

GREEN TO ROASTED: EVALUATING THE EFFECTS OF ROASTING CONDITIONS ON COFFEE'S BIOACTIVE COMPOUNDS

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ABSTRACT

This study evaluates the influence of roasting degree and time–temperature profiles on the physicochemical properties and bioactive compound composition of *Coffea arabica*. Two specialty coffee samples differing in post-harvest processing (wet and dry) were subjected to five roasting conditions: light, medium, dark, low-temperature long-time (LTLT), and high-temperature short-time (HTST), with green coffee serving as control ($n = 16$). Statistical evaluation was performed using analysis of variance (ANOVA, $\alpha = 0.05$), and multivariate relationships were explored by Principal Component Analysis (PCA). Roasting significantly affected all monitored parameters. pH decreased from green coffee (5.33–5.38) to light and medium roasts (4.66–4.92), followed by an increase in dark roasts (5.51–5.74), reflecting the formation and subsequent degradation of organic acids. Dry matter increased from approximately 90.5% in green coffee to ~98% in roasted samples, while water activity decreased from 0.49–0.52 to ~0.19–0.23. Total antioxidant capacity declined with roasting intensity (from ~85–88% DPPH inhibition in green coffee to ~58–61% in dark roast), whereas total polyphenol content showed variability depending on processing method. Chlorogenic acids exhibited substantial degradation, decreasing from ~25–28 $\text{g}\cdot\text{kg}^{-1}$ DM in green coffee to ~7–12 $\text{g}\cdot\text{kg}^{-1}$ DM in dark and HTST samples, while caffeine content remained relatively stable (~7.5–9.1 $\text{g}\cdot\text{kg}^{-1}$ DM). Roasting dynamics significantly influenced compound retention. LTLT roasting preserved chlorogenic acids (~9.4–9.6 $\text{g}\cdot\text{kg}^{-1}$ DM) and antioxidant capacity at levels comparable to medium roast, whereas HTST resulted in the highest degradation (~60–75% loss). PCA confirmed roasting conditions as the primary factor driving compositional variability, with secondary contributions from post-harvest processing. These findings demonstrate that peak temperature is the dominant factor governing bioactive compound stability and highlight the potential of controlled roasting strategies to optimize coffee quality.

Keywords: coffee roasting time, roasting temperature, *Coffea arabica*, bioactive compounds

INTRODUCTION

Green coffee beans are the raw seeds of the *Coffea* plant. Nowadays, coffee beans as a commodity holding a significant influence and share on the world market (Freitas *et al.*, 2024). Green beans are rich in bioactive compounds, including chlorogenic acids, caffeine, and lipids, which contribute to their antioxidant properties and potential health benefits (Farah *et al.*, 2006). The chemical composition of green coffee varies depending on factors such as species, origin, and cultivation practices, influencing the flavor and quality of the final product (Clarke & Macrae, 1985). Unlike roasted coffee, green coffee retains a higher concentration of chlorogenic acids, which are known for their anti-inflammatory and antioxidant effects (Daglia *et al.*, 2000). As the starting material for coffee production, green coffee serves as the foundation for the complex transformations that occur during roasting.

The roasting process is a critical step in coffee production, transforming green coffee beans into the aromatic and flavorful product enjoyed by consumers. During roasting, beans are exposed to high temperatures, typically ranging from 180°C to 250°C, for varying durations depending on the desired roast level (Illy & Viani, 2005). This process triggers a series of complex chemical reactions, including Maillard reactions, caramelization, and pyrolysis, which are responsible for the development of coffee's characteristic flavor, aroma, and color (Baggenstoss *et al.*, 2008). Chlorogenic acids, the primary antioxidants in green coffee, undergo significant degradation during roasting, leading to the formation of phenolic compounds and melanoidins that contribute to the antioxidant activity of roasted coffee (Farah *et al.*, 2005). Additionally, caffeine content remains relatively stable, while lipids and proteins are partially degraded, influencing the sensory profile of the coffee (Gloess *et al.*, 2013). The degree of roasting, categorized as light, medium, or dark, determines the extent of these chemical changes, with darker roasts exhibiting reduced acidity and enhanced bitterness due to prolonged exposure to heat (Moon *et al.*, 2009). Understanding these transformations is essential for optimizing the roasting process to achieve the desired balance of flavor, aroma, and bioactive compounds.

Recent advancements in coffee roasting have introduced innovative techniques aimed at enhancing flavor profiles, improving efficiency, and reducing environmental impact. The roasting process can be modulated not only by the degree of roast but also by the roasting dynamics, including time and temperature. Low-temperature, long-time (LTLT) roasting is characterized by slower heat transfer, allowing for a more gradual development of flavors and preservation of some bioactive compounds such as chlorogenic acids and total polyphenols. This method often results in coffee with a balanced flavor profile and higher antioxidant capacity due to reduced thermal degradation of sensitive compounds. Conversely, high-temperature, short-time (HTST) roasting subjects the beans to rapid and intense thermal exposure, accelerating chemical transformations such as Maillard reactions and caramelization. While HTST roasting enhances the development of certain aromatic compounds and melanoidins, it often leads to greater degradation of polyphenols and chlorogenic acids. Caffeine content, being relatively heat-stable, is typically less affected by the roasting approach but may vary slightly due to weight loss during roasting. The contrasting effects of these methods underscore the importance of tailoring roasting parameters to achieve specific chemical and sensory attributes in coffee (Baggenstoss *et al.*, 2008; Gottstein *et al.*, 2023).

The novelty of this study lies in its mechanistic comparison of conventional roasting with alternative time–temperature strategies (LTLT and HTST), demonstrating that chlorogenic acid degradation is governed primarily by peak temperature rather than roasting time alone. Unlike previous studies focused mainly on roasting degree, this work shows that LTLT slows degradation kinetics and preserves chlorogenic acids despite prolonged exposure, while HTST accelerates their breakdown due to high temperature intensity. This provides new evidence that roasting dynamics can be strategically controlled to modulate bioactive compound retention. Technologically, the study introduces LTLT and HTST as practical approaches for tailoring antioxidant capacity and chemical composition, supported by combined chemical and multivariate analysis, thus contributing to data-driven optimization of coffee roasting processes.

MATERIALS AND METHODS

Raw Material

We analyzed samples of 100% *Coffea arabica* of specialty quality. Samples originated from harvesting sites of Colombia. Samples were divided into two main samples (sample A – Colombia wet processed and sample B – Colombia dry processed). To ensure clarity in the experimental design, the total number of samples (n = 12) refers to the number of experimental groups rather than individual roasting batches. Specifically, two initial coffee batches differing in post-harvest processing (wet and dry) were each subjected to six conditions (green coffee and five roasting profiles: light, medium, dark, LTLT, and HTST), resulting in 12 distinct sample groups. For each roasting condition, the process was performed in five independent roasting replicates (100 g per batch) to ensure process reproducibility. These replicates were subsequently homogenized and combined into a representative composite sample, which was used for all subsequent analyses. This approach was applied to minimize variability associated with small-scale roasting while maintaining representative and analytically robust samples for each experimental condition. Detailed description is shown in Table 1.

Table 1 Raw material description

Sample ID	Country	Variety	Processing	Altitude (mamsl)
A	Columbia	C1, C2,	W	1300 - 1800
B	Colombia	C1, B	D	1500 - 1700

Note: C1 – caturra; C2 - Catuai; B – Bourbon; D – dry processing; W – wet processing; mamsl - meters above mean sea level

Roasting process

Batches of green coffee were roasted using laboratory roaster Sample PRO 100 Series roaster (Coffee PRO Direct, Hong Kong). To monitor the roasting time and temperature, we used the NI – TC01 (National Instruments Corp., USA). Each batch was roasted to five different forms of coffee -Light roast (A1 and B1), Medium roast (A2 and B2), Dark roast (A3 and B3). Additionally, each sample group was roasted using two specific processing techniques High Temperature-Short Time (AHTST and BHTST). Low Temperature-Long Time (ALTLT and BLTLT). Set Roasting conditions and profiles are shown in Table 2 and Figure 1 respectively. Each sample of 100 g (batch) were roasted using conditions shown in Table 2). After the roasting process samples were cooled down with air and after reaching room temperature, the accuracy of the roasting level was measured with Coffee Roast Analyzer RoastRite RA-720BF with NIR sensor (Acronova Technologies, Inc. New Jersey, USA). Roasting results are shown in Figure 2A and 2B.

Table 2 Roasting Profiles and Conditions for Coffee Samples: Roasting Time, Temperature, and Crack Stages

Roasting profile	Roasting time	Starting temperature (°C)	Roasting temperature °C		Crack (time, °C)	
			Min (°C)	Max (°C)	First Crack	Second crack
Light	4 min 40 s	180	134.8	205.5	3 min 30s 175.4	-
Medium	6 min	180	135.4	225.8	3 min 30s 175.4	5 min 40 s 220 °C
Dark	6 min 40 s	180	141.1	235.1	3 min 30 s 185	5 min 215 °C
LTLT	16 min	140	100.6	185	14 min 08 s 181.2	16 min 185 °C
HTST	6 min	215	117.8	220.1	4 min 49 s 190	4 min 50 s 190 °C

Note: HTST - high temperature-short time; LTLT - low temperature-long time; min – minute; s– seconds; Min – minimum of temperature; Max – maximum of temperature; °C

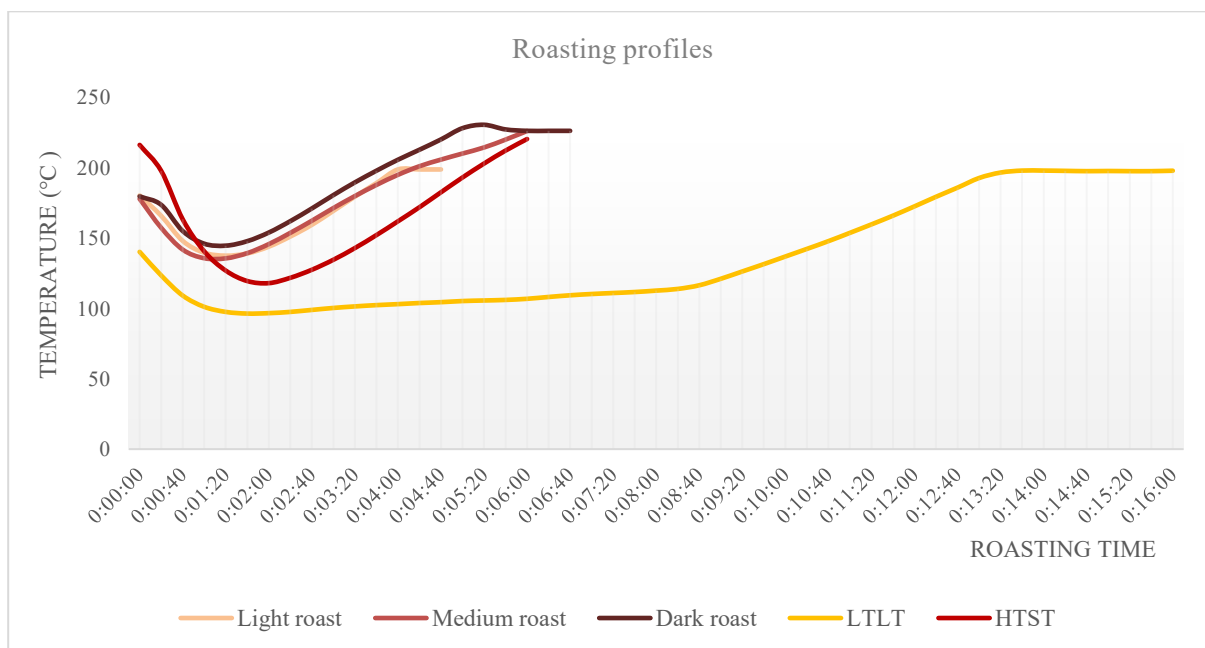


Figure 1 Roasting profiles. Note: (LTLT = long time-low temperature, HTST = high temperature-short time)



Figure 2A Visual results of Colombia wet processed roasting.



Figure 2B Visual results of Colombia dry processed roasting

Grinding and extract preparation

To facilitate homogenization due to the firm structure of green coffee beans, the samples were pre-frozen at $-20\text{ }^{\circ}\text{C}$ for 30 minutes prior to analysis. Homogenization was performed using a Grindomix GM 200 (Retsch, Haan, Germany) at 10,000 rpm, with processing times of 60 seconds for roasted beans, and 120 seconds for green beans to achieve the desired particle size. The resulting homogenized material was subsequently sieved through a 1 mm mesh sieve (Retsch, Germany) to ensure uniform particle size distribution. The extracts were prepared using precisely 7 g of samples weighted with Kern 120-5DM balance (Kern & Sohn GmbH, Balingen, Germany) and 120 mL of demineralized water at $95\text{ }^{\circ}\text{C}$. The mixture was stirred occasionally during the 5-minute extraction process. The resulting solutions were filtered using Grade-390 Sartorius filter paper (Sartorius Lab Instruments GmbH & Co. KG, Göttingen, Germany) and 25 mm PVDF syringe filters, pore size $0.45\text{ }\mu\text{m}$ (Agilent Technologies, Germany). The cooled, filtered extracts were then used for subsequent analyses.

Determination dry matter (DM %) and water activity a_w

Determining dry matter content was conducted using a KERN DAB 100-3 moisture analyzer (KERN & SOHN GmbH, Balingen, Germany), with results expressed as a percentage (%). Samples weighing 5 g were used for the analysis. The drying process was carried out under standardized conditions, utilizing a drying program with a temperature of $110\text{ }^{\circ}\text{C}$. The next parameter analyzed was water activity. We used the Water Activity Meter Fast-Lab to determine a_w in the extracts.

Determination of pH

The pH values were determined using a pH meter, type pH 70 (XS Instruments, Carpi, Italy). The measurement was performed at a sample temperature of $25\text{ }^{\circ}\text{C}$, and pH was determined by triplicate. The pH meter was calibrated using Hamilton Buffer Solution (Hamilton Bonaduz AG, Bonaduz, Switzerland), pH 4.01; 7.00; and 10.01.

Determination of total antioxidant capacity

In this study, the antioxidant activity of the samples was determined using the DPPH radical scavenging assay, based on the method described by **Brand-Williams et al. (1995)** with modifications according to **Poláková et al. (2023)**. The assay involved preparing a DPPH working solution by dissolving 0.025 g of DPPH in 96% ethanol and diluting it in a 1:9 ratio (Centralchem, Bratislava, Slovakia, 96%). A volume of 3.9 mL of this solution was transferred into a glass cuvette to measure the initial absorbance (A_0) at 515.6 nm (T80 UV/VIS Spectrometer; PG Instruments, Ltd.; Luttermouth, UK). Subsequently, 100 μL of the sample extract was added to the DPPH solution, stirred, and allowed to react for 10 minutes. The absorbance after the reaction (A_t) was recorded at the same wavelength. Ethanol served as a blank, and its absorbance (A_s) was included in the calculation. The percentage of DPPH radical inhibition, representing the antioxidant activity, was calculated using the formula:

$$\% \text{ inhibition DPPH} = \frac{(A_0 - A_s) - (A_t - A_s)}{(A_0 - A_s)} \times 100$$

Where:

- A_0 is the initial absorbance of the DPPH solution; A_s is the absorbance of ethanol (blank); A_t is the absorbance after 10 min.

Determination of total polyphenols content

The total polyphenol content (TPC) was quantified as grams of gallic acid equivalents (GAE) per kilogram of dry matter. According to the **Lachman et al. (2003)** with modifications according to **(Demianová et al., 2021)**. A double-beam UV-VIS spectrophotometer (T80 UV/VIS Spectrometer; PG Instruments, Ltd., Luttermouth, UK), equipped with an eight-position cuvette holder, was utilized for the analysis. Measurements were conducted using type S/G/10 glass cuvettes (Exacta+Optech GmbH, Munich, Germany). To prepare the stock solution, 100 mg of gallic acid was accurately weighed using a precision balance (Sartorius Lab Instruments GmbH & Co. KG, Göttingen, Germany) and dissolved in demineralized water, with the volume adjusted to 100 mL in a volumetric flask. A working solution was then prepared by diluting 1 mL of the stock solution with distilled water to a final volume of 200 mL. The calibration curve was established using gallic acid concentrations ranging from 5 to 200 $\text{mg}\cdot\text{L}^{-1}$, and the blank solution consisted of Folin-Ciocalteu reagent and distilled water without any standard or sample. The calibration curve demonstrated a strong linear relationship, with a correlation coefficient of $R^2 = 0.998$. Sample preparation for measurement involved pipetting 50 μL of extract into a 50 mL volumetric flask. A diluted Folin-Ciocalteu reagent (1:2 v/v with distilled water) was prepared, and 2.5 mL of this reagent was added to the flask containing the extract. Subsequently, 5 mL of a 20% Na_2CO_3 solution was added, and the flask was topped up with distilled water to reach a final volume of 50 mL. The mixture was left at room temperature for two hours to allow the blue-colored complex to form. The absorbance of the samples was recorded at 765 nm.

Determination of caffeine and chlorogenic acids

The methodology for the determination of caffeine and chlorogenic acids by HPLC-DAD (High-Performance Liquid Chromatography with Diode-Array Detection) was adapted from **Bobková et al. (2021)**. Analyses were performed using the HPLC Agilent Infinity 1260 (Agilent Technologies GmbH, Waldbronn, Germany) equipped with a DAD detector (1260 DAD VL+). The separation was performed using a LiChroCART 250-4 Purospher STAR, with an RP-18 end-capped column ($250\text{ mm} \times 4\text{ mm} \times 5\text{ }\mu\text{m}$; Merck KGaA, Darmstadt, Germany). Methanol (A) and 0.1% solution of formic acid in ddH₂O (v/v) (B) were used as a mobile phase. The separation was performed at gradient elution (0–2 min: 20% A + 80% B); in the 2–15 min period, the ratio of mobile phases was gradually changed to a final value of 40% A + 60% B, and the post time and equilibration were changed back (20% A + 80% B: 3 min). The flow rate was $1\text{ mL}\cdot\text{min}^{-1}$, and the injection volume was 3 μL . The temperature was set at $40\text{ }^{\circ}\text{C}$. The detection wavelengths were set at 240 and 280 nm. Obtained data were processed using the Agilent OpenLab ChemStation program. The following reagents were used as standards: caffeine, chlorogenic acid, neochlorogenic acid, and cryptochlorogenic acid (HPLC purity, >99%, Merck KGaA, Darmstadt, Germany).

Statistical analysis

The statistical analysis was conducted to evaluate the differences among groups using Analysis of Variance (ANOVA) at a significance level of 0.05. Violin plots were utilized to visualize the distribution and variability of the data across groups, providing a clear representation of outliers and central tendencies. Principal Component Analysis (PCA) was performed to reduce dimensionality and visualize the clustering patterns and variance explained by the principal components. The analysis was conducted using Python version 3.11.6. The analysis utilized the following Python packages: scipy (version 1.11.3) and statsmodels (version 0.14.0) for statistical tests, matplotlib (version 3.8.0) and seaborn (version 0.13.0) for data visualization, and scikit-learn (version 1.3.1) for PCA.

RESULTS AND DISCUSSION

For the data visualization we used violin plots to show detailed representation of data distribution, including variability, and the density we used violin plots, which reveal the full shape of the data distribution, making them useful for identifying or subtle patterns. By mirroring the KDE (Kernel Density Estimate) along the vertical axis, violin plots create a symmetrical shape that highlights the density of data, offering a comprehensive view of the dataset.

Antioxidant properties of green coffee beans were previously proved by various authors (**Montenegro et al., 2021**; **Masek et al., 2020**). The main antioxidants of green coffee are chlorogenic acids, polyphenols, trigonelline, and caffeine (**Masek et al. 2020**; **Analianasari et al., 2022**). However, not all of these can react with DPPH radical. Chlorogenic acids (CQAs) are highly reactive with DPPH radicals due to their phenolic hydroxyl groups, which can donate hydrogen atoms. Other polyphenols present in green coffee, apart from CQAs, also exhibit radical scavenging activity. But caffeine and trigonelline poses minimal or limited scavenging activity towards DPPH (**Gulcin and Alwaseel, 2023**; **Jaisankar and Arivarasu, 2020**; **Liang and Kitts 2014**; **Díaz-Hernández et al. 2022**; **Bashir et al., 2023**).

As shown in Figure 3, the highest percentage of DPPH scavenging was observed in green coffee samples regardless the post-harvest processing (dry/wet). Needless

to emphasize that post-harvest processing caused the significant difference in antioxidant capacity of green coffee (Table 3). Violin plots showed the highest variability in TAC in green samples. These results also suggest that origin both botanical, geographical, and altitude of harvesting sites might play a significant role in the constituents' concentration. Roasting profiles (i.e., light, medium, dark, low-temperature long-time, or high-temperature short-time) influence the balance between preserving existing antioxidants and forming new ones. Studying antioxidant capacity helps identify roasting conditions that maximize health benefits without compromising flavor. Light and medium roasting caused a decrease in TAC compared to the green beans. Wider distribution suggests more variability in antioxidant levels as roasting progresses. Narrower distribution compared to light and medium profiles, indicating a reduction in antioxidants due to higher roasting levels. LTLT and HTST profiles show the TAC comparable to medium roasted coffee. Studies show that HTST roasting can enhance certain antioxidant properties by promoting the Maillard reaction, which generates melanoidins with notable antioxidant activity (Baggenstoss et al. 2008; Jung et al., 2017).

Chlorogenic acids (CQAs), represented in this study by chlorogenic, cryptochlorogenic, and neochlorogenic acids, were the most abundant in green coffee, reaching mean concentrations of 27.65 and 25.07 g·kg⁻¹ DM for chlorogenic acid in dry- and wet-processed samples, respectively. Upon roasting,

CQAs underwent a series of thermally driven transformations governed by both temperature intensity and exposure time. During light roasting, chlorogenic acid content decreased to 16.29 g·kg⁻¹ DM (dry) and 14.06 g·kg⁻¹ DM (wet), indicating initial acyl migration and isomerization among caffeoylquinic acid isomers, alongside the onset of lactonization reactions, which convert caffeoylquinic acids into chlorogenic acid lactones (Farah et al., 2005; Moon et al., 2009). These reactions occur without complete destruction of the quinic acid backbone and are favored at moderate roasting temperatures.

As roasting progressed to medium and dark profiles, CQAs degradation intensified, with chlorogenic acid declining to 14.86–10.69 g·kg⁻¹ DM (medium) and further to 11.98–7.10 g·kg⁻¹ DM (dark). This pronounced loss reflects the dominance of ester bond cleavage between caffeic acid and quinic acid, followed by decarboxylation and fragmentation of quinic acid derivatives, producing low-molecular-weight phenolics that are no longer detected as intact CQAs by HPLC-DAD (Farah et al., 2006; Jeon et al., 2019; Awwad et al., 2021). At higher roasting degrees, these reactions are accompanied by pyrolytic degradation and covalent binding of phenolic fragments to melanoidins, explaining the simultaneous decrease in CQAs and partial preservation of antioxidant capacity observed in darker roasts (Baggenstoss et al., 2008).

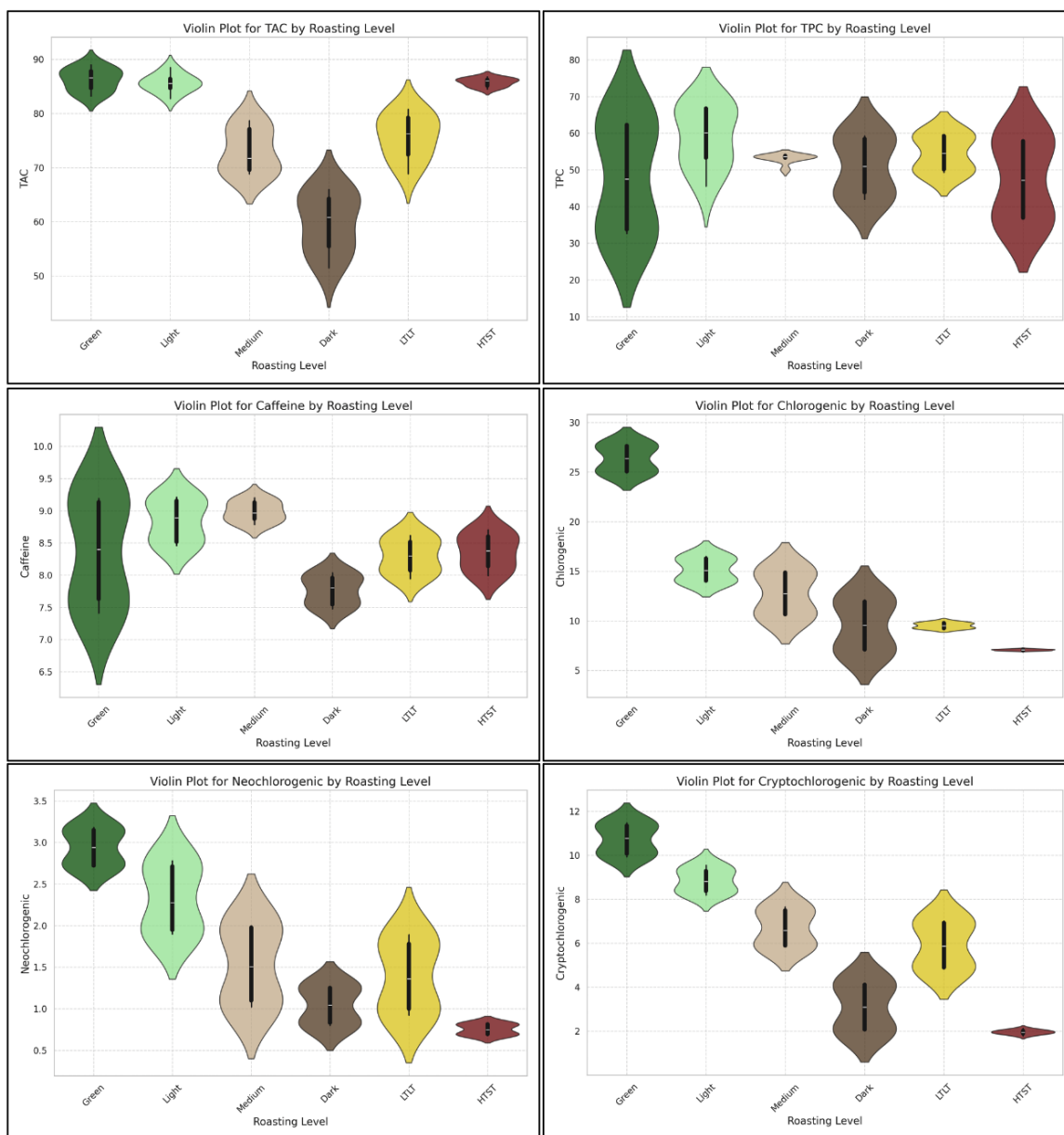


Figure 3 Changes in bioactive compounds caused by the roasting conditions regardless of the post-harvest processing. Note: TAC is expressed in % of DPPH inhibition, TPC in mg of gallic acid equivalent per g of dry matter (mg GAE/g), caffeine and chlorogenic acids in mg/g.

Distinct patterns emerged under alternative roasting strategies. Low-temperature long-time (LTLT) roasting retained chlorogenic acid at levels of 9.40–9.64 g·kg⁻¹ DM, comparable to medium-roasted samples, suggesting that reduced peak temperature slows reaction kinetics and limits extensive ester cleavage despite prolonged heat exposure. In contrast, high-temperature short-time (HTST) roasting

resulted in the lowest CQAs concentrations, with chlorogenic acid reduced to approximately 7.02–7.14 g·kg⁻¹ DM, corresponding to an overall loss of roughly 60–75% relative to green coffee. This indicates that rapid exposure to elevated temperatures promotes accelerated lactonization followed by irreversible thermal decomposition, confirming that maximum temperature is a critical driver of CQAs

breakdown (Baggenstoss et al., 2008; Gottstein et al., 2023). Notably, differences between dry- and wet-processed coffees persisted across all roasting profiles, demonstrating that post-harvest processing might influence CQAs distribution and matrix interactions, thereby modulating susceptibility to thermal degradation during roasting. However, to robustly validate this observation, further studies employing a larger set of comparable samples processed under wet and dry conditions are required.

Caffeine is probably the most important and valuable compound found in coffee. As such, caffeine is highly thermostable and does not break down or lose its potency during roasting process or subsequent brewing (Grzelczyk et al., 2022). Caffeine content in our samples remains relatively stable across roast profiles, traditional as well as novelty ones. This is in line with current literature and other authors' findings (Olechno et al., 2021; Lindsey et al., 2024). Apparent variations among samples are more likely explainable by mass loss concentration effects than different roasting conditions (Grzelczyk et al., 2022).

On the other hand, chlorogenic acids (CQAs) are thermolabile and undergo degradation or transformation when subjected to high-temperature processing, such as coffee roasting. In our study we observed chlorogenic, cryptochlorogenic and neochlorogenic acid concentration in coffee samples. All CQAs were the most prevalent in green coffee and decreased gradually with higher traditional roasting degree. Those changes were expected and are supported by Jeon et al. (2019) or Awwad et al. (2021). If we look closer at novelty roasting methods, LTLT roasting method was able to retain CQAs concentration on level comparable to medium roast. On the contrary, HTST proved to be the most devastating roasting process from the CQAs concentration point of view as the levels observed were showed up to ~60-75% loss depending on individual acid and processing method as post-harvest processing effect (wet vs dry) persists even after roasting. Although the present study demonstrates observable differences associated with post-harvest processing (Table 3), these results are intended to highlight the potential influence of processing method on coffee composition; however, we acknowledge that a more comprehensive and statistically robust interpretation would require a larger set of samples with comparable origin and controlled processing conditions.

The degradation behavior of chlorogenic acids (CQAs) observed in this study is consistent with previously reported thermal transformation pathways occurring during coffee roasting. CQAs are known to be highly thermolabile, with their degradation primarily driven by temperature intensity rather than roasting duration (Farah et al., 2005; Moon et al., 2009; Jeon et al., 2019). At early roasting stages, CQAs undergo acyl migration and isomerization among caffeoylquinic acid isomers, accompanied by the formation of chlorogenic acid lactones through intramolecular esterification (Farah et al., 2005). These intermediates contribute to the sensory profile, particularly bitterness, but are not fully quantified as native CQAs. With increasing thermal load, ester bond cleavage and decarboxylation reactions dominate, leading to the formation of caffeic acid and quinic acid derivatives, which are further degraded or transformed into low-molecular-weight phenolics (Farah et al., 2006; Jeon et al., 2019). Simultaneously, a portion of these degradation products becomes incorporated into high-molecular-weight melanoidins formed via Maillard reactions, explaining the partial retention of antioxidant capacity despite substantial CQA losses (Baggenstoss et al., 2008).

Previous studies report CQA reductions of up to 50–90% depending on roasting severity, which agrees with the losses observed under HTST conditions in the present work (Moon et al., 2009; Awwad et al., 2021). Importantly, recent findings emphasize that roasting kinetics can be modulated to balance degradation and preservation, with lower peak temperatures slowing reaction rates and limiting irreversible breakdown (Gottstein et al., 2023). In line with this, our results confirm that LTLT roasting enables partial retention of CQAs, whereas HTST accelerates their degradation, supporting the concept that peak temperature is the dominant factor controlling CQA stability and transformation pathways during roasting.

Changes in physical-chemical parameters

Measured acidity, in our case pH, of coffee is directly connected to content of organic acids, including chlorogenic acids (CQAs). When compared, we observed differences in pH between the dry and wet processing in all roasting methods, excluding the LTLT method. Both dry and wet processing method follow the pH development trend described by Anokye-Bempah et al. (2024). Firstly, decrease of the pH in light and medium roast which is caused by formation of various organic acids, which are important for sensory profile and could carry some health benefits (Farah & De Paula Lima, 2019; Yeager et al., 2021), and following decrease in dark roast, caused by decomposing the organic acids by long-lasting roasting temperature. Novelty approaches roasting, LTLT and HTST, showed pH more like light or medium roast. On the other hand, we dry matter (DM) is steadily increasing as water activity (aw) is decreasing with the roasting degree from green coffee to dark roast. In this case, novelty approaches show DW and aw values closer to dark roast. Higher DW and lower aw are important parameters for microbial stability and therefore the safety, quality and shelf life of such valuable commodity as coffee (Alp & Bulantekin, 2021; De Abreu et al., 2025). This emphasize that novelty roasting approaches, LTLT and HTST, show great potential to keep and preserve sensory parameters and potential health benefits, which stem from organic acid volume, and increased microbial quality and safety, and potential prolonged shelf life of dark roast coffee.

TAC and TPC

Dry processed (natural) coffee typically retains higher total phenolic content (TPC) and antioxidant activity compared to wet-processed (washed) coffee (Cwiková et al., 2022), as we proved in our study in which TPC content of dry processed samples were significantly higher in green coffee and after every roasting process, except LTLT. On the other hand, TAC is more affected by roasting process than processing method. Highest TAC was observed in green coffee, slightly decreasing in light roasted and then we observe steeper decrease in medium and dark roasted coffee as previously reported by (Yashin et al., 2013). In this case, novelty method LTLT showed TAC comparable to medium roast while HTST reached TAC comparable to light roast. Since Folin–Ciocalteu responds not only to phenolics but also Maillard-derived compounds, divergence from CQAs trends is expected (Dominguez-López et al., 2023).

Table 3 Significant differences between selected parameters regarding the post-harvest processing and roasting profile.

Category	pH	DM	aw	TAC	TPC	Caffeine	Neochlorogenic	Cryptochlorogenic	Chlorogenic
Green Dry	5,33 ^a	90,49 ^a	0,49 ^a	87,67 ^b	62,06 ^b	8,58 ^a	3,15 ^b	11,37 ^b	27,65 ^b
Green Wet	5,38 ^a	90,56 ^a	0,52 ^b	84,80 ^a	50,55 ^a	9,15 ^b	2,73 ^a	10,09 ^a	25,07 ^a
Category	pH	DM	aw	TAC	TPC	Caffeine	Neochlorogenic	Cryptochlorogenic	Chlorogenic
Light Dry	4,77 ^b	95,79 ^b	0,39 ^b	86,61 ^a	66,63 ^b	8,54 ^a	2,70 ^b	9,34 ^b	16,29 ^b
Light Wet	4,66 ^a	95,96 ^a	0,35 ^a	84,59 ^a	51,54 ^a	9,15 ^b	1,94 ^a	8,35 ^a	14,06 ^a
Category	pH	DM	aw	TAC	TPC	Caffeine	Neochlorogenic	Cryptochlorogenic	Chlorogenic
Medium Dry	4,87 ^a	97,25 ^b	0,23 ^a	73,51 ^a	53,42 ^a	8,85 ^a	1,96 ^b	7,49 ^b	14,86 ^b
Medium Wet	4,92 ^b	97,17 ^a	0,26 ^b	72,67 ^a	53,62 ^a	9,12 ^b	1,09 ^a	5,91 ^a	10,69 ^a
Category	pH	DM	aw	TAC	TPC	Caffeine	Neochlorogenic	Cryptochlorogenic	Chlorogenic
Dark Dry	5,51 ^a	97,92 ^a	0,19 ^a	58,78 ^a	58,55 ^b	7,56 ^a	1,26 ^b	4,12 ^b	11,98 ^b
Dark Wet	5,74 ^b	97,63 ^a	0,23 ^b	60,83 ^a	43,39 ^a	7,98 ^b	0,83 ^a	2,07 ^a	7,10 ^a
Significant	Yes	No	Yes	No	Yes	Yes	Yes	Yes	Yes
Category	pH	DM	aw	TAC	TPC	Caffeine	Neochlorogenic	Cryptochlorogenic	Chlorogenic
LTLT Dry	4,93 ^a	97,56 ^b	0,21 ^a	75,13 ^a	59,16 ^b	8,54 ^b	1,79 ^b	6,92 ^b	9,40 ^a
LTLT Wet	4,93 ^a	97,14 ^a	0,22 ^a	76,27 ^a	49,98 ^a	8,06 ^a	0,99 ^a	4,91 ^a	9,64 ^a
Category	pH	DM	aw	TAC	TPC	Caffeine	Neochlorogenic	Cryptochlorogenic	Chlorogenic
HTST Dry	4,85 ^a	97,56 ^a	0,20 ^a	85,74 ^a	57,79 ^b	8,60 ^b	0,81 ^b	2,02 ^a	7,14 ^b
HTST Wet	4,98 ^b	98,10 ^b	0,21 ^a	85,79 ^a	36,93 ^a	8,11 ^a	0,69 ^a	1,90 ^a	7,02 ^a

Note: Columns with different indices a and b are significantly different at $\alpha=0.05$.

Principal Component Analysis (PCA) revealed a clear differentiation of coffee samples primarily driven by roasting conditions, confirming that thermal processing is the dominant factor shaping chemical composition. The first principal component (PC1) explained the majority of variance and was strongly

associated with the degradation of chlorogenic acids and changes in antioxidant capacity, effectively separating green coffee samples from roasted ones. Green samples clustered distinctly due to their high content of native bioactive compounds, while progressively roasted samples (light, medium, dark) showed a

gradual shift along PC1, reflecting increasing thermal degradation and transformation of phenolic constituents. The second principal component (PC2) contributed to finer discrimination among roasting strategies, particularly highlighting differences between conventional and alternative roasting approaches. Notably, LTLT samples clustered closer to medium-roasted coffee, indicating partial preservation of chlorogenic acids and antioxidant-related attributes despite prolonged roasting time. In contrast, HTST samples formed a more distinct cluster, suggesting that high peak temperatures induce more pronounced chemical alterations, consistent with accelerated degradation pathways. Additionally, a subtle separation between dry- and wet-processed samples was observed within roasting groups, indicating that post-harvest processing exerts a secondary but detectable influence on chemical composition. However, this effect was less pronounced compared to roasting conditions. Overall, the PCA results support the conclusion that both roasting intensity and time–temperature dynamics govern the compositional profile of coffee, with peak temperature emerging as a critical factor influencing chemical transformations. Overall, the PCA highlights roasting conditions as a dominant factor governing compositional changes in coffee, with both roasting degree and time–temperature dynamics contributing to sample differentiation.



Figure 4 PCA visualization of the multivariate differentiation of coffee samples based on roasting profiles

CONCLUSION

This study confirms that coffee roasting is a decisive driver of chemical change, shaping both the stability of bioactive compounds and the overall physicochemical profile of *Coffea arabica*. As expected, increasing roasting intensity led to progressive moisture loss, reduced water activity, altered acidity, and a marked decline in chlorogenic acids, reflecting their thermal sensitivity. These trends were consistently captured by both targeted analyses and multivariate evaluation, which clearly separated samples according to roasting conditions. Beyond conventional roasting levels, the results highlight the importance of roasting dynamics. Low-temperature long-time roasting allowed partial preservation of chlorogenic acids and antioxidant capacity, yielding a composition comparable to medium roasts despite extended processing. In contrast, high-temperature short-time roasting accelerated chlorogenic acid degradation and produced a distinct chemical profile, underscoring peak temperature as a key factor governing phenolic stability. Differences arising from post-harvest processing remained evident across all roasting profiles, emphasizing the lasting influence of the raw bean matrix. Overall, the findings demonstrate that roasting strategies can be deliberately adjusted to balance chemical integrity, antioxidant potential, and desired transformations. Such control offers practical opportunities to tailor coffee quality while aligning sensory attributes with nutritional and technological considerations.

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