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CHEMICAL AND SENSORY QUALITY OF SPECIALTY COFFEES MARKETED IN MINAS GERAIS, BRAZIL

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Abstract: The law of supply and demand is a fundamental concept in buying and selling relationships, and describes the interaction between the availability of a product or service (supply) and the willingness of consumers to purchase it (demand). In the specialty coffee market it is no different, the best beans, normally harvested on a small scale, are the most desired and, therefore, people pay more for them, therefore coffees with different levels of quality have different values, although very high values potentially can demotivate the consumer when purchasing a product. Thus, the aim of this study is to evaluate the selling price and sensory quality linked to the chemical composition and physical characteristics of specialty coffees marketed in Minas Gerais, Brazil. For that purpose, 20 specialty roasted coffees commercialized as specialty coffees in coffee shops in Belo Horizonte and Lavras, MG, were randomly purchased. The quality of the products was evaluated by sensory analysis, color determination (Agtron), and the profile of volatile and bioactive compounds. All coffees were classified as specialty coffees, with sensory scores from 81.1 to 87.8 points. The volatile compound profile allowed identification of the compounds related to the coffees with sensory scores ≥ 84.5 points and < 84.5 points. Bioactive compounds, selling price, and Agtron color were not related to the sensory quality of the coffee samples evaluated.

Keywords: *Coffea arabica* L., selling price, bioactive compounds, volatile compound profile, Agtron

QUALIDADE QUÍMICA E SENSORIAL DE CAFÉS ESPECIAIS COMERCIALIZADOS EM MINAS GERAIS, BRASIL

Resumo: A lei da oferta e demanda é um conceito fundamental nas relações de compra e venda, e descreve a interação entre a disponibilidade de um produto ou serviço (oferta) e a disposição dos consumidores em adquiri-lo (demanda). No mercado de cafés especiais não é diferente, os melhores grãos, normalmente colhidos em pequena escala, são os mais desejados e, por isso, paga-se mais por eles, portanto cafés com diferentes níveis de qualidade apresentam valores diferentes, contudo valores muito elevados potencialmente desmotivam o consumidor a comprar um produto. Sendo assim, o objetivo deste estudo é avaliar o preço de venda e a qualidade sensorial atrelados à composição química e às características físicas de cafés especiais comercializados em Minas Gerais, Brasil. Para tanto, foram adquiridos aleatoriamente 20 cafés especiais torrados comercializados como especiais em cafeterias de Belo Horizonte e Lavras, MG. A qualidade dos produtos foi avaliada por análise sensorial, determinação de cor (Agtron) e perfil de compostos voláteis e bioativos. Todos os cafés foram classificados como especiais, com notas sensoriais de 81,1 a 87,8 pontos. O perfil de compostos voláteis permitiu identificar os compostos relacionados aos cafés com escores sensoriais ≥ 84,5 pontos e < 84,5 pontos. Os compostos bioativos, o preço de venda e a cor Agtron não estiveram relacionados com a qualidade sensorial das amostras de café avaliadas.

Palavras-chave: *Coffea arabica* L., preço de venda, compostos bioativos, perfil de compostos voláteis, Agtron

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INTRODUCTION

Coffee is a crop of great economic importance, and it produces one of the most widely consumed beverages in the world. A total of 170.3 million 60-kg bags were consumed in the 2021/22 crop year, with projected growth of 3.3% over the previous crop year (ICO, 2022).

Though traditionally sold as a commodity, since 2000, coffee has followed the trend of highlighting quality, and specialty coffees have gained space in the market, meeting consumer demands and requirements (Schuit *et al*., 2021). According to the Specialty Coffee Association (SCA), specialty green coffee beans must be free of primary defects, and up to five equivalent secondary defects are tolerated. After roasting, the coffee must be free of quaker (immature) beans. In sensory analysis performed by certified judges, the beverage evaluated for fragrance/aroma, flavor, acidity, body, aftertaste, balance, uniformity, absence of defects (clean cup), sweetness, and overall impression. The coffees must have a minimum score of 80 points according to the international methodology proposed by The Coffee Quality Institute (CQI) (Lingle, 2011).

The specialty coffee market has shown notable growth through new products, market research, and an increase in specialty coffee shops (Guimarães *et al*., 2018). Brazilian consumers identified "excellent aroma", "freshly ground", and "concern with sustainability" of the coffee as essential characteristics for sale of the coffee beverage. However, as groups of consumers (experts, enthusiasts, and general public) diversify, other characteristics become important, due to the consumption profile. The general public considered "strong/full-bodied", "vacuum-packed", and "having the ABIC seal" as relevant aspects for quality coffee. Enthusiasts considered "strong/full-bodied" as important, and experts considered "specialty coffee" and "small producer" as significant points for identifying quality. This shows that the consumer profile affects the desire and demand for specialty coffees in the domestic market (ABIC, 2022).

It is known that the chemical and physical changes that occur during the coffee roasting process provide the beverage with its flavor and aroma. Precise control of time and temperature is crucial in the process because these factors affect coffee organoleptic properties, as well as the intensity and relative concentration of the chemical compounds in the beans, determinants of the quality parameters of the beverage (Pramudita *et al*., 2017). Other parameters that can be used to monitor the roasting process are bean color and aroma. During the roasting process, the color of the coffee bean changes from green to yellow and from yellow to shades of brown, ending up as dark brown. These color changes are due to the degradation and/or formation of chemical compounds that occur due to temperature (Anastácio *et al*., 2022). In the industry, roasting quality is typically evaluated by a master roaster who determines the degree of coffee roasting according to sensory properties (color, aroma, and flavor) and physical parameters of the process (air temperature and roasting time) (Silva *et al*., 2022).

The study of the chemical composition of specialty coffee enables better understanding of the aspects related to its quality. Chromatographic analysis methods have become relevant tools for the detection and quantification of different chemical compounds in coffee that may be related to the sensory profile of the beverage (Pereira *et al*., 2020). The aromatic sensory profile is very important to indicate authenticity among coffees, and the basic taste sensations of coffee are formed by volatile compounds that are present in the beans and are precursors of aroma (Knysak, 2017). Bioactive compounds also make an important contribution to flavor. Caffeine, for example, contributes to the bitterness and body of the beverage (Casas *et al*., 2017). Trigonelline plays a vital role in the composition of coffee flavor and aroma; its degradation helps form volatile compounds that benefit the beverage (Prakash *et al*., 2022). Chlorogenic acids (CGAs) provide acidity, astringency, and bitterness to the coffee beverage (Aachary; Eskin, 2017).

The law of supply and demand is a fundamental concept in buying and selling relationships, and describes the interaction between the availability of a product or service (supply) and the willingness of consumers to purchase it (demand). In the specialty coffee market it is no different, the best beans, normally harvested on a small scale, are the most desired and, therefore, people pay more for them, therefore coffees with different levels of quality have different values, although very high values potentially can demotivate the consumer when purchasing a product. Thus, the objective of this study was to evaluate the sensory quality, selling price, and chemical and color characteristics of twenty roasted coffees sold in Minas Gerais, Brazil, as specialty coffees of the *Coffea arabica* species.

MATERIALS AND METHODS

For this study, twenty roasted *Coffea arabica* L. specialty coffees of different brands, regions, producers, cultivars, and processing methods were randomly purchased in coffee shops in Belo Horizonte and Lavras (Minas Gerais, Brazil). Nineteen were purchased as roasted beans, and one as roasted and ground (coffee identified by the letter F).

To evaluate the physical, sensory, and chemical quality of the roasted specialty coffees, the profiles of color, sensory analysis, bioactive compounds, and volatile compounds were analyzed.

Sensory Analysis

Sensory analysis was conducted by five judges certified as Q-graders according to the recommendations of the SCA Protocols - Cupping Specialty Coffee (Lingle, 2011). The sensory quality evaluation was performed using methodology for the aroma, flavor, acidity, and body attributes. The intensity scales of the attributes and the final sensory score were obtained according to the methodology described by

Salvio *et al*. (2023). Ethical approval for the involvement of human subjects in this study was granted by 63934322.3.0000.5148 the Ethics Commitee on Human being Research of the Federal University of Lavras, Reference number 5.966.787, 03/27/2023.

Color Analysis

The color of the roasted coffee beans was evaluated using a Delta Color colorimeter/spectrophotometer, model Delta Vista d.0˚, with measurement through reflectance and spectral range between 400nm and 700nm, calibrated with a D65 light source and observation angle of 10˚. This instrument has its own calibration program for coffee in the Agtron (Ag) parameter, which is used in the official roasting color classification system of the SCA (Specialty Coffee Association).

For the analysis, approximately 13 g of ground roasted coffee was inserted (fine grinding, for filtered coffee) without compacting it, filling the container provided by the devise. The reading was performed in triplicate. The mean of the results on the Agtron scale was obtained.

Volatile Compound Profile

The volatile compounds were determined by gas chromatography. The roasted coffee beans were ground in a 11A basic grinder (IKA, Brazil) for about 1 minute, with the addition of liquid nitrogen to facilitate grinding and prevent oxidation of the samples. Samples of 2 g of ground coffee were packed in hermetically sealed vials.

The volatile compounds were extracted using static headspace of the GC-MS device, model QP - 2010 SE (Shimadzu), equipped with an NST-100 column (30 m × 0.25 mm × 0.25 µm) with a polyethylene glycol phase similar to Carbowax®, using the methodology described by Rabelo *et al.* (2021).

Data were analyzed and compounds were identified using the GCMS solution software (version 4.42, Shimadzu Corporation, Japan) and the NIST NIST/EPA/NIH 2014 database. Chemicals were identified by comparing the MS spectra with the database. The results were expressed as relative percentage area, which corresponds to the peak area for each identified compound as a proportion of the total chromatogram area of all detected peaks.

Bioactive Compounds

The non-volatile compounds caffeine, trigonelline, and chlorogenic acid were determined by High Performance Liquid Chromatography (HPLC), according to a methodology from Borém *et al.* (2023). The roasted coffee beans were ground in a basic 11A grinder (IKA, Brazil) for about 1 minute, with the addition of liquid nitrogen to facilitate grinding and prevent oxidation of the samples. Samples of 0.25 g of ground roasted coffee were extracted in 25 ml of distilled water at boiling point and placed in a water bath with boiling water for 3 minutes. The extract was filtered through regular filter paper and then filtered through a 0.45 µm membrane.

The compounds present were determined in an Agilent chromatograph, model 1260 Infinity II, with an ultraviolet detection system, C18 chromatographic column, and wavelength of 272 nm. The mobile phase consists of 85% A (aqueous solution of 1% acetic acid) and 15% B (methanol), with a flow rate of 1 $ml.min^{-1}$. A standard curve was prepared using caffeine, trigonelline, and 5-caffeeolquinic acid (5-CQA) standards for identification and quantitative analysis.

Experimental design and data analysis

The experiment was performed according to a completely randomized design with three replications. Analysis of variance (ANOVA) was performed on the results obtained in the analysis of color, selling price, sensory score, and intensity of the sensory attributes using the SISVAR software, version 5.3 (Ferreira, 2011). When significant differences were found in the F test, the Scott-Knott test was applied.

To better understand the relationship of treatments with chemical composition, sensory quality, and color, principal component analysis (PCA) was performed using the statistical software CHEMOFACE, version 1.4 (Nunes *et al*., 2012). An m × n matrix was constructed with the chemical compound content identified, the color, price and the sensory attributes for the m samples evaluated. Autoscaling was used to pre-treat the data, and then graphs were generated.

RESULTS AND DISCUSSION

The mean results obtained for sensory score, attribute intensities, and selling price are presented in Table 1. All the coffees acquired for this study had a final score above 80 points; therefore, they were classified as specialty coffees according to the SCA. These coffees were already sold commercially as specialty coffees.

However, the coffee identified as K stands out as it obtained the significantly highest sensory score, in addition to the greatest intensities of the attributes considered positive for the specialty coffee beverage, such as sweetness, acidity, body, and aftertaste.

A significant difference was identified between the final scores and the intensity of the sweetness, acidity, body, and aftertaste attributes among the commercial specialty coffee samples. However, the intensities of the bitterness and astringency attributes showed no significant difference. Bitterness is the perception considered opposite to sweetness, and astringency is the complex sensation accompanied by a retraction of the skin or mucous membrane of the mouth (Sakata *et al*., 2022). These two attributes are desirable at low intensity concerning the specialty coffee beverage, as was found in the sensory analysis of commercial coffees.

Table 1: Mean results obtained for sensory analysis (score and intensity of the attributes: sweetness, acidity, body, astringency, bitterness, and aftertaste) and selling price (R$/250g) of commercial specialty coffees.

Coffee sample	Score	Sweetness	Acidity	Body	Astringency	Bitterness	Aftertaste	Selling Price
A	83.0 d*	4.9 b	5.9 b	5.0 b	0.7 a	0.7 a	4.7 b	R$ 35.00 h
B	83.0 d	5.5 b	5.7 b	5.3 b	0.8 a	1.5 a	4.4 b	R$ 32.00 i
C	84.4 c	5.2 b	6.5 a	5.0 b	0.4 a	0.4 a	4.3 b	R$ 65.00 a
D	82.8 d	5.5 b	6.6 a	5.5 b	1.3 a	0.9 a	4.5 b	R$ 29.90 j
E	83.0 d	5.2 b	5.3 b	5.2 b	0.4 a	0.5 a	4.8 b	R$ 27.90 k
F	82.8 d	5.3 b	6.1 b	5.5 b	0.9 a	1.5 a	4.9 b	R$ 29.90 j
G	82.2 e	5.2 b	5.6 b	5.3 b	0.7 a	1.3 a	4.7 b	R$ 55.00 c
H	84.7 c	5.7 b	6.7 a	5.9 a	0.5 a	0.7 a	4.8 b	R$ 59.00 b
I	85.1 c	5.5 b	6.3 a	5.4 b	0.2 a	0.5 a	5.1 b	R$ 55.00 c
J	86.3 b	6.4 a	7.2 a	6.0 a	0.2 a	0.5 a	5.7 a	R$ 59.00 b
K	87.8 a	7.6 a	7.6 a	6.9 a	0.0 a	0.3 a	6.5 a	R$ 52.00 d
L	84.6 c	6.9 a	7.2 a	6.2 a	0.3 a	0.8 a	5.6 a	R$ 48.00 f
M	84.0 c	5.5 b	5.8 b	5.4 b	0.4 a	1.1 a	4.8 b	R$ 45.00 g
N	84.7 c	6.7 a	6.8 a	6.8 a	0.1 a	0.5 a	5.6 a	R$ 48.00 f
O	85.8 b	6.8 a	7.0 a	6.6 a	0.2 a	0.3 a	6.1 a	R$ 50.00 e
P	84.7 c	5.6 b	6.7 a	5.6 b	1.2 a	1.4 a	4.9 b	R$ 43.80 g
Q	83.3 d	4.6 b	5.2 b	4.9 b	0.5 a	1.4 a	3.7 b	R$ 43.80 g
R	84.1 c	6.0 a	6.2 a	5.5 b	0.1 a	0.5 a	4.7 b	R$ 43.80 g
S	85.0 c	6.2 a	6.9 a	5.7 b	0.5 a	0.7 a	5.8 a	R$ 43.80 g
T	81.1 e	4.1 b	4.6 b	4.4 b	0.8 a	1.8 a	3.8 b	R$ 27.90 k
Mean	84.12	5.72	6.30	5.61	0.51	0.87	4.97	R$ 44.70

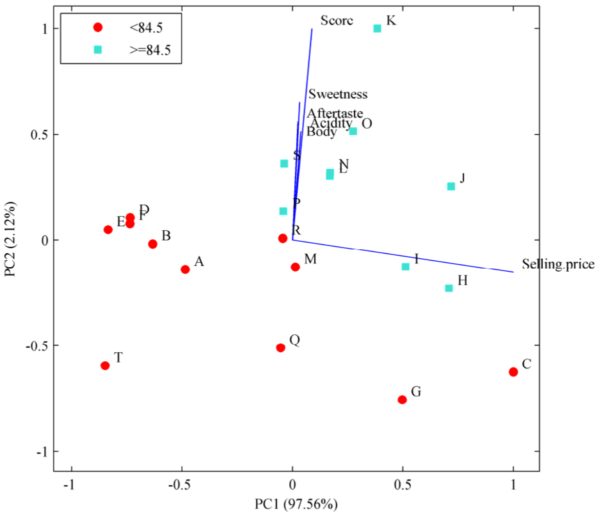
* Means followed by the same lowercase letter in the column do not differ by the Scott-Knott test at 5% probability of error.

Source: Prepared by the authors (2023)

Furthermore, a distinction can be noted between the selling price for 250g packages of the evaluated coffees. Selling prices were from R$ 27.90 to R$ 65.00/250g, with an average selling price of R$ 44.70/250g. The specialty coffees differ in quality and in price from the lower quality coffees sold on the market.

To better understand the quality of the commercial coffees and the selling price, principal component analysis (PCA) was carried out (Figure 1) with the intensities of the attributes that showed significant difference among the samples studied (sweetness, acidity, body, and aftertaste), sensory score, and the selling price of the coffee (R$/250g). The samples were classified according to the final score obtained: less than 84.5 points (<84.5), 11 coffees, and greater than or equal to 84.5 points (≥84.5), 9 coffees. The choice of the cut-off score of 84.5 was the closest overall average score for the coffees (84.12), as can be seen in Table 1.

Figure 1: Principal Component Analysis (PCA) of sensory score, intensity of the sensory attributes of sweetness, acidity, body, and aftertaste of sensory analysis of commercial specialty coffees, and the price paid, ranked according to sensory score.



Where, ●: commercial coffees scoring below 84.5 points, ■: commercial coffees scoring 84.5 points or higher; Commercial coffees evaluated: ●A,●B, ●C, ●D, ●E, ●F, ●G, ■H, ■I, ■J, ■K, ■L, ●M, ■N, ■O, ■P, ●Q, ●R, ■S, ●T; Sensory attributes of sweetness, acidity, body, and aftertaste, and the selling price.

Source: Prepared by the authors (2023)

In this PCA analysis, it was possible to differentiate the commercial coffees according to price that explains 97% of the distribution, while note and sensory attributes explain 3%, the interaction between these variables is capable of separating a group of coffee that comprises notes greater than or equal to 84.5 points. Moreover, the sweetness, acidity, body, and aftertaste attributes are closely related to the sensory score, since their vectors are superimposed. Due to the dimension of the vector, the sensory score was mainly responsible for dispersion of the centroids (coffee samples) in the vertical direction, while the selling price vector was responsible for dispersion of the centroids in the horizontal direction.

The commercial coffees that scored higher than 84.5 obtained the highest intensities of sweetness, acidity, body, and aftertaste. The coffees that scored lower than 84.5 were opposite or distant from the vectors of the intensities of the attributes. This contrasts with the quality and price relation, in which the samples of coffee C and G are located close to the vector of selling price and have sensory scores lower than 84.5 points.

In sensory analysis, the C sample had high acidity, sweetness, and body, and regular aftertaste, acquiring a final score of 84.4 points. However, it was the most expensive coffee in this study, with a selling price of R$ 65.00 for 250g of roasted coffee. In contrast, the ■K coffee sample stood out through intense sweetness, acidity, body, and aftertaste, with a consequent high sensory score of 87.8 points; yet, it was purchased for a significantly lower price than the ○C sample. Thus, in this case, the higher sensory quality of the specialty coffee is not represented by a higher sales price.

Significant differences were found not only in the sensory quality of the specialty commercial coffees, but also in their color (Agtron scale), as shown in Table 2. There were significant differences among the roasting patterns of the commercial specialty coffees studied. The roasting profiles ranged from Agtron #36.0 to #67.7, with an average of #56.0.

Agtron roast profiles in coffee range from very light to very dark, a scale decreasing from #95 to #25, respectively. In the Agtron scale, the range of #95 to #85 describes roasts from very light to light; #85 to #75, light to moderately light; #75 to #65, moderately light to medium light; #65 to #55, medium light to medium; #55 to #45, medium to moderately dark; #45 to #35, moderately dark to dark; and #35 to #25, dark to very dark (Agtron; SCAA, 2010). Thus, coffee sample J had the highest Agtron value (#67.7) and was classified as a moderately light to medium-light roast, according to the descriptions presented above, while coffee sample T had the lowest Agtron value (#36.0) and can be classified as a moderately dark to dark roast. Furthermore, the average color of the coffees analyzed is considered as medium roast, with the Agtron value of #56.0. According to the SCAA (2015), the Agtron standard for gourmet coffee roasting is #63, and for commercial coffee it is #48. That said, samples were found with lighter and darker roasts than the standards defined by the SCAA.

Many physical and chemical changes occur during coffee roasting. The method and intensity of roasting depend on the origin of the coffee beans and consumer preferences. Colorimetric differences in roast profiles are associated with chemical reactions in green coffee beans during roasting. Depending on its intensity, roasting produces more or less drastic changes in the compositional characteristics of green coffee beans. For example, a very light roast profile produces an unpleasant coffee aroma and flavor, without the aroma of roasted coffee. In contrast, a very dark roast carbonizes the coffee and leads to undesirable flavors and a burnt aroma (Yergenson; Aston, 2020).

Table 2: Mean results obtained for color analysis of commercial specialty coffees.

Coffee sample	Agtron
A	#58.0 c
B	#54.3 c
C	#59.3 c
D	#58.3 c
E	#57.0 c
F	#59.3 c
G	#56.0 c
H	#61.7 b
I	#59.3 c
J	#67.7 a
K	#57.3 c
L	#56.0 c
M	#57.7 c
N	#41.7 d
O	#37.7 e
P	#61.7 b
Q	#56.7 c
R	#61.7 b
S	#62.3 b
T	#36.0 e
Mean	#56

* Means followed by the same lowercase letter in the column do not differ by the Scott-Knott test at 5% probability of error.

Source: Prepared by the authors (2023)

In addition to color change, roasting intensity also affects important attributes of the coffee beverage, such as body, aroma, and acidity. Body is the tactile sensation the coffee has in the mouth, and it generally increases during roasting; it is less intense in light roasts and more intense in dark roasts, although it decreases again in very dark roasts (Davids, 2003). The aroma is also modified according to the degree of roasting because of the large variety of chemical compounds generated in small amounts at different times during roasting (Sunarharum *et al*., 2014). Acidity initially increases with roasting intensity, then reaches a peak and begins to decrease. Most roasts are finished at some point after this peak (Yergenson; Aston, 2020). Therefore, medium roasts enhance the flavor and aroma of the coffee beverage, preserve the acidity, and have characteristic bitterness and body for the sensory profile of specialty coffees.

However, sensory analysis consists of a complex process based on the experiences and sensory memory of the judges, which can generate some inconsistency in the results (Pereira *et al*., 2019). In addition, although color analysis of roasted coffee is directly related to sensory and chemical quality, it is only a physical characterization of the samples. As such, an alternative theoretical method is to find chemical indicators based on volatile compounds in order to objectively assess coffee quality. Coffee aroma and flavor are formed by a complex mixture of approximately three hundred volatile compounds, mainly consisting of the aliphatic hydrocarbon classes, sulfur compounds, pyrazines, pyridines, oxazoles, pyrroles, furans, aldehydes, esters, alcohols, ketones, and phenols (Borém *et al*., 2021; Flament, 2002; Poyraz *et al*., 2016).

In this study, twenty-four volatile compounds were identified in the samples of commercially roasted specialty coffees (Table 3). These are seven furans (furan, 2-methyl-; 2-methyltetrahydrofuran-3-one; furfural; furfuryl formate; 2-furanmethanol, acetate; 2-furancarboxaldehyde, 5-methyl-; 2-furanmethanol), five pyrazines (pyrazine; pyrazine, methyl-; pyrazine, 2,5-dimethyl-; pyrazine, 2,6-dimethyl-; pyrazine, ethyl-), three aldehydes (butanal; butanal, 2-methyl-; butanal, 3-methyl-), three ketones (2,3-pentanedione; 1-hydroxy-2-butanone; ethanone, 1-(2-furanyl)-), one ketoacid (pentanoic acid, 4-oxo-), one acid (acetic acid), one pyrrole (1H-pyrrole, 1-methyl), one pyridine (pyridine), one thiol (propane,1-thiol), and one diazole (imidazole).

The characteristics of the beverage are strongly affected by the degree of roasting of the coffee, in which the light roast has the most accentuated and vibrant acidity, expressing the individual qualities of the coffees. The medium roast strikes a balance between acidity and body, accentuating the aroma and flavor of the coffee. The dark roast, in turn, has pronounced body and bitterness, masking subtler aspects of acidity, flavor, and aroma (ITC, 2022). Volatile compounds are also associated with beverage quality, because they are related to aroma and flavor, which are the main factors for identifying the characteristics of the beverage.

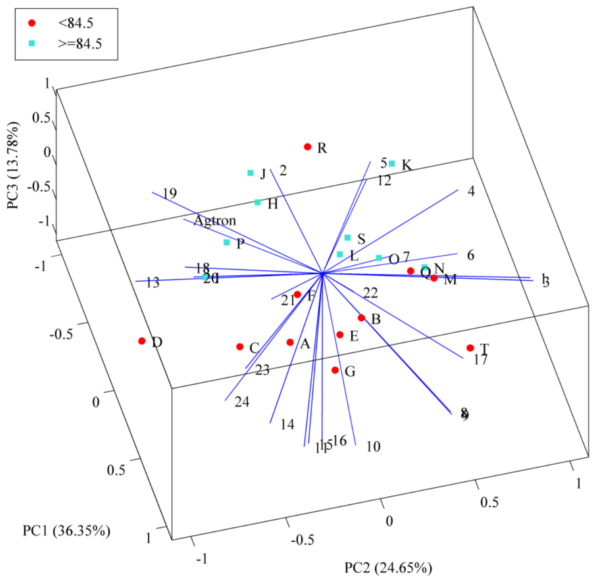
Subsequently, the volatile compounds were analyzed together with the Agtron color values by means of principal component analysis (PCA), presented in Figure 2. In addition, the same classification of commercial coffees was used according to the final score of coffees that obtained less than 84.5 points (<84.5) and those that obtained greater than or equal to 84.5 points (≥84.5).

Table 3: Mean relative area (%) of peaks of volatile compounds in commercial specialty coffees.

Coffee samples	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	7.16	0.00	1.65	8.37	2.38	1.70	4.69	1.29	9.37	1.58	10.84	0.00	2.24	1.49	1.30	1.46	0.91	7.34	9.87	2.16	2.02	1.41	4.05	13.16
B	8.85	0.00	1.79	9.85	3.04	1.72	4.96	1.30	9.10	1.52	10.25	0.00	2.09	1.39	1.27	1.27	1.12	6.77	9.20	1.39	1.20	1.77	3.84	12.27
C	6.37	0.00	1.56	8.77	2.79	1.78	4.76	0.91	5.89	1.79	11.52	0.00	2.79	1.72	1.49	1.61	1.17	9.70	11.77	1.76	1.84	0.00	4.40	13.42
D	3.65	0.00	0.84	5.47	1.99	1.59	3.83	0.86	6.38	1.60	10.40	0.00	2.88	1.46	1.32	1.48	0.00	10.42	16.28	2.02	1.74	1.62	4.81	17.11
E	7.91	0.18	1.70	8.50	3.18	1.91	4.64	1.24	9.60	1.67	10.74	0.00	2.12	1.40	1.32	1.43	1.15	7.13	9.11	1.53	1.39	1.52	3.66	12.91
F	7.47	0.00	1.62	10.16	3.61	1.82	4.38	1.05	6.56	1.65	9.77	0.00	2.29	1.25	1.10	1.21	1.08	8.22	11.84	1.96	1.30	1.34	3.99	14.47
G	8.75	0.21	1.83	8.04	2.58	1.84	4.32	1.29	9.64	1.84	11.68	0.00	1.96	1.55	1.49	1.62	1.15	6.28	8.91	1.88	1.81	1.74	3.90	12.24
H	4.26	11.38	1.23	8.66	3.75	1.77	3.57	0.79	4.57	1.32	7.49	0.00	2.19	0.90	0.85	1.06	0.00	5.46	20.74	1.75	1.39	1.30	2.63	9.16
I	4.92	0.19	1.23	7.26	2.44	2.09	4.78	0.93	4.42	1.53	9.57	0.00	3.54	1.34	1.07	1.10	1.06	11.60	14.76	1.73	2.12	0.92	3.15	14.57
J	6.01	5.89	1.34	9.73	4.21	1.65	5.25	0.59	3.84	0.89	7.38	0.00	2.32	0.89	0.82	0.94	0.00	7.79	19.84	2.02	1.05	1.76	3.05	10.24
K	11.76	0.00	2.01	10.76	3.33	2.50	5.42	0.83	4.95	1.13	3.84	4.70	2.23	1.01	0.89	1.03	1.02	8.96	9.86	1.53	1.78	1.30	3.37	10.30
L	10.75	0.00	2.01	10.30	2.90	2.17	6.16	0.90	5.92	1.23	9.75	0.00	2.12	1.26	1.07	1.15	0.97	8.27	8.76	2.47	1.95	1.53	3.93	10.70
M	10.26	0.61	2.02	15.23	3.79	1.87	4.66	1.17	7.83	1.67	10.12	0.00	1.62	1.14	1.11	1.37	1.15	5.01	8.77	1.24	1.24	1.47	2.64	9.71
N	11.67	0.00	2.03	10.33	3.36	2.24	4.76	1.20	9.49	1.48	9.09	0.00	1.73	1.11	0.99	1.06	0.95	7.57	7.90	1.34	1.64	1.27	3.26	10.84
O	10.83	0.79	1.97	11.20	3.54	1.92	4.87	0.83	6.26	1.37	9.05	0.00	1.92	1.18	1.07	1.21	1.08	7.93	10.03	1.51	1.91	1.16	3.84	10.12
P	4.79	4.64	1.30	7.08	2.53	1.38	3.65	0.71	5.55	1.34	8.71	0.00	2.42	1.09	0.97	1.02	0.00	7.52	20.88	1.60	1.40	2.18	2.78	11.02
Q	11.04	0.19	2.02	11.99	3.73	2.22	5.34	1.08	7.89	1.46	9.82	0.00	1.94	1.24	1.14	1.28	1.07	6.97	7.62	1.35	1.35	1.29	2.67	10.94
R	5.33	13.21	1.53	13.71	7.23	1.39	3.03	0.60	3.05	1.08	6.49	0.00	1.72	0.98	0.80	0.89	0.00	5.80	16.37	1.66	1.49	0.88	1.53	8.12
S	7.01	6.14	1.43	11.44	3.74	1.74	4.08	0.96	6.84	1.36	8.60	0.00	1.92	1.04	1.01	1.18	0.86	5.32	14.92	1.24	0.92	1.39	2.09	9.77
T	12.36	0.00	2.17	7.82	2.87	2.22	4.15	1.67	12.72	1.90	9.96	0.00	1.51	1.17	1.20	1.35	1.36	4.97	5.41	1.40	1.43	1.82	2.59	13.54

Source: Prepared by the authors (2023)

Figure 2: Principal component analysis (PCA) of volatile compounds and the Agtron color scale of commercially roasted specialty coffees ranked according to sensory score.



Where, ●: commercial coffees scoring below 84.5 points, ■: commercial coffees scoring 84.5 points or higher; Commercial coffees evaluated: ●A,●B, ●C, ●D, ●E, ●F, ●G, ■H, ■I, ■J, ■K, ■L, ●M, ■N, ■O, ■P, ●Q, ●R, ■S, ●T; Volatile compounds: (1) furan, 2-methyl-; (2) pentanoicacid, 4-oxo-; (3) butanal; (4) butanal, 2-methyl-; (5) butanal, 3-methyl-; (6) Imidazole; (7) 2,3-pentanedione; (8) 1H-pyrrole, 1-methyl; (9) pyridine; (10) pyrazine; (11) pyrazine, methyl-; (12) 2-methyltetrahydrofuran-3-one; (13) propane,1-thiol; (14) pyrazine, 2,5-dimethyl-; (15) pyrazine, 2,6-dimethyl-; (16) pyrazine, ethyl-; (17) 1-hydroxy-2-butanone; (18) furfural; (19) aceticacid; (20) furfurylformate; (21) ethanone, 1-(2-furanyl)-; (22) 2-furanmethanol, acetate; (23) 2-furancarboxaldehyde, 5-methyl-; and (24) 2-furanmethanol.

Source: Prepared by the authors (2023)

The volatile compound analysis and Agtron were able to differentiate the coffees according to the final score, between those with scores greater than or equal to 84.5 points and those with scores lower than 84.5 points. The grouping of coffees with scores greater than or equal to 84.5 with a smaller amount of volatile compounds can be seen in the upper region of the graph; next to this grouping is sample ●R, which scored less than 84.5. In the lower region of the graph are the samples with sensory scores lower than 84.5. The Agtron e SCAA (2010) roasting recommendation is to roast between #65 and #45 (medium light to moderately dark) to enhance aroma and flavor. Only four coffees (J, N, O, and T) are not within that recommended range –■J is lighter than recommended and the others are darker. The coffee identified as ●T (the darkest roast of all those analyzed) differs from the others in all the analyses performed, possibly because in the dark roast, the coffee becomes less acidic, more bitter, and less full-bodied, which caused it to be undervalued in sensory analysis. In addition, in more intense roasts, there is considerable modification of the chemical matrix of the coffee, which was also identified in the analysis of volatile compounds.

The volatile compounds responsible for separating the samples into the group with sensory scores lower than 84.5 points are the compounds 1H-pyrrole, 1-methyl; pyridine; and pyrazine, as they were found with larger relative areas in these samples. The compound 1H-pyrrole, 1-methyl has smoky, woody, and herbal scents (TGSC, 2023). Flament (2002) found that the pyridine compound has a hot, burning, and smoky scent; and the pyrazine compound has a sweet, pungent scent. Thus, coffees with sensory scores lower than 84.5 points exhibited smoky, burnt, woody, herbal, and sweet notes.

The volatile compounds responsible for separating the coffee samples into the group with sensory scores greater than or equal to 84.5 were the volatile compounds pentanoic acid, 4-oxo- and butanal, 3-methyl-. The compound pentanoic acid, 4-oxo- has a sweet, caramel, sour smell (Flament, 2002) and a sweet, sour, vanilla flavor (TGSC, 2023). The volatile compound butanal, 3-methyl- is described as having a peachy and fatty smell, along with a fruity, dry, green, chocolatey, nutty, and cocoa flavor (TGSC, 2023). Therefore, the coffees with the highest scores had sweet (caramel and vanilla), acidic, and fruity (peach) notes; these descriptions make the coffee flavor and aroma more complex, which differentiated these samples from the coffees with a score of less than 84.5 points.

Furthermore, there is a strong relationship between the vector of the volatile acetic acid compound and the vector of the Agtron color scale. Among the coffees studied, those with a lighter roasting color were found to have the largest relative areas of acetic acid. Acetic acid is associated with more perceptible acidity in the coffee beverage, and it has a sour, pungent smell (Flament, 2002) and a sour, pungent, and overripe fruity flavor (TGSC, 2023). This acid is formed during the roasting process, and its main precursor is the sucrose present in the green coffee beans. Throughout the roasting process, the acetic acid concentration increases up to the medium degree of roasting and then starts to decrease as roasting continues (Ginz*et al*., 2000).

This result is in agreement with the studies having shown that better quality coffees have fewer volatile compounds (Toci; Farah, 2008, 2014). Ribeiro *et al*. (2009) reported the compounds 3-methylbutanal and 2,3-pentanedione as markers of good quality beans; these compounds were also identified in this study in the group of coffees that obtained higher scores. Pyridine and methyl pyrrole, which have been identified as negative quality markers (Toci; Farah, 2008), appear in the coffees that scored lower. Pyridine has also been described as a compound characteristic of dark roasts (Franca *et al*., 2009), and this compound is present in larger quantities in the sample with the darkest roast, ●T.

The concentrations of bioactive compounds (trigonelline, chlorogenic acids, and caffeine) found in commercially roasted specialty coffees are presented in Table 4 and were analyzed using PCA, shown in Figure 3. The classification according to the sensory score of the samples was also used for this analysis.

Table 4: Mean concentrations (g.100$g_{d.m.}^{-1}$) of trigonelline, chlorogenic acids and caffeine in commercial specialty coffees.

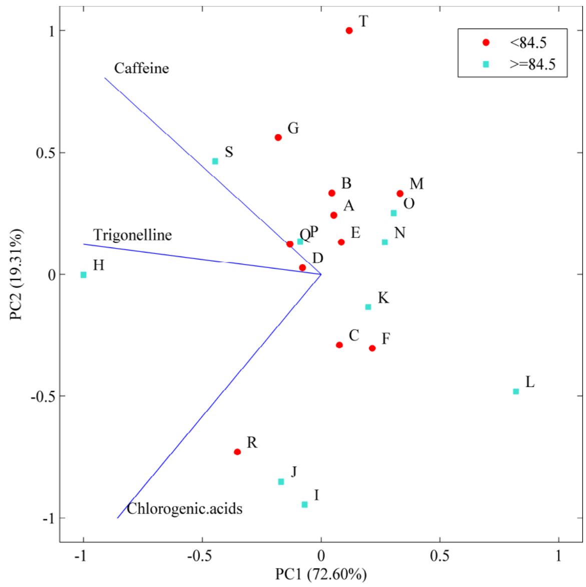
Coffee samples	Trigonelline	Chlorogenic Acids	Caffeine
A	1.0457	1.2706	2.1058
B	1.0408	1.2542	2.1383
C	1.0395	1.4719	2.0368
D	1.0458	1.4628	2.1790
E	1.0434	1.2616	2.0355
F	1.0363	1.4084	1.9845
G	1.0566	1.2752	2.2461
H	1.0707	1.9902	2.5850
I	1.0552	1.6515	1.8271
J	1.0402	1.8533	2.1070
K	1.0336	1.3384	1.9963
L	1.0118	1.0777	1.6194
M	1.0200	1.1741	2.1082
N	1.0412	1.1266	1.9143
O	1.0311	1.1607	2.0370
P	1.0466	1.3937	2.1574
Q	1.0561	1.4273	2.1809
R	1.0402	1.8754	2.1627
S	1.0506	1.5546	2.4646
T	1.0389	1.0201	2.2699

Source: Prepared by the authors (2023)

The bioactive compounds were not grouped according to the sensory quality of commercial specialty coffees, unlike the volatile compounds.

Green coffee beans have abundant bioactivity, and this has mainly been attributed to phenolic compounds, such as chlorogenic acids (Pimpley *et al*., 2020). However, during the roasting process, several modifications occur in the chemical matrix, such as the degradation of bioactive compounds through depletion of phenolic compounds and formation of Maillard reaction products (Alongi *et al*., 2020). In green coffee the levels are chlorogenic acids 2.80-5.42 g/100 g, trigonelline 0.80-1.30 g/100 g and caffeine 0.85-3.00 g/100 g. For roasted coffee the chlorogenic acid content varies from 1.30-3.54 g/100 g. Trigonelline also reduces to around 0.72-1.03 g/100; however, caffeine is a more stable compound during the roasting process. It has levels of 0.88-1.53 g/100 g (Tarigan *et al*., 2022). The three bioactive compounds, chlorogenic acids (CGA), caffeine and trigonelline, affect the quality of the cup of coffee and are closely linked to the formation of volatile compounds in coffee. Trigonelline plays a vital role in the formation of coffee aroma; it is a precursor of several volatile compounds, including pyridines and pyrroles, which contribute to pleasant aroma (Prakash *et al*., 2022), especially in lighter roasts. Chlorogenic acids are degraded during roasting, forming acidic and phenolic derivatives responsible for the acidity, astringency, and bitterness of the coffee beverage (Cheng *et al*., 2016). Therefore, they are important compounds in the formation of the aroma of roasted coffee. The volatile phenols are products derived from the degradation of chlorogenic acid and have already been confirmed as predictors of the acidity and aftertaste attributes (Wang *et al*., 2020). Caffeine, on the other hand, has a bitter taste and a nutty or chestnut aroma, and may or may not show a sensation of astringency. (Pino; Vegro, 2008).

Figure 3: Principal component analysis (PCA) for bioactive compounds of commercially roasted specialty coffees ranked according to sensory score.



Where, ●**:** commercial coffees scoring below 84.5 points, ■: commercial coffees scoring 84.5 points or higher; Commercial coffees evaluated: ●A, ●B, ●C, ●D, ●E, ●F, ●G, ■H, ■I, ■J, ■K, ■L, ●M, ■N, ■O, ■P, ●Q, ●R, ■S, ●T; Bioactive compounds: trigonelline, chlorogenic acids, and caffeine.

Source: Prepared by the authors (2023)

The sensory complexity of coffee is related to several factors that affect flavor and bioactive components, such as the production environment, post-harvest processing, the degree of roasting, and the method of beverage preparation (Worku *et al*., 2018). There is correlation between the bioactive compounds and the sensory quality of coffee, due to the participation of these compounds in roasting and the formation of aroma and flavor (Bolca; Emire, 2020). Yet, because of several variables that affect the concentration of trigonelline, chlorogenic acids, and caffeine, no variability was observed in the profile of bioactive compounds according to the sensory quality of commercial specialty coffees.

CONCLUSIONS

The characteristics of the beverage were affected by the degree of roasting and also by the chemical compounds present. The coffees considered to be of better sensory quality had volatile compounds as 3-methylbutanal and 2, 3-pentanedione as markers of good quality. It was not possible to relate the quality of the coffees with the Agtron color or with the bioactive compounds.

Prices vary greatly between samples of specialty coffees sold in the state of Minas Gerais, where the higher quality of the drink does not necessarily reflect the higher price of the coffee.

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DECLARATIONS OF INTEREST:

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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