for quality control and inspection proposes and can be important in the food industry.

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