

FT-IR as a strategy for controlling coffee marketed in Huila (Colombia)

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ABSTRACT

In addition to offering excellent cup quality and specialty coffees, Huila (Colombia) is the country's primary producer of coffee. However, it is essential to note that there is no entity that evaluates and certifies these specialties in the stores or in the coffee commercialized in the department, so it is necessary to assess its physical, chemical, and organoleptic quality. Therefore, this research assessed whether the coffees meet the characteristics established by the Specialty Coffee Association (SCA). In this work, 17 samples of roasted coffee beans were analyzed, and physicochemical tests (moisture, pH, and °Brix) were carried out. FTIR-ATR spectra were taken, and the content of caffeine (C) and chlorogenic acids (CGA) was determined. Finally, the samples were evaluated according to the SCA methodology. Moisture was within the optimum range for marketing roasted coffee beans (<4%). In the samples evaluated, CGA and C contents ranged between 10.472 ± 0.262 and 8.330 ± 0.138 (mg CGA/g coffee) and between 14.184 ± 0.384 and 7.772 ± 0.391 (mg C/g coffee) respectively. Statistically significant differences were found in relation to the post-harvest processing method for the dry, semi-wet, and wet samples obtained from coffee shops. Of the samples evaluated, 64.70 % were classified as specialty coffee. The samples with the highest scores in this group are processed by dry and semi-dry methods. On the other hand, 42.7% of these specialty coffees correspond to the southern zone of the department of Huila, as this is where the largest production of coffee is concentrated.

Key words: Adulterated Coffee; FTIR-ATR; physicochemical properties; specialty coffee.

1 INTRODUCTION

The department of Huila is recognized as the largest coffee producer in Colombia, with a production of 2,237,400 bags of 60 kg of excelso-coffee for the year 2023 (Huila Coffee Growers Committee, 2024). Likewise, the coffee market has gained prominence in recent years due to its development and production worldwide, which is reflected in the growing demand for specialty and high-quality coffees (Freitas et al., 2024a). Therefore, since its introduction, the term *specialty coffee* has not been concretely defined (Specialty Coffee Association - SCA, 2021). Thus, *specialty coffee* is defined as a coffee or a coffee experience recognized for its distinctive attributes, for which it has a significant additional value in the market (SCA, 2021). In turn, its specialty classification is given by the evaluation of ten attributes established by the Specialty Coffee Association (SCA) (Fernández-Alduenda et al., 2021).

These attributes are related to the type of processing used in post-harvest, as in the case of processing, which corresponds to the set of operations carried out after harvesting the fruit to obtain parchment coffee. There are types of processing: dry, semi-dry, and wet (Henao, Gutiérrez & Medina, 2017). Each represents specific physicochemical and sensory characteristics that relate to cup quality (Henao, Gutiérrez & Medina, 2017). Beans processed through dry milling can develop more complex and fruity flavors due to drying with the cherry and mucilage intact (Freitas et al., 2024a). Similarly, beans processed through the semi-dry method represent sweet, fruity, and less acidic flavor profiles,

while those processed through wet milling result in a more acidic, brighter, and cleaner beverage. This also provides better fermentation control (Elhalis et al., 2023).

Coffee is a complex combination of chemical substances developed in the roasting process, which includes the Maillard and caramelization reactions (Elhalis et al., 2023; Freitas et al., 2024b), responsible for the formation of the characteristic aroma, flavor, and color of the coffee bean. Likewise, the final roasting time determines the sensory profile of coffee in terms of organic acid composition, chlorogenic acid derivatives (CGAs), caramelization of sugars, volatile composition, lipid migration, and melanoidin production (Belchior et al., 2020; Wei & Tanokura, 2015). Such a composition is related to the main attributes evaluated in sensory analysis. Chlorogenic acid is one of the main acids and, together with proteins, amino acids, phenolic compounds, lipids, and polysaccharides, is a precursor of the aroma of green and roasted coffee beans (Freitas et al., 2024b). These components contribute to the bitter taste, acidity, and astringency of coffee when brewed (Pereira et al., 2021; Seninde & Iv, 2020). In addition, CGAs act as precursors in the formation of phenols and catechols, and generate strong antiviral, antidiabetic, antioxidant, and neuroprotective activity, among others (Kamiloglu et al., 2021; Wale et al., 2024).

Caffeine (C) provides the characteristic bitterness of coffee and is present in concentrations that vary according to genetic variety, origin, and preparation method (Elhalis et al., 2023; Wale et al., 2024). In addition, it is a central nervous system stimulant that improves short-term memory, increases

alertness, and reduces fatigue (Wale et al., 2024). Likewise, it has been associated with the reduction of cases of myocardial infarction, some types of cancer, and diabetes, as well as with the prevention of Alzheimer's, Parkinson's, asthma, depression, and cardiovascular problems (Messina et al., 2015; Monis et al., 2022). For these reasons, the consumption of high-quality coffee generates a positive effect on human health.

However, this product is susceptible to adulterations caused by different contaminants and/or foreign matter such as coffee processing by-products (coffee husks, parchment, used coffee grounds, among others), cheaper beans (barley, corn, soybeans and others) and lower quality coffees (*pasilla*) (Reis et al., 2013; Varão Silva et al., 2021), which may represent conditions for human consumption. For this reason, the trade of this product should be monitored and controlled.

In Huila, there is no organization that monitors and controls specialty coffees in the market, mainly in specialty stores, which limits the ability to determine the quality and safety of the product. Consumption in these stores is based on the credibility of their owners, ignoring the authenticity and veracity of the coffee. This contrasts with other food products that are regulated by the National Institute for the Vigilance of Medicines and Food (INVIMA). The INVIMA verifies the safety of the products but does not guarantee that they are specialty coffees.

The SCA is an entity that establishes parameters and quality standards for specialty coffees at an international level. However, within its functions, it does not contemplate the certification and/or validation of coffees marketed in establishments that call themselves *specialty stores*, which represents a great difficulty both for the definition of the term *specialty coffee* as well as for the responsibility and visibility that this product acquires in its commercialization at a worldwide level.

For this reason, complementary analytical techniques are available to ensure the authenticity and traceability of coffee. Fourier transform infrared spectroscopy (FTIR-ATR) is a widely used technique to measure coffee quality quickly and accurately (Barrera et al., 2019; Varão Silva et al., 2021). There are other techniques to identify and quantify the main components of coffee, such as high-performance liquid chromatography (HPLC-DAD), whose use applies mainly to the determination and quantification of CGA and C present in coffee (Rigo Bonnin et al., 2018). Given the above, the objective of this research was to evaluate the so-called *specialty coffees* marketed in specialty stores in the central and southern areas of the department of Huila, in an attempt to guarantee the traceability and authenticity of this product.

2 MATERIAL AND METHODS

2.1 Characterization and sample collection

Eight municipalities in the Department of Huila (Colombia) were visited, where 17 samples of roasted coffee

beans were compared between May-June 2023 and stored for 1 month (Table 1), distributed throughout the central zone (Pital, Garzón, Tarqui and Guadalupe) and the southern zone (Timaná, Pitalito, Palestina and San Agustín) From the fieldwork carried out in the evaluation area. Different varieties and processes of specialty coffee were identified in each of the stores visited.

2.2 Physicochemical characteristics: measurement of moisture, pH, and soluble solids content (°Brix).

The moisture content of the samples was determined by the dielectric (indirect) method, using a bean moisture meter Kett (PM-450). The pH and soluble solids content were determined mixing ground coffee (2.25 g) with 50 ml of water at 80 °C. Subsequently, the coffee was cooled to room temperature, and direct measurements were performed with a pH-meter (Orion Star A111).

2.3 Determination of FTIR-ATR spectra

The coffee samples were ground using a Bunn mill (G3 HD BLK, Springfield, USA) to a particle size between 150 and 250 µm. Infrared spectra were recorded following the methodology proposed by Barrios-Rodríguez et al. (2022), using a Cary 630 FTIR spectrophotometer (Agilent, Santa Clara, California, USA) equipped with a DLATGS detector and an ATR sampling accessory. Readings were taken in the wavelength range of 4000 to 650 cm⁻¹, and 16 scans were performed using 1 g of ground coffee per reading. The measurements were taken in triplicate, and one sample of *pasilla* coffee (lower quality coffee beans) was taken as a reference for each zone. Once the spectra were obtained, they were exported to the Excel format for analysis. All samples were analyzed in triplicates.

2.4 Determination of CGA and C

The determination and quantification of CGA and C were performed by high-performance liquid chromatography (HPLC) with a diode array (DAD), according to the methodology proposed by Barrios-Rodríguez et al. (2020); Sánchez-Riaño et al. (2024). 1 g of sample roasted coffee was mixed in 200 mL of UHQ water (type 1, 18.2 MΩ cm), extracted for 20 min in a water bath at 90 °C, and cooled to room temperature, and brought to a volumetric volume of 250 mL. Finally, the extracts were filtered through a 0.20 µm nylon membrane filter and stored in 2 mL amber vials. Chromatographic conditions for quantification were as follows: 10 µl of filtered extract was injected into the HPLC system (Agilent Technologies 1260 Infinity II) The flow condition was isocratic with methanol: water type 1 (Merck, Darmstadt, Germany) 50:50. A 120 EC-

3 RESULTS

3.1 Physicochemical characteristics

The moisture of the 17 samples was between 1.933 ± 0.057 and 1.100 ± 0.100 , as shown in Table 1. The pH values were between 4.876 ± 0.015 and 5.146 ± 0.015 , and statistically significant differences related to the postharvest processing method were observed (Cortés-Macías et al., 2022).

On the other hand, significant differences were found in the content of total soluble solids, which ranged between 1.300 ± 0.264 and 0.700 ± 0.00 °BRIX.

3.2 Analysis of FTIR spectra

The spectra of roasted and pasilla coffee samples from the department of Huila are presented in Figures 1 (central zone) and 2 (southern zone).

On the other hand, the 1700-1550, 1600-1300, and 1450-1240 cm^{-1} bands have been associated with the main compounds in coffee, such as C, CGAs and trigonelline, respectively (Barrios-Rodriguez et al., 2022).

However, Figure 1 indicates significant overlaps between the pasilla, ZCP1, ZCP2, ZCGP4, and ZCG7 samples, as opposed to ZCP3, ZCT5, and ZCG6. These samples show a large imbalance, with very low absorbance heights compared to the other samples. This behavior may be related to errors in the acquisition of the spectra and can be discarded in the graph due to its abnormality. On the other hand, in Figure 2, samples

C18 Poroshell column, 150×4.6 mm and $4 \mu\text{m}$ (Agilent Technologies, California, USA), a flow rate of 1 mL/min was used with a system equipped with a quaternary pump (G7111A), integrated autosampler with a temperature-controlled column oven at 30°C (G7129A). Caffeine was detected at 272 nm and chlorogenic acid at 325 nm with a diode array detector (G7117C). The reference materials used were: caffeine (CAS: 58-08-2; Merck, Darmstadt, Germany) and chlorogenic acid (CAS: 327-97-9; Sigma Aldrich Inc., St. Louis, USA). The chromatographic data were processed with OpenLab ChemStation software version LTS 01.11.

2.5 Sensory Analysis

Sensory analysis was carried out by a trained panel of three judges from the Centro Surcolombiano de Investigación en Café (CESURCAFÉ), following the SCA cupping protocol (Fernández-Alduenda et al., 2021), with some modifications and a distribution of five cups for each sample.

2.6 Statistical analysis

Data were processed from using analysis of variance (one-way ANOVA) with a confidence level of 95%. Mean comparison analyzes were performed to identify statistically significant differences in the parameters evaluated between different categories. Statistical procedures were carried out using StatGraphics Centurion XVI. (Manugistics Inc., Rockville, MD, USA).

Table 1: Characterization and physicochemical characteristics of the 17 coffee samples.

Municipality	Codes	pH	Moisture	SST (°BRIX)
Pital	ZCP1	4.950 ± 0.006^b	1.900 ± 0.200^h	1.133 ± 0.208^{bcd}
	ZCP2	4.953 ± 0.006^b	1.900 ± 0.173^h	1.233 ± 0.351^{cd}
	ZCP3	5.100 ± 0.030^g	1.300 ± 0.100^{bc}	1.266 ± 0.378^d
Guadalupe	ZCGP4	4.966 ± 0.006^{bc}	1.533 ± 0.057^{de}	0.800 ± 0.360^{ab}
Tarqui	ZCT5	5.020 ± 0.010^{de}	1.300 ± 0.100^{bc}	1.300 ± 0.264^d
Garzón	ZCG6	4.970 ± 0.01^{bc}	1.266 ± 0.152^{ab}	1.300 ± 0.100^d
	ZCG7	4.950 ± 0.01^b	1.466 ± 0.057^{cd}	0.900 ± 0.100^{abc}
Timaná	ZST8	5.233 ± 0.050^i	1.100 ± 0.100^a	0.733 ± 0.208^a
	ZST9	5.030 ± 0.010^f	1.633 ± 0.115^{def}	0.800 ± 0.200^{ab}
	ZST10	4.976 ± 0.015^{bc}	1.933 ± 0.057^h	0.900 ± 0.100^{abc}
Pitalito	ZSP11	5.146 ± 0.015^h	1.266 ± 0.115^{ab}	0.800 ± 0.000^{ab}
	ZSP12	5.050 ± 0.010^f	1.933 ± 0.057^h	1.033 ± 0.208^{abcd}
	ZSP13	5.020 ± 0.026^{de}	1.667 ± 0.057^{efg}	0.866 ± 0.115^{ab}
Palestina	ZSPA14	4.876 ± 0.015^a	1.567 ± 0.057^{de}	0.900 ± 0.100^{abc}
San Agustín	ZSSA15	5.046 ± 0.025^f	1.833 ± 0.057^{gh}	0.700 ± 0.000^a
	ZSSA16	4.910 ± 0.020^a	1.800 ± 0.173^{fgh}	1.033 ± 0.115^{abcd}
	ZSSA17	4.993 ± 0.011^{cd}	1.800 ± 0.100^{fgh}	0.966 ± 0.115^{abcd}
Total		5.012 ± 0.087	1.600 ± 0.285	0.980 ± 0.260

Different letters in the same column indicate statistically significant differences (p-value <0.05).

ZST9 and ZSP11 show the lowest absorbance levels of the entire spectrum, which may be due to the physicochemical composition of coffee, which directly influences the final quality of the beverage (Barrios-Rodríguez et al., 2021; Belchior et al., 2020).

The two bands corresponding to C and coffee lipids (2900 and 2855 cm^{-1}) (Barrios-Rodríguez et al., 2022; Belchior et al., 2020), represented in the samples of Figures 1 and 2, show large overlaps that make it difficult to identify differences in absorption levels. In the 1030 cm^{-1} peak, the

predominant absorption levels of the pasilla sample are observed. In this regard, Barrios-Rodríguez et al. (2022) report that the band between 1032 and 988 cm^{-1} is related to the ether group in corn cellulose. In addition, the distinction and displacement of the bands in that region, reported for the pasilla and the samples evaluated, can be associated with the final quality of the coffee and with possible adulterations (adding lower quality coffee beans). However, in this study, the samples were purchased in beans to mitigate this possibility.

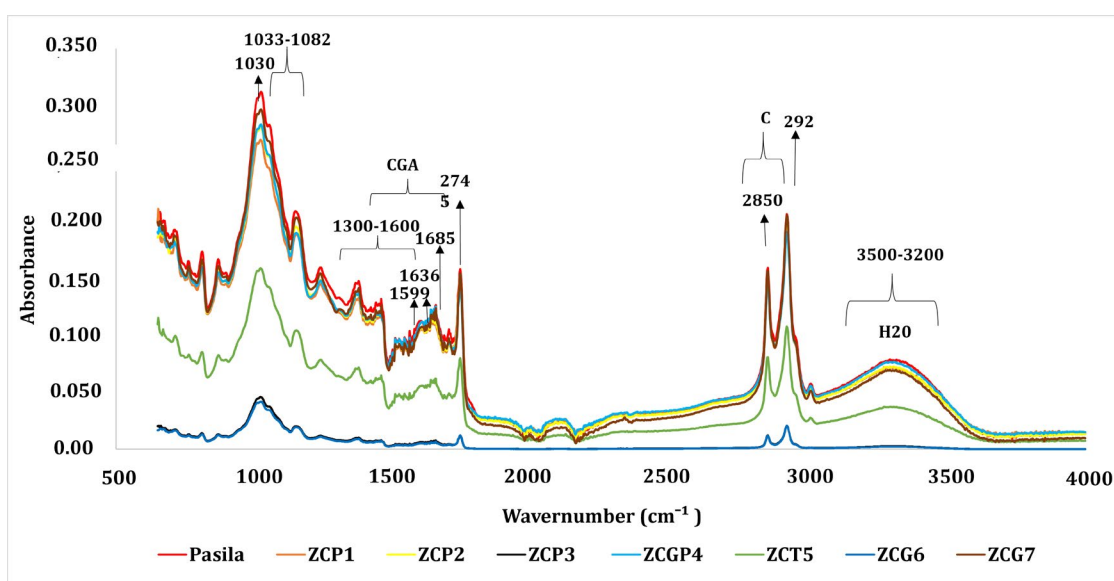


Figure 1: Average total spectra for samples from the central zone of the department of Huila.

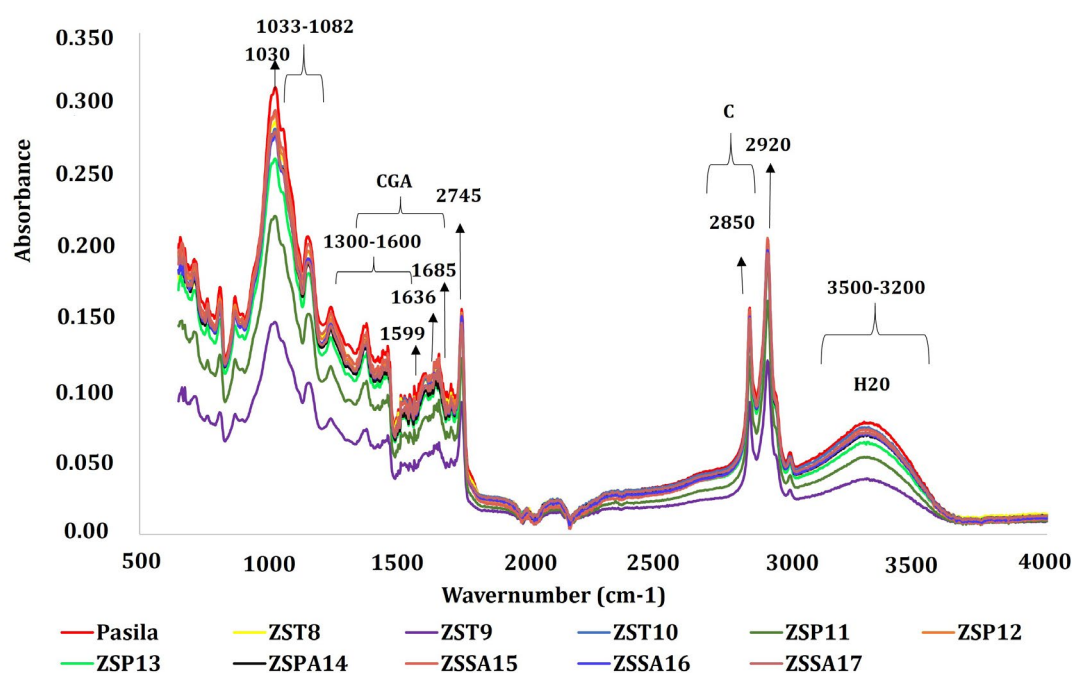


Figure 2: Average total spectra for the samples from the southern zone of the department of Huila.

On the other hand, in the region between 1400 and 900 cm^{-1} , *i.e.*, the fingerprint region, C-O group vibrations of alcohols, ethers, esters, carboxylic acids, and anhydrides are described (Belchior et al., 2020; Varão Silva et al., 2021). The absorption levels of the pasilla sample stand out markedly, as they are higher than those of the samples in Figures 1 and 2.

The region between 1700 and 600 cm^{-1} , associated with the levels of carbohydrates, trigonelline, and CGA, can present reductions after roasting (Belchior et al., 2020; Craig et al., 2014). Variations in this region are due to the physicochemical composition of coffee, as indicated by the spectrum in Figures 1 and 2, which in turn influences the organoleptic characteristics and quality of the final product. At first glance, it is difficult to discriminate with precision the aforementioned components, given the significant overlaps and similarities that are evident in the spectra of the coffee and pasilla samples, but there are statistical analyses that allow us to distinguish with precision and accuracy the differences between these parameters. Additionally, in samples ZCP3, ZCT5, ZCG6, ZST9 and ZSP11, the absorption levels were very low along the spectrum, so in this study, analytical techniques of greater precision were used to validate the related information.

3.3 Determination of CGA and C

Table 2 presents the values of C and CGA for the coffee samples evaluated. The concentration of these components is between 10.472 ± 0.262 and 8.330 ± 0.138 , and between 14.184 ± 0.384 and 7.772 ± 0.391 , respectively.

Statistically significant differences were found in the CGA and C content of the samples, which were associated with grain type, origin, roasting degree, and extraction method (Elhalis et al., 2023; Wale et al., 2024; Wei & Tanokura, 2015).

3.4 Sensory analysis

Samples were evaluated according to the SCA cupping protocol, with some exceptions, as shown in Table 3.

Of the samples evaluated, 64.70 % were classified as specialty coffee, where 41.17 % corresponded to traditionally processed coffees (washed). However, the highest values in the specialty classification corresponded to coffees with other types of processing (*honey* and *natural*) making samples ZCT5 and ZCG7 stand out. According to Figure 3, these samples stand out in attributes such as uniformity, clean cup, sweetness, and fragrance/aroma. Similarly, in Figure 4, samples ZSP12, ZSPA14 and ZSSA17 have similarity with the aforementioned attributes, differing from samples ZCP2, ZCGP4, ZST8, ZST9, ZST10 and ZSP13, classified as non-special.

However, samples classified as special, ZCT5 and ZCG7 (*honey* and *natural*) did not show statistically significant differences with ZCG6, ZSP12, and ZSPA14 (washed), since such classification depends on factors such as fermentation time and roasting level, among others (Barrios-Rodriguez et al., 2021; Freitas et al., 2024a). This generates significant overlaps in descriptors such as fragrance/aroma, flavor, aftertaste, and acidity.

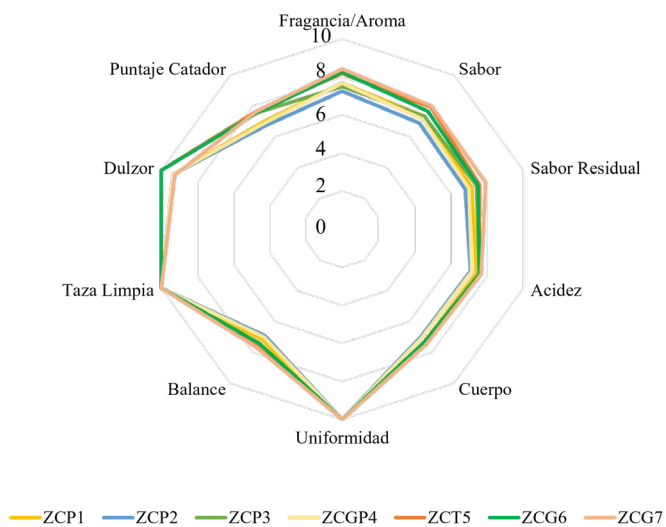
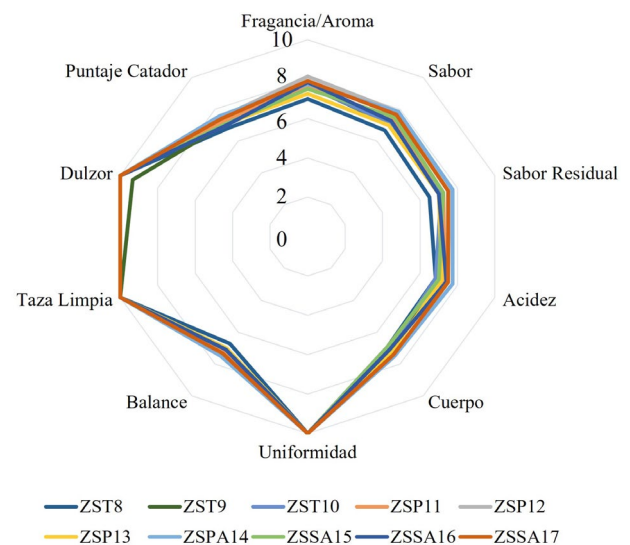
Table 2: Caffeine and CGA content.

Municipality	Codes	Caffeine*	CGA*	Process/variety
Pital	ZCP1	9.110 ± 0.074^b	11.378 ± 0.170^{ef}	Washed/--
	ZCP2	9.632 ± 0.111^{bcde}	10.199 ± 0.073^c	Washed / Caturra
	ZCP3	9.265 ± 0.052^{bc}	9.132 ± 0.035^b	Washed / --
Guadalupe	ZCGP4	10.472 ± 0.262^f	10.982 ± 0.201^{de}	Washed / Castillo
Tarqui	ZCT5	9.980 ± 0.001^{cdef}	12.934 ± 0.019^i	Honey/ Bourbon Rosé
Garzón	ZCG6	9.334 ± 0.444^{bc}	10.372 ± 0.500^{cd}	Washed / Bourbon Rosé
	ZCG7	10.345 ± 0.038^{ef}	11.250 ± 0.244^e	Natural/ Bourbon Rosé
Timaná	ZST8	9.415 ± 0.516^{bcd}	7.772 ± 0.391^a	Washed / Blend
	ZST9	10.344 ± 0.117^{ef}	11.438 ± 0.064^{ef}	Washed / Castillo
	ZST10	10.142 ± 0.645^{def}	14.184 ± 0.384^j	Washed / Bourbon Rosé
Pitalito	ZSP11	9.697 ± 0.465^{bcde}	12.239 ± 0.623^{hi}	Natural/ Tabi
	ZSP12	9.296 ± 0.136^{bc}	9.879 ± 0.161^c	Washed / Bourbon Rosé
	ZSP13	9.958 ± 0.825^{cdef}	11.01 ± 0.922^{de}	Washed /--
Palestina	ZSPA14	8.330 ± 0.138^a	10.314 ± 0.169^{cd}	Washed / Bourbon Rosé
San Agustín	ZSSA15	9.798 ± 0.513^{bcdef}	12.089 ± 0.218^{gh}	Washed / Castillo
	ZSSA16	9.387 ± 0.108^{bcd}	11.626 ± 0.185^{efg}	Washed / Tabi
	ZSSA17	10.340 ± 0.075^{ef}	12.034 ± 0.129^{gh}	Natural/ Bourbon Rosé
Total		9.696 ± 0.612	11.108 ± 1.476	

Different letters in the same column indicate statistically significant differences (p-value <0.05); *mg/g coffee for C and CGA respectively.

Table 3: Final score of the coffees evaluated and their classification according to the SCA.

Municipality	Codes	Final score	Process/variety	Classification under SCA protocol
Pital	ZCP1	80.250 ± 2.046 ^c	Washed/--	≥80 – is considered specialty coffee
	ZCP2	77.833 ± 1.258 ^{ab}	Washed / C*	<80 – is not considered specialty coffee
	ZCP3	82.333 ± 0.381 ^{def}	Washed / --	≥80 – is considered specialty coffee
Guadalupe	ZCGP4	79.333 ± 0.946 ^{abc}	Washed / C*	<80 – is not considered specialty coffee
Tarqui	ZCT5	83.916 ± 0.520 ^f	Honey/ BR*	≥80 – is considered specialty coffee
Garzón	ZCG6	83.334 ± 1.628 ^f	Washed /BR*	≥80 – is considered specialty coffee
	ZCG7	84.07 ± 1.488 ^f	Natural/ BR*	
Timaná	ZST8	77.466 ± 2.552 ^a	Washed / B*	<80 – is not considered specialty coffee
	ZST9	79.666 ± 1.282 ^{bc}	Washed / C*	
	ZST10	79.933 ± 1.282 ^c	Washed / BR*	
Pitalito	ZSP11	81.216 ± 1.328 ^{cde}	Natural/ T*	≥80 – is considered specialty coffee
	ZSP12	83.466 ± 0.450 ^f	Washed / BR*	<80 – is not considered specialty coffee
	ZSP13	79.75 ± 1.089 ^{def}	Washed /--	
Palestina	ZSPA14	83.666 ± 0.144 ^f	Washed / BR	≥80 – is considered specialty coffee
San Agustín	ZSSA15	80.333 ± 0.381 ^{cd}	Washed / C*	≥80 – is considered specialty coffee
	ZSSA16	80.666 ± 1.040 ^{cd}	Washed / T*	
	ZSSA17	82.75 ± 0.661 ^{ef}	Natural/ BR*	

**Figure legend:** Fragrance/Aroma, flavor, aftertaste, acidity, body, uniformity, balance, clean cup, sweetness, taster score.**Figure 3:** Graphical representation of the attributes of coffee samples from the central zone.**Figure legend:** Fragrance/Aroma, flavor, aftertaste, acidity, body, uniformity, balance, clean cup, sweetness, taster score.**Figure 4:** Graphical representation of the attributes of the coffee samples from the southern zone.

4 DISCUSSIONS

4.1 Physicochemical characteristics

These results are within the established standards (Instituto Colombiano de Normas Técnicas y Certificación (ICONTEC), 2007) or roasted or ground coffee, *i.e.*, values lower than 4 %. However, statistically significant differences

were found, possibly associated with the roasting level in the samples evaluated, where the moisture content decreased as the roasting level increased (Cortés-Macías et al., 2022). Samples ZST8 and ZSP11 reported the lowest values of this parameter.

The pH statistically significant differences related to the postharvest processing method were observed (Cortés-Macías et al., 2022). Samples ZSPA14 and ZSSA16 showed

the lowest pH values, which could be associated with the accumulation of lactic and acetic acid generated by lactic acid bacteria and yeasts during fermentation and long drying periods (Cortés-Macías et al., 2022; Elhalis et al., 2023) where samples ZCG7 and ZSSA17, processed through dry milling, also stood out. The pH values were also associated with the degree of roasting of the coffee, which sometimes increased with the roasting level (Barrios-Rodríguez et al., 2021; Cortés-Macías et al., 2022). However, it is necessary to verify this statement by examining characteristics such as color to demonstrate the exact incidence of this factor.

Additionally, at the total soluble solids content; these differences also are related to the types of coffee processing, where dry and semi-dry methods have a special incidence; beans processed by these methods develop a sweet, fruity, and less acidic profile (Elhalis et al., 2023). This is why the ZCT5 sample reported the highest value in this parameter, compared to ZSSA15.

However, according to (Freitas et al., 2024b) soluble solids concentrations decreased with higher roasting temperatures due to the loss of chemical components during the high-temperature roasting process, this may be related to sample ZST8.

4.2 Analysis of FTIR spectra

The 3500-3200 cm^{-1} region belongs to the H-O-H single bonds of water (Craig et al., 2014), and the two bands at 2900 and 2855 cm^{-1} correspond to the C-H group vibrations, related to both C and lipids in coffee (Barrios-Rodríguez et al., 2022; Belchior et al., 2020). The peak at 2850 cm^{-1} has been associated mainly with C (Barrios-Rodríguez et al., 2021; Craig et al., 2014). In this study, the values for the aforementioned compounds in coffee were shifted to 2920 and 2850 cm^{-1} , respectively.

The wavelength between 1600 and 1700 cm^{-1} is related to the presence of CGA due to the stretching of the C=O bond (Barrera et al., 2019; Barrios-Rodríguez et al., 2022). Similarly, the 1750 cm^{-1} wavelength is associated with the vibration of the carbonyl group of carboxylic acids and ketones. The former are precursors of coffee acidity and aroma (Belchior et al., 2020), while ketones contribute to characteristic aromas such as woody, cooked fruit, and almonds. In addition, this region has been associated with the aliphatic acid vibration (Belchior et al., 2020), largely related to the aromatic profile of coffee. Also, the three predominant peaks corresponding to the carbonyl group (C=O) at 1685 cm^{-1} , the ethylene group (C=C) at 1636 cm^{-1} , and the phenyl ring at 1599 cm^{-1} are characteristic of CGA. The presence of other carbonyl compounds in the 1800-1680 cm^{-1} region, such as aldehydes, is related to the specific organoleptic properties of coffee (Belchior et al., 2020; Wang et al., 2011).

The region between 1680 and 1630 cm^{-1} is associated with carbonyl-amide group vibrations, and trigonelline also

generates absorbance peaks in this region (Belchior et al., 2020). During the roasting process, trigonelline decomposes into pyridines and pyrroles. The former are responsible for the characteristic aroma of roasted coffee (Belchior et al., 2020). Additionally, the peak observed between 1082 and 1033 cm^{-1} could be related to cellulose and quinic acid (Barrios-Rodríguez et al., 2021). Finally, carbohydrates generally present absorption bands between 1400 and 900 cm^{-1} , *i.e.*, the well-known *fingerprint region*, which is responsible for most of the spectral bands (Barrios-Rodríguez et al., 2022; Belchior et al., 2020).

4.3 Determination of CGA and C

The sample ZCGP4 (table 2) recorded the highest C content, and ZST10 reported the highest level of CGA. However, samples ZCP3, ZCT5, ZCG6, ZST9, and ZSP11, evaluated with the FTIR method, were not relevant in this aspect, since their absorbance levels at the wavelengths associated with C and CGA (Figures 1 and 2) did not indicate similarities with those of the other samples. However, the determination and quantification of these compounds by HPLC-DAD established that these samples lie within the ranges described.

Additionally, samples ZCG7 and ZSSA17 showed higher values for C due to dry processing compared to ZSPA14 (washed). This behavior is like that observed by Cortés-Macías et al. (2022). In addition, the coffee cherry fermentation process generates several chemical compounds such as aldehydes, esters, alcohols, and ketones, which, together with the compounds evaluated in this study (C and CGA), contribute significantly to the aroma and flavor of roasted beans and brewed coffee (Seninde & Iv, 2020). Consequently, the C and CGA content is closely related to the roasting process. The lower values for these two compounds can be attributed to their release in the gas phase during roasting, as a result of the cracking of the coffee beans (Cortés-Macías et al., 2022; Elhalis et al., 2023; Wale et al., 2024).

When discussing changes in the main components of green and roasted coffee, Wei and Tanokura (2015) state that CGA can experience a significant decrease, going from a percentage range of 5.5-8.0 to one of 1.2-2.3 (of the dry weight of the beans), while trigonelline and C can remain stable in percentage ranges between 1.0-1.2 and 0.5-1.0 and between 0.9-1.2 and 0-1.0 respectively (Velásquez & Banchón, 2022). Therefore, the final roasting time determines the physicochemical composition of coffee, especially due to the reduction of the aforementioned compounds and others such as sucrose, free amino acids, and melanoidins, in addition to the degradation of proteins and polysaccharides (Belchior et al., 2020; Wei & Tanokura, 2015). The above had a great impact on the values of the samples evaluated in this study and is directly related to the final quality of the beverage, so

it should be considered as one of the processes of greater care and dedication in coffee production.

4.4 Sensory analysis

The method of post-harvest processing of coffee is closely related to cup quality (Cortés-Macías et al., 2022). Each type of process generates different organoleptic characteristics in the final product. According to Seninde and Iv (2020), coffees processed by dry (natural) processing are differentiated by having vanilla flavor attributes and a floral aroma. However, these descriptors were not relevant for the samples evaluated. Meanwhile, Cortés-Macías et al. (2022) described attributes associated with ‘chocolate’ and ‘caramel’ flavors, as well as a ‘medium fruity body’. These attributes coincide with the profiles found in samples ZCG7, ZSP11 and ZSSA17 (table 3). Likewise, *honey* coffees are characterized by a lasting sweet fruity flavor, with low acidity compared to washed coffee (Seninde & Iv, 2020), which coincides with that described for samples ZCT5, ZCG6 and ZSP12.

On the other hand, due to the growing demand for specialty coffee in Colombia, the implementation of new types of coffee processing has become indispensable (Jacobi et al., 2024). Hence, different varieties and processes are related to the samples of this study (table 3). Fifty percent of the samples evaluated correspond to the Bourbon Rosé variety, 21.4% to the Castillo variety, and 14.3% to the Tabi variety. The rest corresponded to unidentified varieties, as their information was not on the product label. Although specialty coffees in Colombia acquire an extra value due to this denomination, not all of them are marketed responsibly. This is evident in aspects such as the basic information on the product label, which should include the origin and provenance of the coffee, its variety, its height, its INVIMA registration, and the degree of roasting. *Specialty* stores that commercialize this type of coffee do not usually follow up on these key aspects, which compromises the veracity of the information provided to the consumer.

5 CONCLUSIONS

The study identified pH and moisture as key parameters influencing the final beverage quality, with significant differences depending on the post-harvest processing method. Chlorogenic acid (CGA) and caffeine (C) content varied among samples in FTIR and HPLC analyses. Coffees processed using dry and semi-dry methods obtained the highest scores as specialty coffees (64.70%), primarily from the southern Huila region of Colombia. Finally, further studies with more precise techniques are needed for better characterization.

6 AUTHOR CONTRIBUTIONS

Conceptual idea: Barrera-Bermeo, O.; Lugo-Moreno, A.; Methodological design: Lugo-Moreno, A; Vargas, D.;

Barrera-Bermeo, O., Data collection: Lugo-Moreno, A; Vargas, D. Data analysis and interpretation: Lugo-Moreno, A; Barrera-Bermeo, O; Vargas, D. Writing and editing: Lugo-Moreno, A; Barrera-Bermeo, O.

7 DATA AVAILABILITY STATEMENT

Data available upon request to authors.

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