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Impact of coffee-cherry fermentation time on physicochemical, spectral and sensory characteristics of Arabica coffee beans in two agroecological zones of Huila, Colombia

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ABSTRACT

This study investigated how coffee-cherry holding (pre-pulping in-fruit fermentation) time (0–96 h) modulates the chemical composition (caffeine, trigonelline, chlorogenic acids quantified by HPLC) and the infrared spectral fingerprints (FTIR/FTNIR) of Arabica coffee produced in two contrasting agroecological zones (ZAE 1 and ZAE 5) in Huila, Colombia.

A randomized block design was used, testing five fermentation durations across the two zones. Physical quality parameters (defect rate, yield), sensory attributes (SCA protocol), chemical composition (caffeine, trigonelline, chlorogenic acids via HPLC), and spectral profiles (FTIR/FTNIR) were assessed. Results showed that extended fermentation times (≥72 h) increased physical defects and decreased the proportion of sound beans. Caffeine and trigonelline levels remained stable, while chlorogenic acids varied significantly with fermentation time and agroecological zone. FTNIR effectively captured process kinetics (PC1 =70%), and FTIR provided functional chemical specificity. Sensory scores ranged from 78 to 86, with ZAE 1 displaying more consistent profiles over time, whereas ZAE 5 showed greater fluctuation. The findings indicate that there is no universal optimal fermentation time; however, a 24–48 h window is considered a safe operational range, adjustable to local conditions and under basic process control (temperature, pH, °Brix). The study recommends the development of predictive multivariate models to adapt fermentation strategies based on microenvironmental conditions and improve postharvest decision-making.

1. Introduction

Fermentation in fruit is a critical stage in coffee quality control (Meira Borém et al., 2023), where the microbial ecology of the fruit (de Sousa et al., 2023), the physicochemical conditions of the substrate, and technological decisions in wet processing converge. It has been shown that time and temperature modify fermentation kinetics, pectin extraction, and the formation/degradation of metabolites with sensory impact (dos Santos Gomes et al., 2025), although the magnitude and direction of these effects depend on the production context and the management

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applied (Borém et al., 2024). On the other hand, the use of inoculants (yeasts and lactic acid bacteria) and bioreactors has sought to increase reproducibility and modulate volatile and sensory profiles, with promising but still heterogeneous results between matrices and environments (Afriliana et al., 2024; Haile & Kang, 2019; Mardhatilah et al., 2023).

In Colombia, the scaling up of controlled fermentations in stirred bioreactors between 10–30 °C has been documented, showing that temperature-controlled processes require an additional 2–13 h compared to spontaneous fermentation to achieve complete mucilage degradation, with differences in final pH (Peñuela Martínez et al., 2023a). In terms of microbial diversity, a metataxonomic study conducted on 20 farms in Quindío showed that *Enterobacteriaceae* genera were replaced by *Leuconostoc*, *Lactobacillus*, and *Acetobacter* towards the end, associated with a drop in pH and the formation of alcohols and esters in the green grain (Peñuela-Martínez et al., 2023g). Controlling temperature also microbial kinetics quality in altitudinal gradients: at 15 °C, higher cup scores were observed than at 30 °C and in spontaneous fermentations, with a consistent effect at various altitudes (Peñuela-Martínez et al., 2023c). In addition, oxygen availability and time affect performance: self-induced anaerobic fermentations of shorter duration obtained the best integrated physical and sensory quality indices, while prolonged times penalized these indices (Peñuela-Martínez et al., 2025). By variety, trials with Castillo, Cenicafé-1, and Tabi indicated similar fermentation behaviors among materials, scores greater than 82 SCA points, and no significant differences between 15 °C, 30 °C, and spontaneous fermentation (Peñuela-Martínez and García-Duque, 2023b). These studies lay the groundwork for research that can be taken to farms so that it can be used by coffee growers, adding value to coffee quality while avoiding risks that cause sensory defects.

A frequently underestimated component is the climate, which conditions the biochemistry of the fruit and the dynamics of the process. In Huila, the selected agroecological zones show significant contrasts: ZAE 1 (average altitude 1477 m) has 1300–1600 hours of sunshine per year, 1200–1600 mm of precipitation per year, and ~94 days of water deficit during flowering; ZAE 5 (1459 m) has 1400–1600 hours/year of sunshine, 1400–1800 mm/year of precipitation, and a daily thermal accumulation for fruit formation of 2300–2800 degrees (Peña et al., 2012). These microenvironmental gradients can alter the content and state of the mucilage, enzymatic activity, and microbial establishment, conditioning the response to the same fermentation time in fruit.

Despite progress, gaps remain: (i) a lack of controlled comparisons by ZAE that isolate the effect of time on fruit before pulping; (ii) results for the relationship between specific chemical compounds (caffeine, trigonelline, chlorogenic acids) and sensory quality by ZAE; and (iii) lack of multiscale readings that integrate chromatography, FTIR/FTNIR spectroscopy, and chemometrics to explain, rather than describe, variability between zones and processes. This study addresses these gaps by evaluating, in batches of *Coffea arabica* L. from Huila, the effect of 0, 24, 48, 72, and 96 h of pre-pulping coffee-cherry holding (in-fruit fermentation) on physicochemical parameters, chemical compounds by HPLC (caffeine, trigonelline, CGA), FTIR/ FTNIR profiles, and sensory quality, comparing ZAE 1 and ZAE 5.

The objective of this study was to identify the effect of fermentation time on coffee fruit, under the hypothesis that the physical, chemical, and sensory quality of the coffee obtained varies depending on climatic conditions.

We propose that the waiting time of the fruit before pulping acts as a post-harvest treatment that may modify (i) the availability of mucilage substrates and (ii) the physicochemical trajectory of the fermentation mass (as reflected by pH and temperature). These process-level differences may be associated with changes in fermentation kinetics and mass transfer of water-soluble constituents, potentially influencing physical defects and the stability/transformations of phenolic esters (e.g., chlorogenic acids) in an environment-dependent manner across ZAEs.

Accordingly, the main contribution of this work is the integrated chemical–spectral characterization of the fermentation-time effect across agroecological zones, combining targeted HPLC markers with FTIR/FTNIR fingerprints and chemometric interpretation. Physical and sensory quality measurements are included as supportive indicators to translate the chemical–spectral findings into practical postharvest decision-making.

Table 1
Characteristics of the farms sampled by agroecological zone (Huila, Colombia).

Characteristic	ZAE 1	ZAE 5
Farm	Villa Suce	Las Torres
Municipality	La Argentina (Huila)	Suaza (Huila)
Location (WGS84)	02°11′41.5083″ N; 75°56′58.2304″ W	01°49′00.4524″ N; 75°51′23.1488″ W
Altitude (m above sea level)	1813	1341
Average annual precipitation (mm)	1477	1508
Average sunshine (h year^{-1})	1438	1486
Average temperature (°C)	18 ± 5	26 ± 5

2. Materials and methods

2.1. Obtaining raw materials

We worked with *Coffea arabica L.*, Castillo variety. The harvest was carried out manually, selecting only ripe fruits, collected from two farms in the department of Huila (Colombia) that represent agroecological contrasts (altitude and environmental conditions), in order to capture variability relevant to fruit fermentation and its post-harvest effect. The

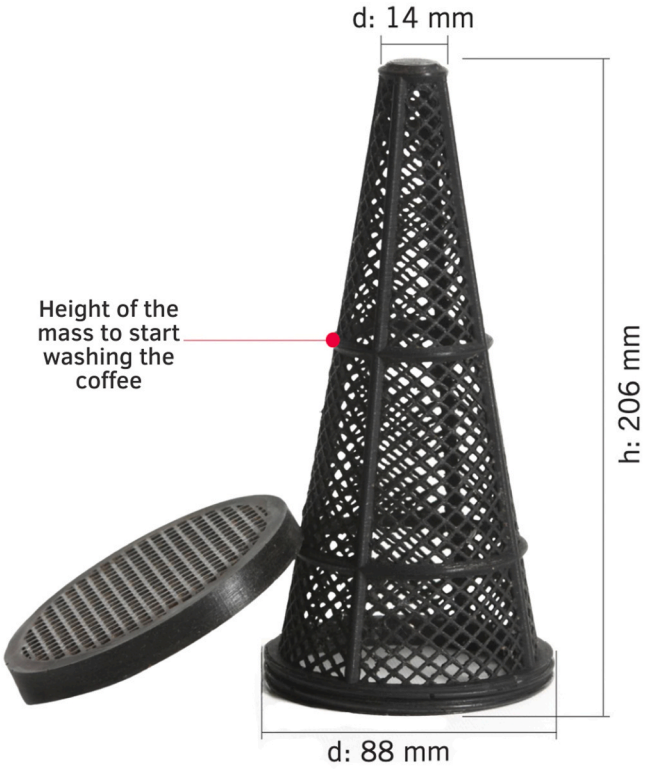

Fig. 1. Fermaestro® device (truncated cone; internal volume 500 mL) used to determine the washing endpoint of mucilage fermentation based on the stabilization of coffee bed height/upper void. The endpoint was reached when the upper void height exceeded 85 mm, corresponding to a mucilage removal rate > 96% (Peñuela-Martínez et al., 2013).

soil and climate characteristics of each area are summarized in Table 1.

2.2. Experimental design and sample size

The study followed a randomized complete block design with a 2 × 5 factorial structure: two agroecological zones (ZAE 1 and ZAE 5) and five pre-pulping coffee-cherry holding times (in-fruit fermentation) (0, 24, 48, 72, and 96 h). In each ZAE (one farm per ZAE), the trial was replicated in three independent blocks (lots processed on separate harvest days), yielding 15 experimental units per ZAE (3 blocks × 5 times) and 30 experimental units in total. Within each block, 180 kg of ripe cherries were harvested and 150 kg were allocated to the five treatments (≈ 30 kg per treatment), which ensured sufficient material for physical, sensory, chemical, and spectral analyses.

2.3. Post-harvest coffee processing

Both farms had adequate infrastructure and operating conditions and clean equipment for coffee processing (pulpers and screens). In each experimental block, 180 kg of ripe coffee cherries were harvested manually, and their quality was assessed using the Mediverdes® tool (Guerrero et al., 2022) and Cromacafé® (Peñuela-Martínez et al., 2022). The fruits were then classified by density using the double bucket technique, and fruit quality was assessed again using the Mediverdes® tool (Guerrero et al., 2022); From this process, 150 kg of coffee were selected to form five treatments: a control (immediate pulping after sorting) and four treatments with different times of 24, 48, 72, and 96 h in fruit before pulping. This pre-pulping stage corresponds to controlled coffee-cherry holding ('in-fruit fermentation'). The 0 h treatment represents immediate pulping after sorting. After pulping, the mucilage fermentation was conducted to the point of washing using the Fermaestro® method (Peñuela-Martínez et al., 2013). This method is based on the change in apparent density of the pulped coffee mass due to the drainage of the degraded mucilage (Fig. 1), which reduces the volume occupied by the mass until it stabilizes (≈11.9–13.1% of the initial volume). To facilitate observation, a truncated cone-shaped perforated device (internal volume 500 mL) was used, with perforations < 6 mm and a minimum perforated area of 55%, which allows fluids to drain and beans to be retained. The device was filled flush with freshly pulped coffee through the larger base, the lid was secured, and it was placed inside the tank with the narrow part facing up. Near the end of fermentation, the device was removed and dropped three times onto the larger base from a height of 3 cm to settle the beans and facilitate reading the upper empty space. The washing point was considered to have been reached when the height of the coffee/empty space in the device stabilized and the empty space exceeded the first mark (final empty space height >85 mm), which corresponds to a mucilage removal rate > 96%. If the threshold was not reached, the device was reinserted and checked every hour until the criterion was met. In this manuscript, in-fruit fermentation' refers to the controlled holding of intact ripe coffee cherries prior to pulping, i.e., the elapsed time between cherry sorting and pulping. Operationally, this is equivalent to 'cherry holding/cherry storage' (also described as fruit reserve) in postharvest practice. We use the expression 'in-fruit fermentation' to emphasize that biochemical and fermentative changes may already start within the intact cherry during this pre-pulping stage; after pulping, fermentation proceeds as mucilage fermentation until the washing endpoint.

2.3.1. Process control and measurements during fermentation

The pH, temperature, and total soluble solids (°Brix) were measured in freshly pulped coffee before washing. The pH and temperature were recorded with a portable meter (HI9814, manufactured by Hanna Instruments SAS, USA) calibrated with pH 4.0, 7.0, and 10.0 buffer solutions. A refractometer (BTX-1 manufactured by Vee Gee Scientific, USA) was used for total soluble solids (°Brix), and a digital probe thermometer (TP101 manufactured by SHTROL, China) was used for the temperature of the mass.

At the end of fermentation, all samples were washed manually four times, followed by density sorting. The washed coffee was sun-dried in marquee-type dryers until it reached between 10% and 12% moisture content using indirect measurement equipment (PM-450 manufactured by KETT, USA).

2.4. Physical analysis of the bean

A representative sample of 250 g of dry parchment coffee was taken, the parchment was removed by threshing, and the fractions were separated: excelso, almond or green coffee; pasilla, defective beans, and coffee below mesh size No. 13 according to standard NTC 5248–2013; and losses, husks, parchment, impurities, and defects. Based on these weights, the percentages of good quality coffee, losses, pasilla, and the yield factor were calculated based on these weights.

2.4.1. Yield factor (YF)

Estimated based on the quantity (kg) of dry parchment coffee (DPC) needed to obtain a 70 kg bag of high-quality coffee (Eq. 1). Calculated based on the high-quality yield of the sample:

$$(YF) = \frac{(250\ \ g\ DPC) * (70\ \ Kg\ bag\ of\ excelso\ coffee)}{Weight\ \ of\ \ green\ \ coffee\ \ without\ \ defects\ \ in\ \ grams} \quad (1)$$

2.4.2. Percentage of good beans (%GB)

This is the percentage of good beans in a sample of dry parchment coffee (DPC) (Eq. 2):

$$\%GB = \frac{M_G\ \ g}{PDC\ \ g} \times 100 \quad (2)$$

Where, M_G is the green coffee beans without physical defects, calculated by subtracting the husks, impurities and defective beans identified in the classification from the parchment.

2.4.3. Percentage of coffee threshing loss (%Ctl)

Corresponds to the mass of the husk, parchment, and unusable materials resulting from threshing (Eq. 3):

$$(\%Ctl) = \frac{(250\ \ g\ DPC)\ \ *\ \ (Total\ weight\ of\ green\ coffee\ after\ threshing)}{(250\ \ g\ \ CPS)} * 100 = \quad (3)$$

Where, DPC denotes dry parchment coffee.

2.4.4. Percentage of pasilla (%P)

Percentage of defects in a freshly threshed sample (Eq. 4).

$$(\%P) = \frac{Weight\ of\ all\ defective\ beans}{Total\ weight\ of\ green\ coffee\ after\ threshing} * 100 \quad (4)$$

2.5. Roasting procedure

Green coffee samples were roasted under standardized conditions following the Specialty Coffee Association (SCA) cupping roast approach to minimize roasting-driven variability prior to sensory and chemical analyses. Roasting was performed in a DR-1 sample roaster (1 kg; PRISMA Coffee Tech, Medellín, Colombia) using a constant batch size of 200 g per run. Roast profiles were continuously monitored and recorded with Artisan v3.4.0, and key events were logged (charge, yellowing/drying end, first crack onset, and drop). All samples were roasted to a medium degree defined by objective color measurement using a Lighttells CM-100 colorimeter (Lighttells, Taiwan), targeting Gourmet scale 51–60. Total roast time was controlled between 10 and 12 min. Each sample was roasted in triplicate under the same operating conditions.

Immediately after reaching the endpoint, beans were discharged and rapidly air-cooled to ambient temperature to stop roasting reactions. Roasted samples were stored in airtight containers protected from light and moisture and allowed to rest prior to cupping according to SCA practice.

2.6. Sensory analysis of coffee

Sensory analysis was conducted following the Specialty Coffee Association (SCA) cupping protocol under controlled conditions (odor-free environment, stable temperature, and standardized cupping materials). A panel of five cuppers participated, including four certified Q Graders and one non-certified cupper with prior experience in coffee evaluation. To reduce sensory fatigue and control order effects, cupping was organized into three randomized sessions, each session evaluating a maximum of 10 samples. Samples were blind-coded and presented in randomized order within each session. Roasted coffee was ground immediately prior to evaluation, cupping grind (EK43s manufactured by Mahlkonig, Germany), and brewed using standardized SCA cupping conditions (coffee-to-water ratio and infusion time), with evaluation performed on the official SCA cupping form considering fragrance/aroma, flavor, aftertaste, acidity, body, balance, uniformity, clean cup, sweetness, overall, and defects (SCAA, 2015). Each cupper scored samples independently; sensory results for each experimental unit were obtained by averaging scores across cuppers within each session and subsequently across the three sessions, yielding a single sensory value per experimental unit for downstream statistical analysis.

2.7. Determination of chlorogenic acids and caffeine in coffee (HPLC–DAD), method validation and quality assurance

The quantification of caffeine, trigonelline and chlorogenic acids in roasted coffee was performed following the method described by Sánchez-Riaño et al., (2024), with minor adaptations. Briefly, 100 mg of ground roasted coffee were extracted in 10 mL of ultrapure water (18.2 MΩ·cm) at 90 °C using ultrasound for 30 min (15 mL tubes), followed by incubation in a shaking incubator (KS 4000 i control, IKA) at 300 rpm and 60 °C for 18 h. Extracts were centrifuged at 4200 rpm (Unicen 21, Orto Aleresa), filtered through a 0.20 μm nylon membrane, and transferred to 2 mL amber vials. Ten μL were injected into an Infinity II 1260 HPLC system (Agilent Technologies, USA) equipped with a Poroshell 120 EC-C18 column (150 × 4.6 mm; 4 μm). Elution was performed under isocratic conditions using methanol:water (20:80, v/v) at 1.0 mL min^{-1} and 30 °C. Detection was carried out using a diode-array detector (DAD) at 272 nm (caffeine and trigonelline) and 325 nm (chlorogenic acids). External calibration was conducted using certified reference standards: chlorogenic acid (Aldrich, C3878, CAS 327–97–9), trigonelline (US Pharmacopeia Reference Standard, 1686411, CAS 6138–40–5), and caffeine (Sigma-Aldrich, PHR1009, CAS 58–08–2). Six-point calibration curves were prepared in the same solvent system used for extract dilution; for caffeine and trigonelline the levels were 50, 80, 100, 150, 200 and 300 mg L^{-1} (ppm), and for chlorogenic acid 20, 50, 80, 100, 150 and 250 mg L^{-1} (ppm). Peak areas were regressed against nominal concentrations by least-squares linear regression and calibration suitability was checked by regression statistics and residual inspection; chlorogenic acids were reported as chlorogenic acid equivalents when integrated as a combined response. Method sensitivity (LOD/LOQ) was estimated from calibration data using the 3.3 σ/S and 10 σ/S criteria, respectively, where σ is the standard deviation of the response and S is the calibration slope, and repeatability was assessed from replicate injections of a mid-level standard and representative sample extracts (expressed as %RSD). Quality assurance during the analytical sequence included blank injections every 10 chromatographic runs to monitor carryover/contamination, together with periodic verification of system stability (retention time and detector response). Data processing was performed using OpenLab ChemStation (v. LTS 01.11, Agilent Technologies), and each ZAE×time combination was analyzed from independent roast replicates (n = 3). The HPLC–DAD procedure is reported in full (sample preparation, instrumental conditions, calibration scheme, and QA/QC) to enhance reproducibility, following detailed reporting practices in the literature

2.8. Determination of FTIR spectra

The mid-infrared (MIR) spectra of roasted coffee samples were acquired following Collazos-Escobar et al., (2024) using an FTIR spectrophotometer (Cary 630, Agilent Technologies, Santa Clara, CA) coupled to a horizontal ATR accessory (Diamond ATR). Prior to measuring all samples, instrument performance was verified through the laser frequency calibration test (x-axis accuracy) by recording the spectrum of a polystyrene film and comparing the observed absorbance band positions with the certified values of the NIST Standard Reference Material (SRM) 1921. Spectra were collected over 4000–650 cm^{-1} at 4 cm^{-1} resolution, scan speed 16, with background correction; each spectrum comprised 900 wavenumbers. To minimize acquisition-related variability, the ATR crystal was cleaned between measurements and consistent sample–-crystal contact was maintained. Spectra were preprocessed using baseline correction followed by multiplicative scatter correction (MSC) (Collazos-Escobar et al., 2023). Each sample was measured in quintuplicate (n = 5 spectra), and the mean spectrum was used for subsequent multivariate analysis.

2.9. Determination of spectra by Fourier transform near-infrared spectroscopy (FT-NIR)

This was performed according to the methodology described by Ordoñez Lozano et al., (2025). Near-infrared spectra were obtained using a Spectrum Two FT-NIR spectrometer (PerkinElmer, Inc., USA), equipped with a continuous sample rotation accessory and interleaved scanning. Control and acquisition were performed using Spectrum IR software, version 10 (PerkinElmer). Approximately 15 g of roasted coffee beans were placed in a Petri dish and placed in the rotating sample holder, ensuring homogeneity through continuous rotation during measurement. Acquisitions were performed in diffuse reflectance mode with a high-resolution InGaAs detector, covering a spectral range of 12000–4000 cm^{-1} (≈ 830–2500 nm). Each spectrum was recorded with a spectral interval of 4 cm^{-1}, resolution of 8 cm^{-1}, and 64 co-averaged scans. Each spectrum included approximately 2000 points, and three independent replicates were obtained for each sample. Quintuple spectra were averaged prior to chemometric analysis.

2.10. Statistical analysis

The experiment followed a randomized complete block design with a 2 × 5 factorial structure (two agroecological zones, ZAE 1 and ZAE 5; and five pre-pulping coffee-cherry holding times (in-fruit fermentation): 0, 24, 48, 72 and 96 h). In each agroecological zone, treatments were replicated in three independent blocks (lots processed on separate occasions), resulting in n = 3 experimental replicates per treatment within each ZAE and 30 experimental units in total (2 ZAE × 5 times × 3 blocks). For FTIR, each experimental unit was measured in quintuplicate (n = 5 spectra) and the mean spectrum was used for chemometric analysis. Sensory evaluation was conducted using three randomized cupping sessions per sample panel, with a maximum of 10 samples per session, assessed by five cuppers (four certified Q Graders and one non-certified cupper). Sensory scores were summarized by averaging across cuppers within each session and then across the three sessions to obtain a single sensory value per experimental unit.

The fermentation trial was conducted in randomized blocks with two agroecological zones (ZAE) (1 and 5) and five fruit fermentation times (0, 24, 48, 72, 96 h). The block (lot within ZAE) was modeled as random. Normality (Shapiro–Wilk) and homoscedasticity (Levene) were

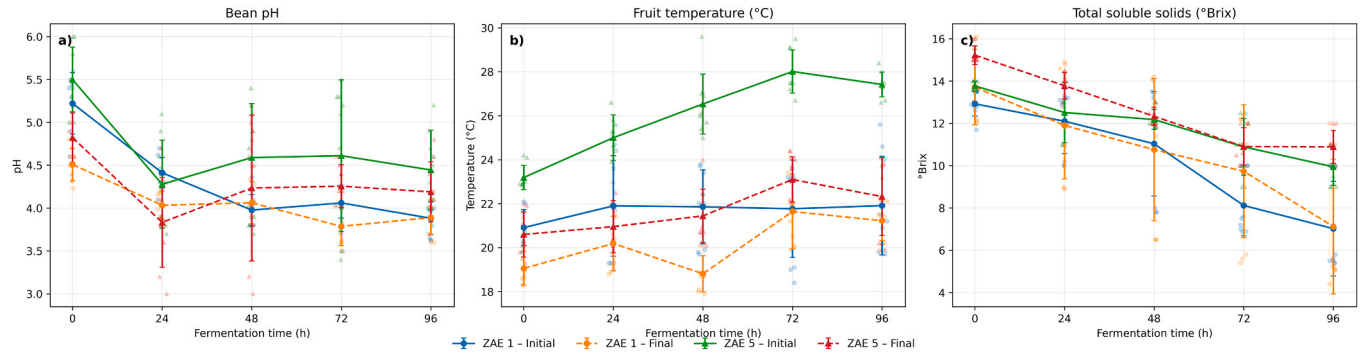

Fig. 2. Evolution of physicochemical parameters measured in the fermentation mass at the beginning (immediately after pulping) and at the end (washing endpoint) of fermentation in two agroecological zones (ZAE 1 and ZAE 5): (a) pH, (b) temperature (°C), and (c) total soluble solids (°Brix). Bars/points represent mean ± standard deviation of three independent experimental replicates (n = 3 blocks/lots) per treatment within each ZAE.

evaluated. For each sensory attribute (aroma, flavor, aftertaste, acidity, body, balance, overall impression, final score), physical attribute (% loss, % raisins, % good quality coffee, yield factor), and chemical attribute (caffeine, trigonelline, chlorogenic acids), the panel maps show the mean and standard deviation of replicates per ZAE combination (1.5) × time (0, 24, 48, 72, 96 h), without smoothing, and chemometric analysis of the FT-NIR/FT-IR spectroscopy data was performed with preprocessing (baseline + MSC) and PCA (Jiao et al., 2020).

To evaluate the effects of agroecological zone (ZAE), fermentation time (Time), and their interaction (ZAE×Time) on each compound, a two-way ANOVA was applied. When significant differences were detected, Tukey's HSD post-hoc test ($\alpha = 0.05$) was used to identify homogeneous groups. In the results table No. 2, uppercase letters denote significant differences between ZAE levels within the same fermentation time, while lowercase letters denote significant differences among fermentation times within the same ZAE. Statistical analyses were performed using standard parametric procedures and significance was set at $p < 0.05$.

3. Results and discussion

3.1. Physicochemical characteristics during fermentation

During the coffee fruit processing, variations in physicochemical characteristics were observed at the beginning and end of fermentation (Fig. 2). These differences were evident between the two agroecological zones evaluated. The pH decreased progressively, with greater acidification in ZAE 1 at 96 h, suggesting fermentation associated with the accumulation of organic acids (De Bruyn et al., 2017). The temperature of the coffee fruit increased in ZAE 5, reaching final values close to 27 °C, while in ZAE 1 it remained more stable at around 22 °C, consistent with differences in the process microenvironment between farms (ambient conditions and heat accumulation in the fermentation mass). With regard to Total Soluble Solids (°Brix), a similar constant decrease

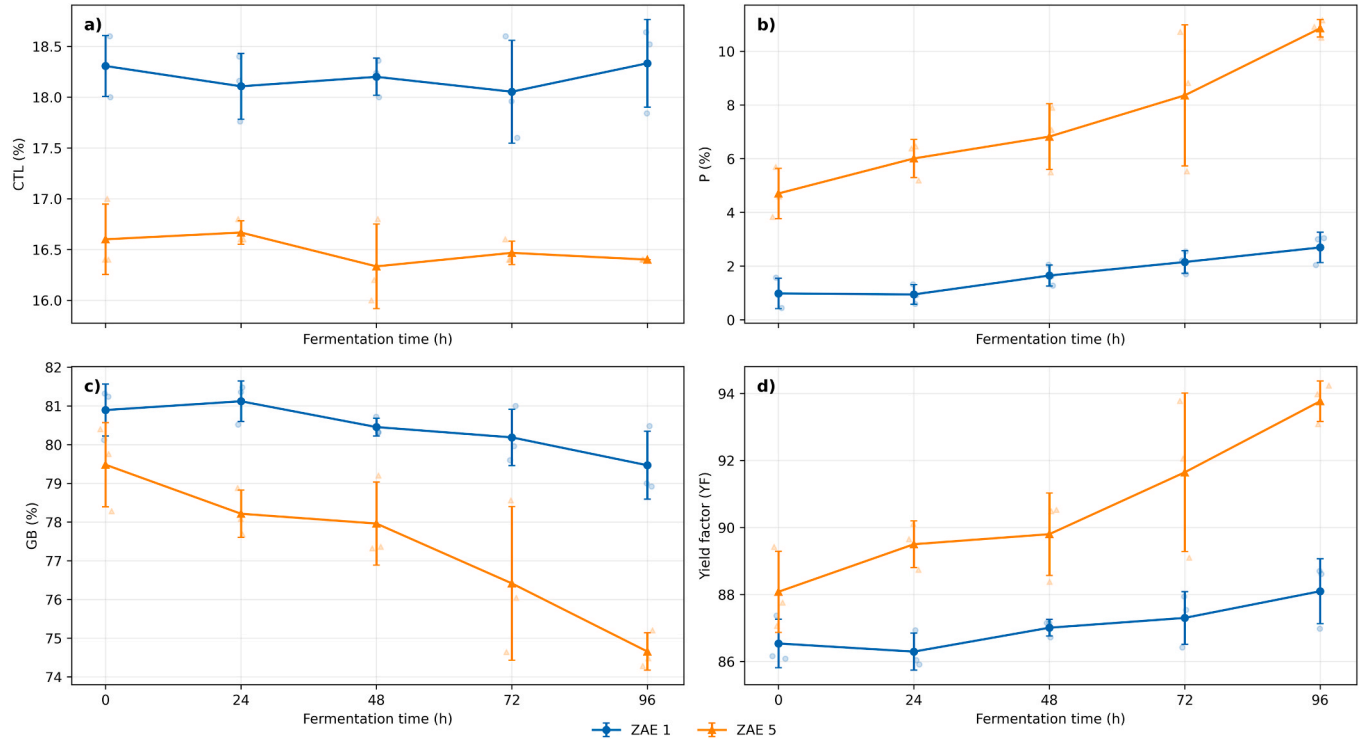

Fig. 3. Physical quality indicators as a function of fruit holding/fermentation time (0–96 h) in two agroecological zones (ZAE 1 and ZAE 5): (a) coffee threshing loss (%Ctl), (b) defective beans (%P, pasilla), (c) good beans (%GB), and (d) yield factor (YF; kg of dry parchment coffee required to obtain a 70-kg bag of excelso green coffee). Bars/points represent mean ± SD of n = 3 blocks/lots per treatment within each ZAE.

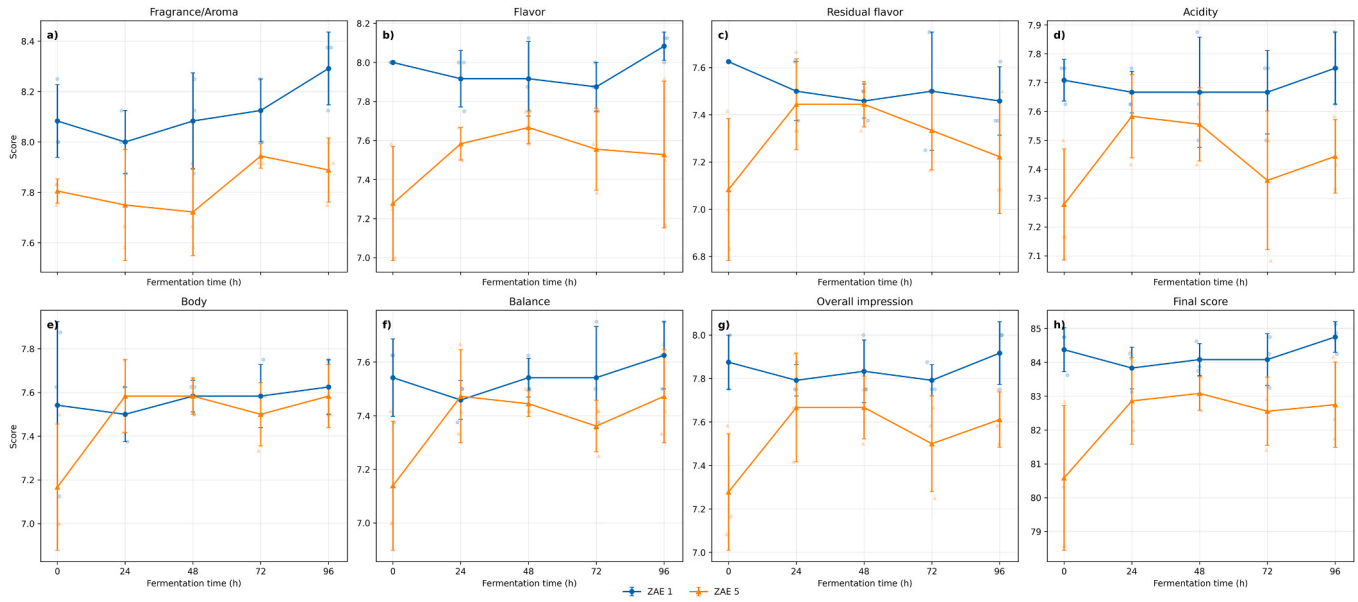

Fig. 4. Evolution of SCA sensory attributes during fruit holding/fermentation (0–96 h) by agroecological zone: (a) fragrance/aroma, (b) flavor, (c) aftertaste, (d) acidity, (e) body, (f) balance, (g) overall impression, and (h) final score (SCA points). Color code: ZAE 1 (blue) and ZAE 5 (orange). Bars/points represent mean ± standard deviation of n = 3 blocks/lots per treatment within each ZAE; sensory values correspond to the aggregated cupping output per experimental unit (three sessions; five cuppers).

was observed for both zones, possibly derived from the release of intracellular soluble compounds from the pulp and mucilage, which are affected by other parameters such as time and temperature, also consistent with substrate utilization during fermentation; time–temperature conditions may favor faster consumption/dilution of soluble constituents, without implying a specific microbial mechanism (Nakyinsige et al., 2025). This behavior is similar to that reported in fermentations with starter cultures, where microbial dynamics intensify and the inclusion of yeasts and lactic acid bacteria accelerates the conversion of sugars into organic acids and other metabolites. Under process control, reductions from 15.8 to 8.45 ° Brix (Polanía Rivera et al., 2024). These results show a partial correlation with previous research on the monitoring of coffee fermentation, which shows a significant decrease in pH, a relative increase in temperature, and fluctuations in total soluble solids (°Brix) according to microbial dynamics and experimental conditions (de Oliveira Junqueira et al., 2019; Janne Carvalho Ferreira et al., 2023).

The progressive pH decrease observed with increasing holding fermentation time is consistent with the accumulation of organic acids produced by microbial metabolism as readily fermentable substrates are consumed; similar physicochemical trajectories (acidification coupled to sugar utilization) have been described in other fruit fermentation systems, including vinegar processes (Baltaci et al., 2024). In wet coffee processing, pH and TSS are widely reported as practical indicators of fermentation progress and microbial activity, and their evolution has been repeatedly documented under controlled and field fermentation conditions (Tirado-Kulieva et al., 2024). In addition, the tendency of the coffee mass temperature to approach ambient conditions as fermentation proceeds has also been reported during prolonged wet fermentations, emphasizing the role of process environment in fermentation kinetics (Sánchez-Riaño et al., 2024).

3.2. *Physical quality of coffee based on fermentation time and agroecological zone*

Fig. 3 shows a comparison of physical parameters for ZAE 1 and 5 for fermentation times from 0 to 96 h, where we see that the percentage of loss (Fig. 3a) varied between ZAE over time; its value can change due to moisture content, the weight of the removed structural layer (cuticle or parchment), rather than fermentation time. The literature maintains that the physical yield of coffee (parchment to green factor, % of defects, and % of good quality coffee) is primarily determined by genetic material (cultivar/genotype) (Partelli et al., 2021), field work (planting density, fertilization, and nutritional management), and drying management (Peñuela-Martínez and García-Duque, 2023b).

The percentage of pasilla (Fig. 3b) tended to increase when the fermentation process was prolonged, especially under less controlled conditions, where there may be a greater risk of over-fermentation and post-harvest failures that induce physical defects and possible sensory defects (vinegary beans, black spots, fractures) (Osorio Pérez et al., 2022; Silva et al., 2024). Several studies confirm that failures in the coffee fermentation process can increase the appearance of defects in the bean and generate economic losses for coffee growers, especially in Colombia, where coffee quality is internationally recognized (Motato Rocha et al., 2024; Peñuela-Martínez et al., 2023d). Inadequate post-harvest practices, such as poorly controlled fermentation, can cause inconsistencies in quality and defects that reduce both the commercial value and the final price of the product; therefore, monitoring and controlling time and temperature during fermentation is critical to avoid defects. In our experiment, the differences between ZAEs suggest that site-specific processing conditions (e.g., temperature profile during fermentation and baseline cherry physiology) can modulate fermentation kinetics and thereby increase the risk of physical defects as holding time extends; however, microbial drivers are not directly demonstrated here because microbial community data were not collected. (Motato Rocha et al., 2024).

The increase in defective beans (pasilla) and the deterioration of physical quality metrics at longer holding times are consistent with previous reports showing that delays between harvest and pulping (“cherry storage/fruit reserve”) can promote uncontrolled fermentations and quality losses, particularly when storage conditions favor microbial growth (Y., Nugroho, 2014; Osorio et al., 2024). Reviews of coffee fermentation further highlight that extended or poorly controlled fermentations can shift microbial activity and metabolite production in ways that increase the likelihood of defects and undesirable attributes, reinforcing the need for well-defined processing windows (Elhalis et al., 2023).

The yield factor (Fig. 3d) showed differences between ZAE 1 and 5.

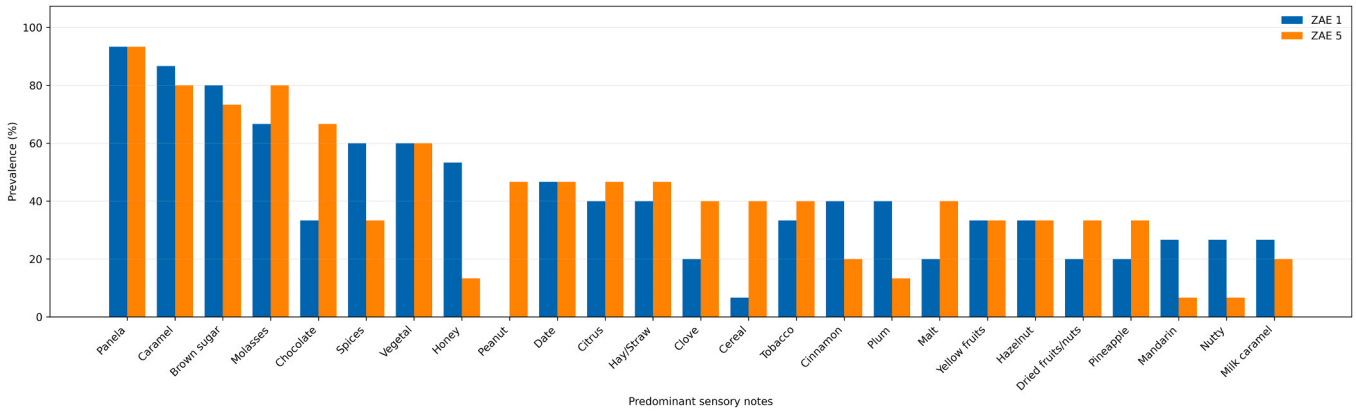

Fig. 5. Relative frequency of sensory descriptors by agroecological zone (ZAE). Descriptor frequency is expressed on a 0–100 scale, where 1 indicates the descriptor was reported in all evaluations and 0 indicates it was never reported, aggregated across fermentation times and cupping sessions for each ZAE.

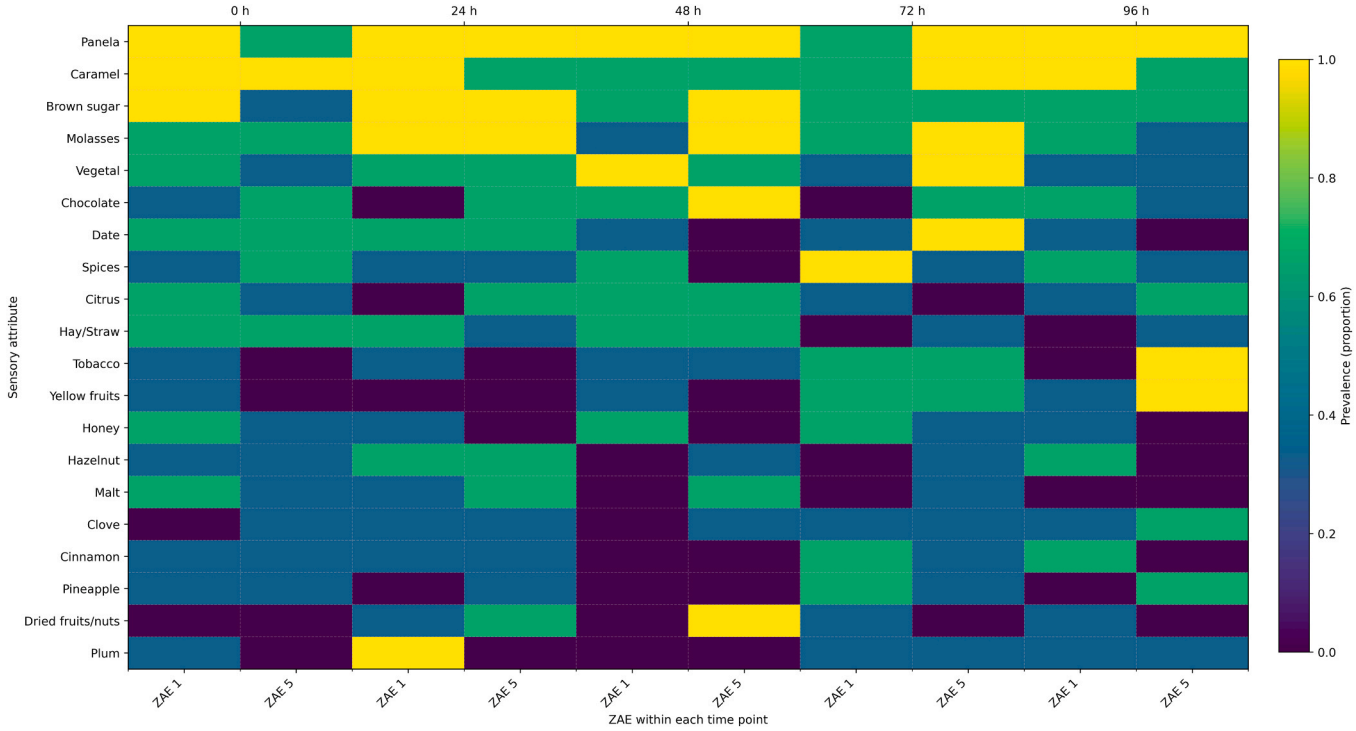

Fig. 6. Temporal dynamics (0, 24, 48, 72, 96 h) of sensory descriptor occurrence by agroecological zone (ZAE). Values represent relative frequency (0−1) of descriptor reporting within each ZAE at each time point, aggregated across cupping sessions and cuppers.

Evidence suggests that, except in cases of over-fermentation or improper handling, fermentation time per se does not substantially alter industrial conversion; rather, the site×process interaction (microclimate, temperature control) determines the small differences detected. Consequently, times exceeding 72 h require exhaustive control to avoid a decrease in physical quality or yield factor (Peñuela-Martínez et al., 2023d).

3.3. *Sensory changes during fruit fermentation: effect of time and agroecological zone (ZAE)*

Sensory analysis of the samples (Fig. 4) showed some differences, for example, in the attributes of fragrance/aroma (Fig. 4a), Flavor (Fig. 4b), and Residual Flavor (Fig. 4c). For ZAE 1, higher and more stable values were maintained over time, while ZAE 5 showed an increase between 24 and 48 h of fermentation in fruit, but as fermentation time increased, these values decreased slightly in their scores (Fig. 4a-c). Acidity (Fig. 4d) showed the same behavior, with a slight increase in acidity values, thus being a better quality characteristic for the sample processed in ZAE 5, while for the sample from ZAE 1, this sensory attribute remained stable. For body (Fig. 4e) and balance (Fig. 4f), the trajectories were equally smooth; ZAE 1 remained above or at the level of ZAE 5.

Taken together, the overall impression (Fig. 4g) and final score (Fig. 4h) confirm the improvement in coffee quality for ZAE 1 and a slight increase in values for ZAE 5 at 24 h, stabilizing after this time. The consistency between attributes (a–g) and aggregate metrics (g–h) suggests that, under these conditions, sensory differences are mainly governed by the ZAE, while the effect of fermentation time is secondary and not uniform across the parameters evaluated.

Studies conducted mainly in Brazil, Guatemala, and Colombia show that, for natural coffees subjected to fermentation, the most marked increases in SCA scores tend to appear after 48 h, with improvements of > 2 points and sensory peaks between 60 and 96 h (Meira Borém et al., 2023; Rocha et al., 2024). In contrast, in wet processes with pulped

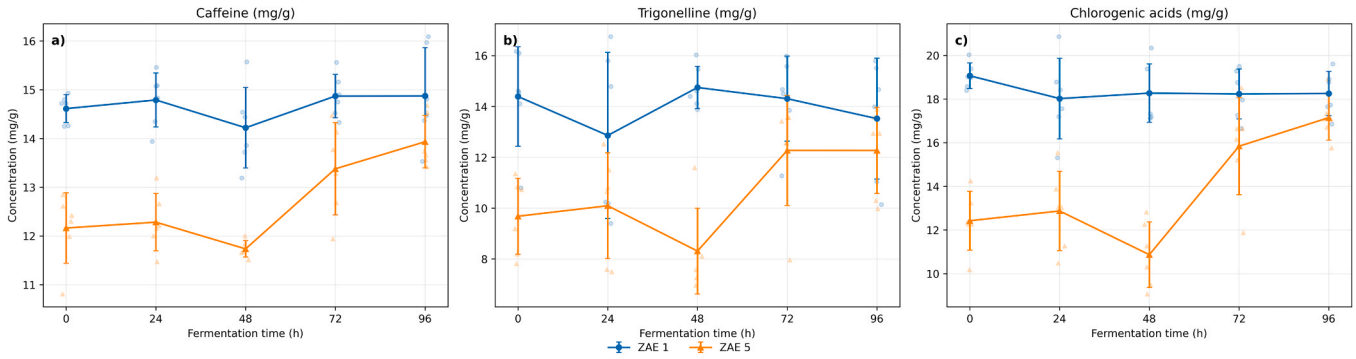

Fig. 7. Box-and-whisker plots showing the variation of bioactive compounds quantified by HPLC across fruit holding/fermentation times (0–96 h) in ZAE 1 and ZAE 5: (a) caffeine, (b) trigonelline, and (c) chlorogenic acids (CGA, reported as chlorogenic acid equivalents). Boxes indicate the interquartile range (IQR), the center line is the median, whiskers extend to 1.5 ×IQR, and points denote outliers. Data correspond to n = 3 blocks/lots per condition.

coffee in Colombia, it has been reported that 18 h of fermentation are sufficient to achieve very high scores (88.5 points) and floral and high acidity profiles, while in Guatemala, some genotypes show no significant differences in score between 24 and 72 h, although there are changes in the flavor profile (Dos Santos-Silva et al., 2022).

The sensory profiles of the samples (Fig. 5) are strongly dominated by sweet notes, such as sugar cane (0.93), caramel (0.83), brown sugar (0.77), and molasses notes (0.73). These are followed by vegetal notes (0.60), dates (0.53), chocolate (0.50), spices (0.47), straw (0.47), and citrus (0.43). This sweet base is present as the main attribute, with real discrimination emerging in secondary descriptors and in their modulation by ZAE and time (Fig. 6). This observation is consistent with studies where, even when fermentation time is increased from 24 to 72 h, the main change is manifested in the nature of the caramel and chocolate notes towards fruity and wine-like notes, rather than in large jumps in the final score (Dos Santos-Silva et al., 2022; Pereira et al., 2020).

The differences between ZAE are perceived in some descriptors. For example, in Fig. 5, it can be seen that the attribute spices (0.60) compared to (0.33) ($\Delta = +0.27$) and cinnamon 0.40 compared to 0.20 ($\Delta = +0.20$). In ZAE 5, chocolate is enriched at 0.67 compared to 0.33 in ZAE 1 ($\Delta = -0.33$), clove 0.40 compared to 0.20 ($\Delta = -0.20$), malt 0.40 compared to 0.20 ($\Delta = -0.20$), and molasses 0.80 compared to 0.67 ($\Delta = -0.13$). The most abundant notes overall show little difference between zones, for example, cane sugar (0.93) in both ZAE zones, and brown sugar with a difference of less than 0.10. In summary, ZAE 1 showed a greater contribution of honey, spicy, and ripe fruit notes, while ZAE 5 was associated with a higher probability of chocolate, clove, malt, and molasses nuances. These differences in sweetness and aromatic complexity are consistent with the literature describing the transition from predominantly chocolate and nutty profiles in shorter fermentations to more fruity, vinous, and spicy profiles when the process is extended to 72–96 h (Brioschi Junior et al., 2021).

The time axis reveals windows of appearance that depend on the ZAE (Fig. 6). In ZAE 1, spices are present after 72 h of fermentation, while in ZAE 5 the same note is high at the start (0.67) and then attenuates (0.33) in 24–96 h. Honey in ZAE 1 is sustained over time at 0.33 between 0.67, while in ZAE 5 it is marginal or nil except at 0 and 72 h 0.33. Chocolate in ZAE 5 reaches a maximum at 48 h (1.00) and decreases to 0.33 at 96 h, in contrast to ZAE 1, where more modest and alternating peaks are observed (0.67 at 48 h and 96 h). Molasses is high and stable in ZAE 5 between 24 and 72 h 1.00 and decreases to 96 h 0.33; in ZAE 1 it shows a more undulating pattern 0.67 at 0 h, 1.00 at 24 h, 0.33 at 48 h, and 0.67 at 72–96 h. Yellow fruits intensify late in both ZAE, with a more marked increase at 72–96 h in ZAE 5 0.67 and 1.00 compared to ZAE 1 0.67 and 0.33. The sweet base of raw cane sugar, caramel, and brown sugar remains high throughout the time range, but with slight fluctuations: for example, in ZAE 1 brown sugar temporarily falls to 0.67 at 48–96 h, while in ZAE 5 it remains at 1.00 between 24 and 48 h and drops to 0.66 at 72–96 h.

Table 2
Effect of fermentation time and agroecological zone (ZAE) on caffeine, trigonelline, and chlorogenic acids quantified by HPLC (mean ± SD) with Tukey HSD homogeneous groups (α = 0.05).

Time (h)	ZAE	Caffeine (mg/g)	Trigonelline (mg/g)	Chlorogenic acids (mg/g)
0	1	14.61 ± 0.29 Aa	14.39 ± 1.96 Aa	19.07 ± 0.59 Aa
	5	12.16 ± 0.72 Bb	9.68 ± 1.49 Ba	12.42 ± 1.35 Bb
24	1	14.79 ± 0.55 Aa	12.86 ± 3.27 Aa	18.02 ± 1.85 Aa
	5	12.28 ± 0.59 Bb	10.10 ± 2.08 Aa	12.87 ± 1.82 Bb
48	1	14.22 ± 0.83 Aa	14.75 ± 0.83 Aa	18.27 ± 1.33 Aa
	5	11.73 ± 0.17 Bb	8.31 ± 1.69 Bb	10.87 ± 1.51 Bb
72	1	14.87 ± 0.44 Aa	14.31 ± 1.67 Aa	18.23 ± 1.14 Aa
	5	13.38 ± 0.95 Ba	12.27 ± 2.16 Aa	15.84 ± 2.22 Ba
96	1	14.87 ± 0.99 Aa	13.52 ± 2.38 Aa	18.25 ± 1.02 Aa
	5	13.93 ± 0.54 Aa	12.27 ± 1.69 Aa	17.15 ± 1.03 Aa
F-ratio$^{p\text{-value}}$				
Time (T)		9.14***	1.96***	8.94***
ZAE (Z)		135.02***	43.68***	145.52***
TxZ		3.59***	3.29***	10.37***

Uppercase letters indicate significant differences between ZAE levels within the same fermentation time (Tukey HSD, $\alpha = 0.05$). Lowercase letters indicate significant differences between fermentation times within the same ZAE (Tukey HSD, $\alpha = 0.05$). p-value: ns: no significant; *** $p < 0.001$. Values are expressed as mean ± SD of three independent experimental replicates (n = 3 blocks/lots) per treatment within each agroecological zone.

3.4. Analysis of caffeine, trigonelline, and chlorogenic acids

In Fig. 7a, caffeine remains stable during the period from 0 to 96 h in both ZAE. The medians show minor variations and no trend, while the interquartile range increases slightly at times, suggesting the existence of microenvironment effects rather than systematic transformations. Comparative studies have shown that certain methods, such as natural, dry, wet, and semi-wet, preserve more caffeine than methods involving washing or prolonged soaking, which helps explain the slight differences (Halagarda & Obrok, 2023; Joët et al., 2010).

In Fig. 7b, trigonelline changes over the prolonged fermentation time; greater variability is observed at specific times at 24 h, which is

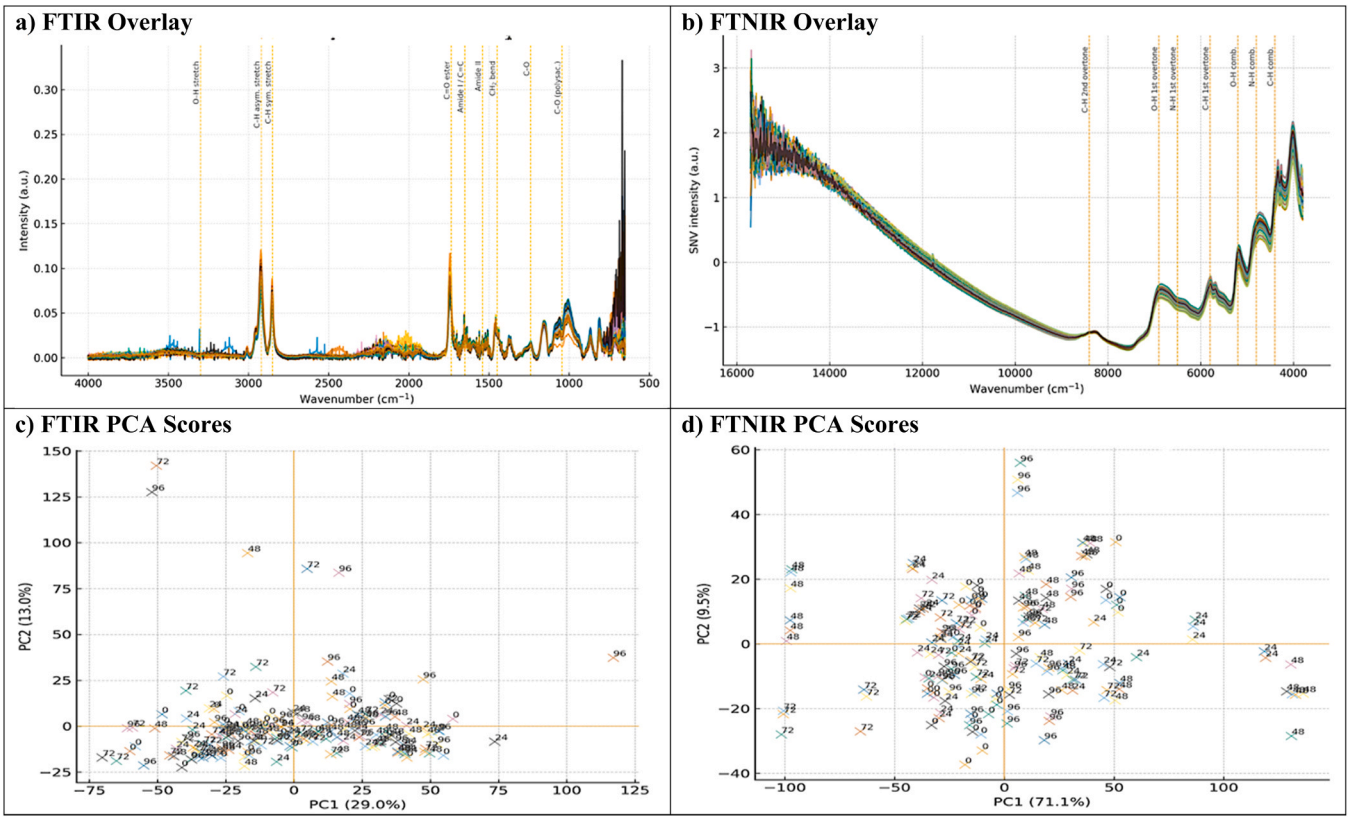

Fig. 8. Spectral fingerprints and PCA discrimination of roasted coffee samples as a function of agroecological zone and fruit holding/fermentation time (0–96 h): (a) ATR-FTIR spectra (4000–650 cm^{-1}) and (b) FT-NIR spectra (12000–4000 cm^{-1}), both after baseline correction and multiplicative scatter correction (MSC); (c) PCA score plot derived from FTIR spectra and (d) PCA score plot derived from FT-NIR spectra. Each point represents one experimental unit (n = 30; 2 ZAE x 5 times x 3 blocks). FTIR spectra were acquired in quintuplicate (n = 5 spectra) per experimental unit and averaged prior to PCA; FT-NIR replicate spectra were averaged prior to PCA (as described in Methods). Explained variance (%) is indicated on the PCA axes. Color/marker coding follows the figure legend to distinguish ZAE (ZAE 1 vs ZAE 5) and fermentation time (0-96 h).

reduced after controlling for outliers, indicating that the changes detected are temporary and probably dominated by specific leaching rather than biochemical conversion specifically at that stage of time. The literature supports that trigonelline is highly water-soluble and thermolabile, with significant losses during washing or soaking and, above all, during roasting (Duarte et al., 2010); therefore, in the fermentation stage, variations in trigonelline due to fermentation time may be modest and sensitive to small changes in pH, temperature, and microbial load, rather than to a linear effect of time (Heo et al., 2020; Konstantinidis et al., 2023).

With regard to chlorogenic acids (CGA), they were the most responsive group among the three markers (Fig. 7c), showing significant ZAE, time and ZAE×time effects (Table 2). Because CGA are predominantly caffeoylquinic acid esters, their non-linear behavior during extended wet contact can plausibly reflect a combination of (i) mass transfer/leaching of soluble phenolics during prolonged aqueous handling and washing, and (ii) temperature- and pH-dependent chemical rearrangements (acyl migration/isomer redistribution) and partial hydrolysis of caffeoylquinic esters. Importantly, ZAE 5 exhibited a warmer process microenvironment (higher fermentation-mass temperature) and a distinct pH trajectory (Fig. 2), which may shift the balance between CGA retention, leaching, and transformation, yielding the stronger time-dependence observed in ZAE 5 compared with the comparatively stable CGA levels in ZAE 1. We emphasize that this is a mechanistic hypothesis; causal attribution to microbial pathways would require dedicated profiling (organic acids, individual CGA isomers/lactones, and microbiome data), which was beyond the scope of the present study. (Purwoko et al., 2022). Post-harvest studies have documented CGA modulations due to wet processing and microbial-acid dynamics in the tank, consistent with the pattern observed (Sinaga et al., 2021). Respectively, the data point to specific effects of ZAE, which differ in their microclimate, crop management, and specific microbial kinetics of the areas that can change the temporal trend of biochemical dynamics (Joët et al., 2010a).

Table No. 2, the results obtained using high-performance liquid chromatography (HPLC) show that the agroclimatic zone (ZAE) was the factor with the greatest explanatory weight on the variation of caffeine, trigonelline, and chlorogenic acids (CGA), followed by the fermentation time of the coffee pulp and a significant ZAE x time interaction ($p < 0.001$). These results suggest that compositional kinetics during fermentation are not universal but rather a multifactorial problem that may depend on the microenvironment associated with each crop zone. ZAE 1 exhibited significantly higher concentrations: caffeine 14.2–14.9 mg/g; CGA 18.0–19.1 mg/g compared to ZAE 5: caffeine 11.7–13.9 mg/g; CGA 10.9–17.2 mg/g. This finding suggests that the discrepancies in concentration levels between the two sampling zones could be attributed to ecophysiological and environmental factors specific to the terroir, which modulate the accumulation of metabolites in the coffee bean rather than merely reflecting a temporary effect of the production process (Cheng et al., 2016).

However, they point out that the fruit fermentation period can cause non-linear variations: occasional decreases and recoveries in sensory notes that are probably linked to the diffusion, leaching, or degradation of water-soluble compounds, the metabolic activity of the grain, and the and potential transformations mediated by the microbiota typically present in the mucilage–endosperm ecosystem, with responses that may differ by zone (De Bruyn et al., 2017; Duarte et al., 2010; Halagarda & Obrok, 2023). This finding is relevant to the study hypothesis, as the

Table 3
Selected mid-infrared (FTIR) wavenumber assignments (cm^{-1}) commonly reported for coffee matrices and used here to interpret diagnostic spectral regions. Assignments are literature-based and should be interpreted as indicative rather than exclusive (multiple constituents may contribute within the same region).

Wavelength (cm^{-1})	Compound	Reference
(3500–3200)	Water	(Rodriguez, Calderon, et al., 2020)
2920	Caffeine, lipids	(Craig et al., 2012a, 2012b; Cremer & Kaletunç, 2003)
2850	Caffeine	(Craig et al., 2012a, 2012b; Cremer & Kaletunç, 2003)
1743	Associated with the carbonyl group as aldehydes related to the organoleptic properties of coffee	(Wang et al., 2009)
1740	Fatty acids or aliphatic esters associated with lipids	(Lyman et al., 2003)
1739	Lipids	(Rodriguez, Calderon, et al., 2020)
1650	Chlorogenic acids	(Rodriguez, Guzman, et al., 2020)
(1600–1300)	Trigonelline	(Craig et al., 2012b; Rodriguez, Calderon, et al., 2020)
(1450–1250)	Chlorogenic acids	(Wang et al., 2009)
(1420 – 1000)	Chlorogenic acids	(Craig et al., 2012b)
(1153–1150)	Polysaccharides	(Craig et al., 2018)
1025	The C-O-C bond of the ester	(Lyman et al., 2003)
	Carbohydrates	(Craig et al., 2012b)
872	Carbohydrates	(Lyman et al., 2003)

significance of Z, T, and Z × T is consistent with a hypothesis of environment-dependent responses. This confirms that optimizing or standardizing times without considering ZAE can skew results, which has direct implications for quality, given that CGAs (and their derivatives) contribute to sensory attributes such as acidity, astringency, bitterness, and the bioactive fraction of coffee (Farah et al., 2006; Joët et al., 2010).

With regard to the limitations of the analysis, it is important to recognize that it focuses on three specific markers in two ZAEs, covering a specific time range. However, no explicit control has been made of critical variables such as the microbial community, intramass temperature, washing, and drying conditions, among others that may affect the results. Consequently, causal mechanisms cannot be attributed in a deterministic manner. Furthermore, the presentation of CGAs may conceal rearrangements between isomers and derivatives with different sensory impacts, which may compromise the timely transformation of CGA, as it is important for improving sensory quality. Taken together, the findings provide evidence for adjusting fermentation windows by zone and propose a practical use of these compounds as markers for traceability and process control. Future lines of research should integrate expanded profiling of CGA isomers and lactones, metabolomics, and microbiology to link pathways and microbes with chemical changes, and multivariate kinetic models that connect chemistry with sensometry at the batch scale (Cheng et al., 2016; De Bruyn et al., 2017; Duarte et al., 2010).

3.5. FTIR and FTNIR spectrum analysis

In FTIR (Fig. 8a), bands consistent with green coffee matrices are observed. Noteworthy are the broad O–H stretch (3300 cm^{-1}), aliphatic C–H stretches (2920–2850 cm^{-1}), the carbonyl region region (1735 cm^{-1}; esters/acids), the Amide I/II region (1650/1540 cm^{-1}) associated with proteins, and the polysaccharide fingerprint (1240–1045 cm^{-1}), according to different authors mentioned in Table 3. After baseline+MSC cleaning and exclusion of outliers, the differences between ZAE 1 and ZAE 5 emerge mainly as modulation of relative intensity in the fingerprint. The reading over time (0–96 h) does not show the band shifts expected in FTIR, but rather adjustments in the intensity ratio; PCA-FTIR (lower left panel) partially orders the samples and suggests that the dominant effect is that of process and microstructure (dispersion, bound water) rather than the formation of new chemical functions.

In FTNIR (annotated overlay), ZAE×time differences are expressed with a higher signal-to-noise ratio at the multivariate level. Diagnostic regions are visible: 1st O–H overtone (~1450 nm or ~6900 cm^{-1}), O–H combination (~1930 nm or ~5200 cm^{-1}), C–H overtones/combinations (≈1720 nm/5800 cm^{-1}; 2300 nm/4400 cm^{-1}) and N–H contributions (≈1510 nm/6500 cm^{-1}). PCA-FTNIR (bottom right panel) concentrates the variance in PC1, consistent with changes in bound water and dispersion during fermentation; times are usually organized along PC1 (evolution) while ZAE shifts the scatter plot (microenvironmental and management differences). Overall, FTNIR better discriminates process kinetics (global changes in matrix and moisture), while FTIR provides functional specificity in fingerprinting (Fig. 9).

Given the strong ZAE effect, we hypothesize that the distinct temperature and acidification trajectories of ZAE 5 could contribute to its CGA pattern. Temperature and pH are key drivers of coffee fermentation kinetics, accelerating microbial succession and organic acid production under warmer conditions (Costa et al., 2025; Vaz et al., 2023). Altitude- and environment-dependent shifts in the coffee microbiota have also been associated with differences in acids and other metabolites during fermentation and postharvest processing (Rojas-Chacón et al., 2024). Such shifts may impact both the extractability and biotransformation of chlorogenic acids: environmental conditions and wet processing can modify CGA levels in green beans (Joët et al., 2010), and caffeoylquinic acids undergo acyl migration/isomerization and hydrolysis in aqueous media with rates influenced by pH and temperature (Alcázar Magaña et al., 2021; Dawidowicz & Typek, 2011). In addition, lactic acid bacteria possess chlorogenate esterases capable of hydrolyzing 5-CQA into caffeic and quinic acids, supporting a plausible microbial contribution under distinct acidification regimes (Bel-Rhlid et al., 2013). Therefore, the higher initial temperature and different pH trajectories in ZAE 5 may shift the balance between CGA retention, leaching, and enzymatic/microbial transformation, leading to the observed non-linear behavior compared with the more stable ZAE 1. This interpretation is presented as a hypothesis because organic acid kinetics, individual CGA isomers, and microbiota composition were not directly measured in the present study.

4. Limitations and scope of interpretation

Because this study did not include microbial community profiling (e.g., sequencing) or volatile/metabolomic measurements, we avoid attributing specific descriptors (e.g., cane sugar, spices, chocolate) to individual microbial taxa or single aroma compounds. Instead, we interpret sensory differences at the level of zone- and time-dependent chemical fingerprints, supported by HPLC markers and FTIR/FTNIR patterns. Future work combining microbiome + volatiles with the present chemical–spectral framework would allow stronger causal links between fermentation dynamics and descriptor-level sensory changes.

5. Conclusions

This study demonstrates that fermentation time in fruit produces zone-dependent changes that are best captured by chlorogenic acids (HPLC) and by FTIR/FTNIR spectral fingerprints interpreted through chemometrics, while physical and sensory metrics provide complementary evidence of practical quality outcomes. Fermentation for up to 72 h allowed high sensory quality to be maintained, with scores ranging from 78 to 86 points on the Specialty Coffee Association (SCA) scale, while times longer than this began to compromise the physical quality of the bean, manifested in an increase in the percentage of parchment and a

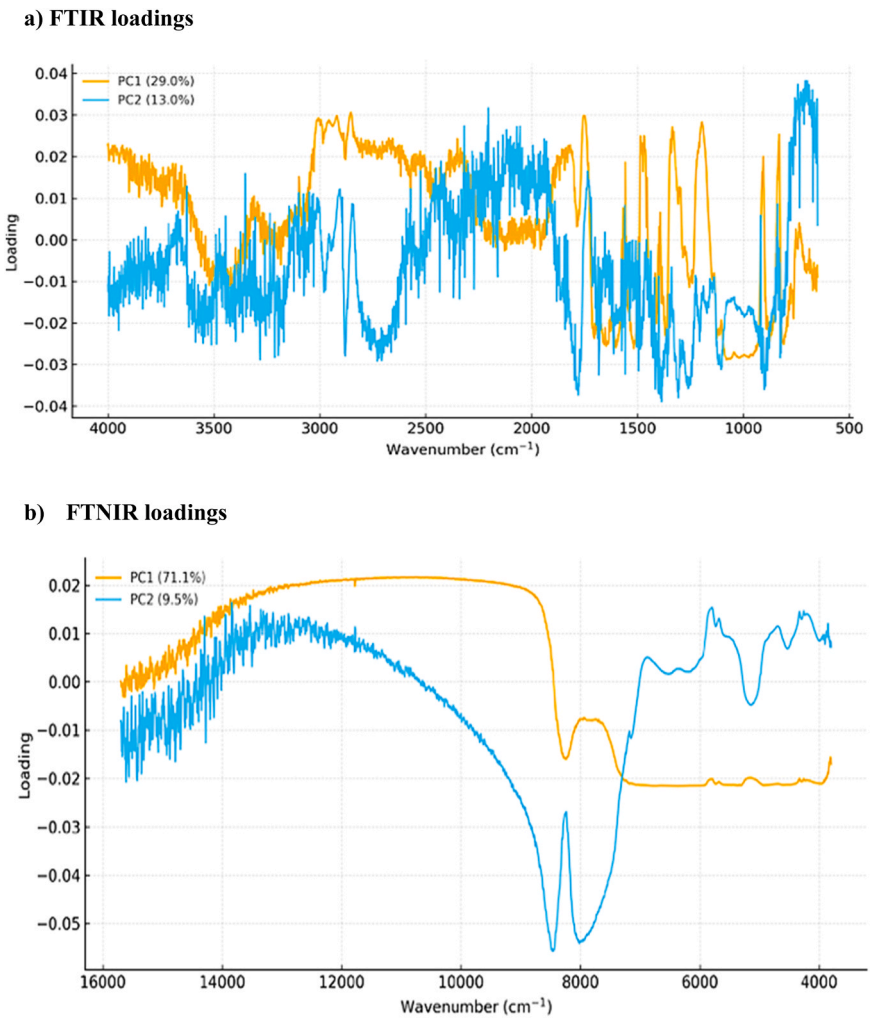

Fig. 9. PCA loadings highlighting the spectral variables that drive discrimination in Fig. 8: (a) FTIR loadings and (b) FT-NIR loadings for PC1 and PC2. Peaks with higher absolute loading values indicate wavenumber regions contributing most to sample separation. Color code: ZAE 1 (blue) and ZAE 5 (orange), consistent with the manuscript convention.

decrease in the integrity of good quality coffee. Likewise, the variation in sensory attributes, such as aroma, flavor, and aftertaste, was mainly influenced by the agroecological zone, with Agroecological Zone 1 (ZAE 1) showing the best results with more stable attributes throughout the process. The difference in microclimatic conditions, such as temperature and pH, and zone-specific temperature/pH conditions were associated with different chemical trajectories and spectral fingerprints; microbiological drivers are plausible but were not directly assessed in this study, affecting the final quality of the product. Finally, monitoring and controlling the fruit fermentation process, taking into account the specific conditions of each zone, is essential for optimizing coffee quality and reducing post-harvest losses, thus supporting evidence-based decision-making to reduce postharvest losses and preserve cup quality.

Ethics statement

Sensory evaluation was conducted with trained adult panelists (four certified Q-graders) following the SCA cupping protocol. Participation was voluntary; the study objectives and procedures were explained in advance, and written informed consent was obtained. No coercion was used, no personal identifiers or sensitive data were collected, and results were reported only in aggregate form. According to Colombian regulations and the institutional policies of the participating institutions, this type of sensory evaluation of a food product is exempt from formal ethics committee approval; therefore, the study was considered exempt from ethics committee review. No vulnerable populations were involved.

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Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the authors used ChatGPT (GPT-5.4 Thinking) solely to improve English grammar, spelling, and readability. The authors reviewed and edited the output as needed and take full responsibility for the content of the publication.

Declaration of competing interest

Aida Esther Peñuela Martínez declares a potential conflict of interest as the inventor of the Fermaestro® method (developed by Cenicafé) used in this study to determine the washing endpoint. Aida Esther Peñuela Martínez reports no personal financial benefit from the use of Fermaestro® in this research and has no paid consultancy, stock ownership, patent licensing income, or royalty arrangements related to

Fermaestro® that could have influenced the study. The study design, data collection, data analysis, interpretation, and manuscript preparation were conducted following standard scientific procedures. All other 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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Data availability

Data will be made available on request.

References

Y, Nugroho, D., 2014. Physical and flavor profiles of Arabica coffee as affected by cherry storage before pulping. Pelita Perkeb. (a Coffee Cocoa Res. J.) 30 (2), 137–158. https://doi.org/10.22302/iccri.jur.pelitaperkebunan.v30i2.7.

Afriliana, A., Allenia, Q.R., Jayus, Giyarto, 2024. Chemical characteristics of original robusta coffee beans from Jember fermented with Saccharomyces cerevisiae starter using the semi-carbonic maceration technique. IOP Conference Series Earth Environmental Science 1356 (1), 012032. https://doi.org/10.1088/1755-1315/1356/1/012032.

Alcázar Magaña, A., Kamimura, N., Soumyanath, A., Stevens, J.F., Maier, C.S., 2021. Caffeoylquinic acids: chemistry, biosynthesis, occurrence, analytical challenges, and bioactivity. Plant J. 107 (5), 1299–1319. https://doi.org/10.1111/tpj.15390.

Bel-Rhlid, R., Thapa, D., Kraehenbuehl, K., Hansen, C., Fischer, L., 2013. Biotransformation of caffeoyl quinic acids from green coffee extracts by Lactobacillus johnsonii NCC 533. AMB Express 3 (1), 28. https://doi.org/10.1186/2191-0855-3-28.

Brioschi Junior, D., Carvalho Guarçoni, R., de Cássia Soares da Silva, M., Gomes Reis Veloso, T., Catarina Megumi Kasuya, M., Catarina da Silva Oliveira, E., Maria Rodrigues da Luz, J., Rizzo Moreira, T., Grancieri Debona, D., Louzada Pereira, L., 2021. Microbial fermentation affects sensorial, chemical, and microbial profile of coffee under carbonic maceration. Food Chem. 342. https://doi.org/10.1016/j.foodchem.2020.128296.

Baltaci, Cemalettin, Yilmaz, Kubra, Ozturk, Seyda, Karpuz, Omer, 2024. Vinegar production from different cherry laurel fruits and investigation of some of their physicochemical properties. J. Food Saf. Food Qual. (JFSFQ) 75 (1), 13–23. https://doi.org/10.53194/0003-925X-75-13.

Cheng, B., Furtado, A., Smyth, H.E., Henry, R.J., 2016. Influence of genotype and environment on coffee quality. Trends Food Sci. & Technol. 57, 20–30. https://doi.org/10.1016/j.tifs.2016.09.003.

Collazos-Escobar, G.A., Barrios-Rodriguez, Y.F., Bahamón-Monje, A.F., Gutiérrez-Guzmán, N., 2023. Uses of mid-infrared spectroscopy and chemometric models for differentiating between dried cocoa bean varieties. Rev. Bras. De. Eng. Agr. ícola e Ambient. 27 (10), 803–810. https://doi.org/10.1590/1807-1929/agriambi.v27n10p803-810.

Collazos-Escobar, G.A., Barrios-Rodríguez, Y.F., Bahamón-Monje, A.F., Gutiérrez-Guzmán, N., 2024. Mid-infrared spectroscopy and machine learning as a complementary tool for sensory quality assessment of roasted cocoa-based products. Infrared Phys. & Technol. 141, 105482. https://doi.org/10.1016/j.infrared.2024.105482.

Costa, G.X.R., Bertarini, P.L.L., Silva, L.C.F., Amaral, L.R., do, Gomes, M., de, S., de Oliveira, L.M., Santos, L.D., 2025. The impact of ambient temperature regulation on Arabica coffee fermentation. Appl. Food Res. 5 (1), 101028. https://doi.org/10.1016/j.afres.2025.101028.

Craig, A.P., Botelho, B.G., Oliveira, L.S., Franca, A.S., 2018. Mid infrared spectroscopy and chemometrics as tools for the classification of roasted coffees by cup quality. Food Chem. 245, 1052–1061. https://doi.org/10.1016/j.foodchem.2017.11.066.

Craig, A.P., Franca, A.S., Oliveira, L.S., 2012a. Discrimination between defective and non-defective roasted coffees by diffuse reflectance infrared Fourier transform spectroscopy. LWT Food Sci. Technol. 47 (2), 505–511. https://doi.org/10.1016/j.lwt.2012.02.016.

Craig, A.P., Franca, A.S., Oliveira, L.S., 2012b. Evaluation of the potential of FTIR and chemometrics for separation between defective and non-defective coffees. Food Chem. 132 (3), 1368–1374. https://doi.org/10.1016/j.foodchem.2011.11.121.

Cremer, D.R., Kaletunç, G., 2003. Fourier transform infrared microspectroscopic study of the chemical microstructure of corn and oat flour-based extrudates. Carbohydr. Polym. 52 (1), 53–65. https://doi.org/10.1016/S0144-8617(02)00266-7.

Dawidowicz, A.L., Typek, R., 2011. The influence of pH on the thermal stability of 5-O-caffeoylquinic acids in aqueous solutions. Eur. Food Res. Technol. 233 (2), 223–232. https://doi.org/10.1007/s00217-011-1513-x.

De Bruyn, F., Zhang, S.J., Pothakos, V., Torres, J., Lambot, C., Moroni, A.V., Callanan, M., Sybesma, W., Weckx, S., De Vuyst, L., 2017. Exploring the impacts of postharvest processing on the microbiota and metabolite profiles during green coffee bean production. Appl. Environ. Microbiol. 83 (1). https://doi.org/10.1128/AEM.02398-16.

de Oliveira Junqueira, A.C., de Melo Pereira, G.V., Coral Medina, J.D., Alvear, M.C.R., Rosero, R., de Carvalho Neto, D.P., Enríquez, H.G., Soccol, C.R., 2019. First description of bacterial and fungal communities in Colombian coffee beans fermentation analysed using Illumina-based amplicon sequencing. Sci. Rep. 9 (1), 8794. https://doi.org/10.1038/s41598-019-45002-8.

de Sousa, L.H.B.P., da Luz, J.M.R., da Silva, M., de, C.S., Moreli, A.P., Veloso, T.G.R., Guarçoni, R.C., Moreira, T.R., Barros, M.V.P., Kasuya, M.C.M., Marcate, J.P.P., Brioschi Júnior, D., Gomes, W., dos, S., Pereira, L.L., Oliveira, E.C. da S., 2023. Relationship between sensory and microbial profiles of fermented coffee by dry and washed methods. Food Chem. Adv. 2, 100259. https://doi.org/10.1016/j.focha.2023.100259.

dos Santos Gomes, W., Partelli, F.L., da Silva Oliveira, E.C., Guimarães, C.V., Simmer, M.M.B., Filete, C.A., Guarçoni, R.C., da Luz, J.M.R., Moreli, A.P., Pereira, L.L., 2025. Fermentation time and temperature induce changes in the volatile and sensory profile of Coffea canephora var. Conilon subjected to carbonic maceration. J. Food Compos. Anal. 143, 107636. https://doi.org/10.1016/j.jfca.2025.107636.

Dos Santos-Silva, J., Silva-Nadaleti, D.H., Angélico-de- Mendonça, J.M., Rodrigues-Carvalho, G., Elias-Botelho, C., Ribeiro-Malta, M., Coto-Markus, S.E., Coto-Osorio, S.F., 2022. Influence of fermentation time on the sensory quality of Arabica coffee genotypes in guatemala. Rev. Fitotec. Mex. 45 (2), 235. https://doi.org/10.35196/rfm.2022.2.235.

Duarte, G.S., Pereira, A.A., Farah, A., 2010. Chlorogenic acids and other relevant compounds in Brazilian coffees processed by semi-dry and wet post-harvesting methods. Food Chem. 118 (3), 851–855. https://doi.org/10.1016/j.foodchem.2009.05.042.

Elhalis, H., Cox, J., Zhao, J., 2023. Coffee fermentation: expedition from traditional to controlled process and perspectives for industrialization. Appl. Food Res. 3 (1), 100253. https://doi.org/10.1016/j.afres.2022.100253.

Farah, A., de Paulis, T., Moreira, D.P., Trugo, L.C., Martin, P.R., 2006. Chlorogenic acids and lactones in regular and water-decaffeinated Arabica coffees. J. Agric. Food Chem. 54 (2), 374–381. https://doi.org/10.1021/jf0518305.

Borém, Flávio M., Salvio, Luís Gustavo A., Correa, Jefferson Luiz G., Alves, Ana Paula C., Dos Santos, Cláudia M., Haeberlin, Luana, Cirillo, Marcelo A., Schwan, Rosane F., 2024. Influence of fermentation time and inoculation of starter culture on the chemical composition of fermented natural coffee followed by depulping. Chem. Sci. 96 (1), 1–17. https://doi.org/10.1590/0001-3765202420240083.

Guerrero, Á., Sanz-Uribe, J.R., Peñuela-Martínez, A.E., Ramírez, C.A., 2022. Mediverdes®: un método para medir la calidad de la recolección del café en el campo. Av. Técnicos Cenicafé 536, 1–8. https://doi.org/10.38141/10779/0536.

Haile, M., Kang, W.H., 2019. Antioxidant activity, total polyphenol, flavonoid and tannin contents of fermented green coffee beans with selected yeasts. Fermentation 5 (1), 29. https://doi.org/10.3390/fermentation5010029.

Halagarda, M., Obrok, P., 2023. Influence of post-harvest processing on functional properties of coffee (Coffea arabica L.). Molecules 28 (21), 7386. https://doi.org/10.3390/molecules28217386.

Heo, J., Adhikari, K., Choi, K.S., Lee, J., 2020. Analysis of caffeine, chlorogenic acid, trigonelline, and volatile compounds in cold brew coffee using high-performance liquid chromatography and solid-phase microextraction—gas chromatography-mass spectrometry. Foods 9 (12), 1746. https://doi.org/10.3390/foods9121746.

Janne Carvalho Ferreira, L., de Souza Gomes, M., Maciel de Oliveira, L., Diniz Santos, L., 2023. Coffee fermentation process: a review. In: Food Research International, 169. Elsevier Ltd. https://doi.org/10.1016/j.foodres.2023.112793.

Jiao, Y., Li, Z., Chen, X., Fei, S., 2020. Preprocessing methods for near-infrared spectrum calibration. J. Chemom. 34 (11). https://doi.org/10.1002/cem.3306.

Joët, T., Laffargue, A., Descroix, F., Doulbeau, S., Bertrand, B., kochko, A. de, Dussert, S., 2010. Influence of environmental factors, wet processing and their interactions on the biochemical composition of green Arabica coffee beans. Food Chem. 118 (3), 693–701. https://doi.org/10.1016/j.foodchem.2009.05.048.

Konstantinidis, N., Franke, H., Schwarz, S., Lachenmeier, D.W., 2023. Risk assessment of trigonelline in coffee and coffee by-products. Molecules 28 (8), 3460. https://doi.org/10.3390/molecules28083460.

Lyman, D.J., Benck, R., Dell, S., Merle, S., Murray-Wijelath, J., 2003. FTIR-ATR analysis of brewed coffee: effect of roasting conditions. J. Agric. Food Chem. 51 (11), 3268–3272. https://doi.org/10.1021/jf0209793.

Mardhatilah, D., Padama, F., Ngatirah, 2023. Development of sustainable Arabica coffee fermentation using yeast starter. IOP Conference Series Earth Environmental Science 1241 (1), 012078. https://doi.org/10.1088/1755-1315/1241/1/012078.

Meira Borém, F., Paula de Carvalho Alves, A., Mendes dos Santos, C., Haeberlin, L., Gustavo Amaral Salvio, L., 2023a. Sensory and chemical analyses of spontaneously fermented coffees. Coffee Sci. 18, 1–12. https://doi.org/10.25186/.v18i.2137.

Motato Rocha, K.E., Gonzalez-Montero, V., Román-Morales, M.O., 2024a. Identification of microorganisms in wet coffee fermentation Coffea Arabica Var Catimor and Castillo in Jardín, Antioquia-Colombia, using culture-dependent methods. Vitae 31 (1). https://doi.org/10.17533/udea.vitae.v31n1a351373.

Nakyinsige, K., Mugerwa, F., Tabula, A., Mugampoza, D., Matovu, M., Bamuwamye, M., 2025. The influence of spontaneous microbial fermentation isolates on physicochemical properties and cup quality of wet processed Arabica coffee (Coffea Arabica). LWT 216, 117343. https://doi.org/10.1016/j.lwt.2025.117343.

Ordoñez Lozano, K.S., Felipe Bahamón Monje, A., Gutierrez Guzman, N., 2025. Predictive model of moisture content in dry parchment coffee beans using near-infrared spectroscopy (FT-NIR). Coffee Sci. 20, 1–9. https://doi.org/10.25186/.v20i.2289.

Osorio Pérez, V., Álvarez-Barreto, C.I., Matallana, L.G., Acuña, J.R., Echeverri, L.F., Imbachí, L.C., 2022. Effect of prolonged fermentations of coffee mucilage with different stages of maturity on the quality and chemical composition of the bean. Fermentation 8 (10), 519. https://doi.org/10.3390/fermentation8100519.

Osorio, V., Pabón, J., Medina, R., 2024. Impact of fruit reserve conditions from harvest to processing on the chemical composition and quality of coffee. Front. Sustain. Food Syst. 8. https://doi.org/10.3389/fsufs.2024.1425599.

Partelli, F.L., Oliosi, G., Dalazen, J.R., da Silva, C.A., Vieira, H.D., Espindula, M.C., 2021. Proportion of ripe fruit weight and volume to green coffee: differences in 43 genotypes of *Coffea canephora*. Agron. J. 113 (2), 1050–1057. https://doi.org/10.1002/agj2.20617.

Peña, A.J., Ramírez, V.H., Valencia, J.A., Jaramillo-Robledo, A., 2012. La lluvia como factor de amenaza para el cultivo del café en Colombia. Av. Técnicos Cenicafé 415. https://doi.org/10.38141/10779/0415.

Peñuela Martínez, A.E., Moreno Riascos, S.P., García Duque, J.F., 2023a. Operating conditions of a bioreactor for fermentation in coffee. Biotecnol. ía En. El Sect. Agropecu. Y. Agroind. 22 (1), 29–39. https://doi.org/10.18684/rbsaa.v22.n1.2024.2231.

Peñuela-Martínez, A.E., García-Duque, J.F., 2023b. Métodos de fermentación modificados y su influencia en la calidad de la bebida. Av. Técnicos Cenicafé 554, 1–12. https://doi.org/10.38141/10779/0554.

Peñuela-Martínez, A.E., García-Duque, J.F., Sanz-Uribe, J.R., 2023c. Characterization of fermentations with controlled temperature with three varieties of coffee (Coffea arabica L.). Fermentation 9 (11). https://doi.org/10.3390/fermentation9110976.

Peñuela-Martínez, A.E., Guerrero, Á., Sanz-Uribe, J.R., 2022. Cromacafé® Herramienta para identificar los estados de madurez de las variedades de café de fruto rojo. Av. Técnicos Cenicafé 535, 1–8. https://doi.org/10.38141/10779/0535.

Peñuela-Martínez, A.E., Moreno-Riascos, S., Medina-Rivera, R., 2023e. Influence of temperature-controlled fermentation on the quality of mild coffee (Coffea arabica L.) cultivated at different elevations. Agriculture 13 (6), 1132. https://doi.org/10.3390/agriculture13061132.

Peñuela-Martínez, A.E., Osorio-Giraldo, C.V., Buitrago-Zuluaga, C., Medina-Rivera, R.D., 2025. Development of fermentation strategies for quality mild coffee production (Coffea arabica L.) based on oxygen availability and processing time. Foods 14 (17), 3001. https://doi.org/10.3390/foods14173001.

Peñuela-Martínez, A.E., Pabón, J., Sanz-Uribe, J.R., 2013. Método fermaestro: para determinar la finalización de la fermentación del mucílago de café. Av. Técnicos Cenicafé 431. https://doi.org/10.38141/10779/0431.

Peñuela-Martínez, A.E., Velasquez-Emiliani, A.V., Angel, C.A., 2023g. Microbial diversity using a metataxonomic approach, associated with coffee fermentation processes in the Department of Quindío, Colombia. Fermentation 9 (4), 343. https://doi.org/10.3390/fermentation9040343.

Pereira, L.L., Guarçoni, R.C., Pinheiro, P.F., Osório, V.M., Pinheiro, C.A., Moreira, T.R., ten Caten, C.S., 2020. New propositions about coffee wet processing: chemical and sensory perspectives. Food Chem. 310, 125943. https://doi.org/10.1016/j.foodchem.2019.125943.

Polanía Rivera, A.M., López Silva, J., Torres-Valenzuela, L.S., Plaza Dorado, J.L., 2024. Development of starter inoculum for controlled Arabica coffee fermentation using coffee by-products (pulp and mucilage broth), yeast, and lactic acid bacteria. Fermentation 10 (10), 516. https://doi.org/10.3390/fermentation10100516.

Purwoko, T., Suranto, S., Setyaningsih, R., Marliyana, S.D., 2022. Chlorogenic acid and caffeine content of fermented robusta bean. Biodiversitas J. Biol. Divers. 23 (2). https://doi.org/10.13057/biodiv/d230231.

Rocha, R.A.R., Cruz, M.A.D., da, Silva, L.C.F., Costa, G.X.R., Amaral, L.R., Bertarini, P.L.L., Gomes, M.S., Santos, L.D., 2024. Evaluation of Arabica coffee fermentation using machine learning. Foods 13 (3), 454. https://doi.org/10.3390/foods13030454.

Rodriguez, Y.F.B., Calderon, K.T.S., Hernández, J.G., 2020. Comparison of sensory attributes and chemical markers of the infrared spectrum between defective and non-defective Colombian coffee samples. Coffee Sci. https://doi.org/10.25186/cs.v15i.1659.

Rodriguez, Y.F.B., Guzman, N.G., Hernandez, J.G., 2020. Effect of the postharvest processing method on the biochemical composition and sensory analysis of Arabica coffee. Eng. Agr. ícola 40 (2), 177–183. https://doi.org/10.1590/1809-4430-eng.agric.v40n2p177-183/2020.

Rojas-Chacón, J.A., Echeverría-Beirute, F., Jiménez Madrigal, J.P., Gatica-Arias, A., 2024. Microorganismos de suelo y su relación con la calidad de la bebida de café: una revisión. Agron. ía Mesoam. 57260. https://doi.org/10.15517/am.2024.57260.

Sánchez-Riaño, A.M., Vega-Oliveros, C., Ladino-Garzón, W.L., Orozco-Blanco, D.A., Bahamón-Monje, A.F., Gutiérrez-Guzmán, N., Amorocho-Cruz, C.M., 2024. Effects of cherries sanitization methods and fermentation times on quality parameters of coffee beans. Heliyon 10 (13), e33508. https://doi.org/10.1016/j.heliyon.2024.e33508.

SCAA, 2015. SCAA protocols cupping specialty coffee. Specialty Coffee Association of America.

Silva, L.C.F., Pereira, P.V.R., Cruz, M.A.D., da, Costa, G.X.R., Rocha, R.A.R., Bertarini, P.L.L., Amaral, L.R., do, Gomes, M.S., Santos, L.D., 2024a. Enhancing sensory quality of coffee: the impact of fermentation techniques on Coffea arabica cv. Catiguá MG2. Foods 13 (5), 653. https://doi.org/10.3390/foods13050653.

Sinaga, H.L.R., Bastian, F., Syarifuddin, A., 2021. Effect of decaffeination and re-fermentation on level of caffeine, chlorogenic acid and total acid in green bean robusta coffee. IOP Conference Series Earth Environmental Science 807 (2), 022069. https://doi.org/10.1088/1755-1315/807/2/022069.

Tirado-Kulieva, V., Quijano-Jara, C., Avila-George, H., Castro, W., 2024. Predicting the evolution of pH and total soluble solids during coffee fermentation using near-infrared spectroscopy coupled with chemometrics. Curr. Res. Food Sci. 9, 100788. https://doi.org/10.1016/j.crfs.2024.100788.

Vaz, C.J.T., de Menezes, L.S., de Santana, R.C., Sentanin, M.A., Zotarelli, M.F., Guidini, C.Z., 2023. Effect of fermentation on the physicochemical characteristics and sensory quality of Arabica coffee. 3 Biotech 13 (12). https://doi.org/10.1007/s13205-023-03768-9.

Wang, J., Jun, S., Bittenbender, H.C., Gautz, L., Li, Q.X., 2009. Fourier transform infrared spectroscopy for kona coffee authentication. J. Food Sci. 74 (5). https://doi.org/10.1111/j.1750-3841.2009.01173.x.