VALDEIR VIANA FREITAS

CHEMICAL AND SENSORY COMPOSITION OF ARABICA AND ROBUSTA COFFEE IN RESPONSE TO MODIFICATIONS IN THE ROASTING PROCESS

Thesis submitted to the Food Science and Technology Graduate Program of the Universidade Federal de Viçosa in partial fulfillment of the requirements for the degree of *Doctor Scientiae*.

Adviser: Paulo Cesar Stringheta

Co-advisers: Marcelo Henrique dos Santos
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ABSTRACT

Freitas, Valdeir Viana Freitas, D.Sc., Universidade Federal de Viçosa, October, 2023. **Chemical and sensory composition of Arabica and Robusta coffee in response to modifications in the roasting process**. Adviser: Paulo Cesar Stringheta. Co-advisers: Marcelo Henrique dos Santos and Márcia Cristina Teixeira Ribeiro Vidigal.

In recent years, the coffee market has experienced remarkable growth, driven by its expansion and production on a global scale. South America, in particular, stands out as one of the main coffee-producing regions, led by Brazil, and is also the largest exporter of this agricultural commodity. Furthermore, it is relevant to emphasize that coffee is one of the most widely consumed beverages worldwide, attracting an increasingly discerning consumer audience regarding product quality. An essential element in the process of transforming green coffee beans into an aromatic and flavorful cup of coffee is the roasting stage. This operation plays a fundamental role in creating the distinctive flavors and aromas found in the final beverage. In this context, the purpose of this study was to investigate the complexity of roasting by conducting a thorough analysis of the physicochemical and sensory changes that occur during this process. For this purpose, six different roasting profiles were employed, where temperature and roasting time were carefully considered and adjusted. The results unveiled intriguing information. It was found that the highest levels of total phenolics, compounds endowed with beneficial antioxidant properties for health, were identified in coffees subjected to specific temperatures, such as 135 °C/20.20 min and 210 °C/9.02 min. These findings not only provide valuable insight into the nutritional profile of roasted coffee but also emphasize the influence of different roasting profiles on these characteristics. Surprisingly, *C. canephora*, known for its more robust and full-bodied character, exhibited superior antioxidant activity compared to *C. arabica* in many of the evaluated roasting profiles. This finding may redefine the traditional view that *C. arabica* always surpasses *C. canephora* in terms of quality. The results showed that roasting profiles, as well as the species, strongly influenced all investigated parameters, particularly the concentration of sugars, organic acids, and melanoidins. Succinic acid was the organic compound with the highest concentrations, with the highest concentration observed in *C. canephora* at 210 °C/11.01 min (224.24 mg/g), with the highest concentrations of organic acids found in this same roasting profile and species (430.39 mg/g). Fructose was the sugar with the highest concentration, particularly in the 210 °C/11.01 min roast, which exhibited 17.14 mg/g. The highest melanoidin content was also found in this same roasting profile and

species. Sensory evaluation, conducted by both experts and consumers, has revealed significant differences in flavor, aroma, and overall quality properties among coffee varieties and various roasting profiles. *C. arabica* has received higher ratings compared to *C. canephora*, particularly with better scores for roasting profiles at 135 °C/20.20 min and 230 °C/17.43 min. These conclusions offer a deeper understanding of the nuances present in the roasting process and its impact on the coffee experience for enthusiasts of this beverage. Therefore, as we delve deeper into the coffee market, it becomes evident that roasting represents an operation that not only transforms the beans but also influences flavor, nutritional value, and consumer perception.

Keywords: *Coffea arabica L. Coffea canephora*. Roasting. Chemical composition. Coffee quality.

RESUMO

Freitas, Valdeir Viana, D.Sc., Universidade Federal de Viçosa, outubro de 2023. **Composição química e sensorial de café arábica e robusta frente a modificações no processo de torração**. Orientador: Paulo Cesar Stringheta. Coorientadores: Marcelo Henrique dos Santos e Márcia Cristina Teixeira Ribeiro Vidigal.

Nos últimos anos, o mercado de café tem vivenciado um notável crescimento, impulsionado pela sua expansão e produção em escala global. A América do Sul, em particular, se destaca como uma das principais regiões produtoras de café, liderada pelo Brasil, e também de maior exportador dessa commodity agrícola. Além disso, é relevante salientar que o café é uma das bebidas mais amplamente consumidas em todo o mundo, atraindo um público de consumidores cada vez mais exigente em relação a qualidade do produto. Um elemento essencial no processo de transformação do grão de café verde em uma xícara de café aromática e saborosa é a etapa de torrefação. Essa operação desempenha um papel fundamental na criação dos sabores e aromas distintivos encontrados na bebida final. Neste contexto, o propósito deste estudo foi investigar a complexidade da torrefação, conduzindo uma análise minuciosa das alterações físico-químicas e sensoriais que ocorrem durante essa etapa do processamento do café. Para tal finalidade, foram empregados seis perfis de torrefação diferentes, onde a temperatura e o tempo de torra foram cuidadosamente definidos. Os resultados desvendaram informações intrigantes. Verificou-se que os níveis mais elevados de fenólicos totais, compostos dotados de propriedades antioxidantes benéficas para a saúde, foram identificados em cafés submetidos a temperaturas específicas, como 135 °C/20,20 min e 210 °C/9,02 min. Essas descobertas não apenas fornecem uma perspectiva valiosa sobre o perfil nutricional do café torrado, mas também enfatizam a influência dos diferentes perfis de torrefação sobre essas características. De forma surpreendente, o *C. canephora*, reconhecido por seu caráter mais robusto e encorpado, apresentou uma atividade antioxidante superior em comparação ao *C. arabica* em muitos dos perfis de torrefação avaliados. Essa constatação pode redefinir a visão tradicional de que o *C. arabica* sempre supera o *C. canephora* em termos de qualidade. Os resultados mostraram que os perfis de torrefação, bem como a espécie modificaram fortemente todos os parâmetros físico-químicos investigados, principalmente as concentrações de açúcares, ácidos orgânicos e melanoidinas. O ácido succínico foi o composto orgânico com as concentrações mais elevadas, com a concentração mais alta observada em *C. canephora* a 210 °C/11,01 min (224,24 mg/g), com as concentrações mais elevadas de ácidos orgânicos encontradas nesse

mesmo perfil de torrefação e espécie (430,39 mg/g). A frutose foi o açúcar com a concentração mais alta, particularmente na torra a 210 °C/11,01 min, que apresentou 17,14 mg/g. O maior teor de melanoidina também foi encontrado nesse mesmo perfil de torrefação e espécie. A avaliação sensorial, conduzida tanto por especialistas quanto por consumidores, evidenciou diferenças notáveis nas propriedades de sabor, aroma e qualidade global entre as variedades de café e os diversos perfis de torrefação, sendo o *C. arabica* mais bem avaliado em relação ao *C. canephora*, com melhores notas nos perfis de torrefação a 135 °C/20,20 min e 230 °C/17,43 min. Essas conclusões oferecem uma compreensão mais profunda das nuances presentes no processo de torrefação e seu impacto na experiência do café para os apreciadores dessa bebida. Portanto, à medida que adentramos mais profundamente no mercado cafeeiro, evidencia-se que a torrefação representa uma operação que não apenas transforma os grãos, mas também influencia o sabor, o valor nutricional e a percepção do consumidor.

Palavras-chave: *Coffea arabica L. Coffea canephora*. Torrefação. Composição química. Qualidade do café.

SUMMARY

1. INTRODUCTION

Global coffee consumption has experienced a remarkable increase in recent years, establishing itself as one of the most widely enjoyed beverages worldwide (Acquaticci et al., 2023; Klaidaeng et al., 2023). In the realm of caffeinated preferences, the predominance of the *Coffea arabica* variety stands out, recognized for imparting superior quality characteristics to the beverage. Coffee made from *C. arabica* beans is appreciated for its smooth flavor and refined sensory attributes, in sharp contrast to the *Coffea canephora* variety. However, this gustatory excellence often translates into a higher price tag in the market (Chindapam et al., 2019; Hall et al., 2022; Poisson et al., 2017). Furthermore, the world of coffee exhibits a wealth of nuances that encompass a diversity of types, influenced by variety selection, processing method, degree of bean roasting, brewing techniques, and even the addition of complementary ingredients (Mehaya & Mohammad, 2020; Pereira et al., 2021; Poltronieri & Rossi, 2016; Worku et al., 2023).

Roasting and other thermal procedures represent essential steps in improving the digestibility and palatability of food products while enhancing the bioavailability of constituents through physicochemical and structural modifications in the food matrix (Baggenstoss et al., 2008; Cortés-Macías et al., 2023; Sruthi et al., 2021). It is worth noting that the degree of roasting plays a fundamental role in defining coffee characteristics, such as antioxidant activity and phenolic compound content (Freitas et al., 2023). However, the influence of roasting on coffee's bioactive compounds remains a topic of ongoing debate. Some research suggests that high roasting temperatures can result in the depletion of phenolic compounds, leading to a reduction in the beverage's antioxidant activity. In contrast, milder roasting tends to preserve antioxidant activity because certain phenolic compounds are heat-resistant, and new non-phenolic compounds are generated during the roasting process (Freitas et al., 2023; Mehaya & Mohammad, 2020; Van der Werf et al., 2014; Wu et al., 2022).

The intrinsic bioactivity of coffee is closely related to phenolic compounds, notably chlorogenic acids, which are more abundant in unroasted coffee beans (Pimpley et al., 2020). However, most coffee preparations involve beans that have undergone the roasting process, significantly altering coffee's bioactivity by reducing phenolic compounds and generating Maillard reaction products (Alongi & Anese, 2018; Alongi et al., 2019; Alongi et al., 2021; Anese et al., 2023). In addition to chlorogenic acids, coffee also contains caffeine, known for its stimulating effect. Epidemiological studies suggest that coffee consumption may be

correlated with a reduced risk of cancer (Silva et al., 2022) and type 2 diabetes (Akash et al., 2014; Shahinfar et al., 2021), with these beneficial properties largely attributed to chlorogenic acids (CGAs), caffeine, and trigonelline (Li et al., 2023).

The roasting phase, essential in coffee processing, directly influences the quality characteristics of the product, including aroma, flavor, and color. During roasting, heat triggers the Maillard reaction, caramelization, and oxidation of certain polyphenolic compounds, contributing to the distinctive traits of coffee beans (Aguiar et al., 2016; Sruthi et al., 2021). However, this process can also lead to the degradation of proteins, polysaccharides, caffeine, trigonelline, and CGAs, as well as the generation of the compound 5-hydroxymethylfurfural (5-HMF), a result of the thermal decomposition of sugars via the Maillard reaction or caramelization (Chaichi et al., 2015; Mehaya & Mohammad, 2020; Freitas et al., 2023; Lopes et al., 2020).

Specifically, roasting, a dry heating process, is a crucial step in coffee production, with variations in roasting conditions, such as temperatures typically ranging from 160-240°C and exposure time to heat of 8-25 minutes, resulting in different flavor profiles, ranging from light to medium and dark roasts (Park et al., 2023; Sruthi et al., 2021). The choice of roasting profile represents a critical decision in achieving the desired flavor and is an essential element in defining the quality of the final product.

The objective of this study was to assess various parameters, including colorimetric indices, chemical composition, antioxidant activity, and total phenolic content in Robusta and Arabica coffees. This study addressed variations in time and temperature during the post-harvest roasting process. Additionally, an attempt was made to establish references for the concentration of sugars and organic acids present. For a more comprehensive approach, this study also investigated the possibility of qualitatively predicting different roasting profiles based on infrared spectra, as well as assessed the sensory quality of the coffees through tastings conducted by trained tasters and consumers.

Artigo 1*

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Coffee: A comprehensive overview of origin, market, and the quality process

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Graphical abstract

Abstract

Context

Coffee is a culture of great economic importance on the global stage. In the international market, the term "specialty coffee" is used to describe a beverage of exceptional quality, distinguished by its unique flavors and characteristics. This superior quality becomes a key factor in accessing markets where consumers are willing to pay an added value for the product. Numerous factors, from cultivation to consumer preferences, play an essential role in determining the final quality of coffee. Obtaining a comprehensive understanding of these factors is essential for effectively managing coffee processing and beneficiation procedures

Scope and approach

This comprehensive review aims to explore various aspects of the coffee post-harvest process, encompassing its production, consumption, and the factors that influence its quality. Special emphasis will be given to the entire quality process involving coffee, with a discussion based on the available scientific literature on the subject.

Key findings and conclusions

The quality of coffee beans is influenced by factors such as harvesting methods, geographical location, climate, and genetic characteristics. Post-harvest processing, including roasting, significantly impacts the chemical composition and sensory attributes of coffee. Chemically, coffee is a complex mixture containing caffeine, chlorogenic acids, sugars, lipids, amino acids, minerals, and vitamins. Understanding these interconnected elements is essential for optimizing coffee production while appreciating its unique characteristics. The review brought innovative information regarding the influence of factors such as harvesting, genetics, and roasting on coffee quality, emphasizing the complexity of its production. Furthermore, it addressed the rich chemical composition of coffee and its impact on sensory attributes and health benefits

Keywords: Coffee Quality; Cultivation; Processing Methods; Roasting; Coffee Chemistry.

1. Introduction

In recent years, the coffee market has gained significant prominence due to its development and worldwide production. South America stands out as one of the major coffee-producing regions, with Brazil leading the production and export of this agricultural commodity. In 2020, the global coffee production was estimated at 175,347 million 60 kg bags, while global consumption reached 167,670 million bags (ICO, 2022). Brazil, as the leader in this market, produced around 69 million 60kg bags in the same year, followed by countries like Vietnam, Colombia, and Indonesia, which also contribute significantly to the coffee market (ICO, 2022). Minas Gerais, Espírito Santo, São Paulo, and Bahia are the Brazilian states that stood out the most in coffee production in 2020 (CONAB, 2022).

Furthermore, the price of coffee beans reached its highest value in a decade, further boosting the Brazilian economy and that of other coffee-producing countries (ICO, 2022). Coffee consumption has also been on the rise over time, with estimates pointing to approximately 166,340 million 60 kg bags consumed worldwide in 2022 (BCA, 2021; ICO, 2022).

This traditional and widely consumed beverage plays a crucial role in the global and Brazilian economy. With the growing demand for high-quality products, the coffee market has expanded to meet consumer preferences. Currently, there are various coffee varieties available, such as freshly ground coffee, instant coffee, instant coffee blends, fresh ground coffee pods, and standard decaffeinated instant coffee (Gosalvitr et al., 2023).

The quality of coffee is influenced by various factors, from agriculture and processing methods to roasting and grinding of the beans, as well as beverage preparation methods and consumer preferences. Grain maturation, harvesting method, geographical location, regional climate, cultivation method, and grain genetics are some of the relevant factors for coffee quality (Pereira et al., 2021; Poltronieri & Rossi, 2016; Worku et al., 2023). The altitude of coffee plantations also plays an important role in the quality of the final product, although there are different perspectives on this factor. Additionally, the region's climate, including temperatures and regular rainfall, can affect coffee production and quality by influencing the development of pests and diseases (Magrach & Ghazoul, 2015; Mukherjee et al., 2012). Grain genetics, represented by species and varieties, is also a determining factor in coffee quality. *Coffea arabica* is the most cultivated and consumed species, known for its fine and exquisite aromas, while *Coffea canephora* has unique characteristics such as higher caffeine content and

distinct flavors (Chindapam et al., 2019; Dong et al., 2015; Hall et al., 2022; Poisson et al., 2017).

The harvesting process and the type of processing also have a direct impact on the final quality of coffee. Dry, wet, or semi-dry processing affects the chemical composition of the beans and, consequently, the sensory properties of the beverage (Cassimiro et al., 2022; Ferreira et al., 2023; Pereira et al., 2015; Ribeiro et al., 2016; Worku et al., 2018).

The roasting process is essential for developing the characteristic flavors and aromas of coffee. Roasting occurs in stages, with Maillard reactions and caramelization being responsible for creating the complex flavors found in the final beverage. The choice of roast level also influences the chemistry and characteristics of the coffee (Freitas et al., 2023; Lee et al., 2015; Sruthi et al., 2021; Worku et al., 2018). Understanding the entire coffee production chain, as well as its scientific aspects, is essential for producers, roasters, and coffee enthusiasts aiming to produce high-quality products appreciated by consumers.

The unique aspect of this review lies in its comprehensive and interdisciplinary approach to coffee production, covering not only traditional aspects such as agriculture and processing but also the scientific factors that influence coffee quality, from grain genetics to chemical reactions during roasting. Additionally, it highlights the impact of coffee on the global and Brazilian economies, including recent data on production and consumption.

2. Scope and approach of the review

The topic addressed is the origin and market, quality and processing, roasting, and chemistry of coffee. The proposal is to provide a scientific approach to these topics, based on studies in the field. The discussion begins with the exploration of the historical and geographical origins of coffee, as well as its relevance in the global market. Economic factors such as production, export, consumption, and market trends are considered, as well as socio-economic and environmental aspects that affect the coffee industry.

Next, the issue of coffee quality and processing is addressed. Quality criteria such as sensory attributes, chemical composition, and physical characteristics of coffee are examined. In addition, processing techniques such as wet processing, dry processing, and semi-dry processing are discussed, along with their influence on the quality of the final product.

The main focus is on coffee roasting and its chemistry. The roasting process is described, including the stages of drying, Maillard reactions, caramelization, and pyrolysis, with an

emphasis on temperature evolution. The complex chemistry involved in roasting is explored, considering the degradation and formation of chemical compounds. The effects of roasting on sensory quality and the antioxidant and anti-inflammatory properties of coffee are also reported.

This scientific approach aims to present information based on recent studies to provide an in-depth understanding of the origin, market, quality, processing, roasting, and chemistry of coffee. The goal is to promote knowledge of this widely consumed and appreciated beverage worldwide.

3. Coffee origin and market

Coffee is a perennial shrub plant belonging to the *Rubiaceae* family, which produces fruits that usually contain two seeds. Coffee seeds, after processing and beneficiation, are commonly consumed in the form of an infusion. Reports indicate that the cultivation of the plant was first carried out by the Arabs, hence the name "*C. arabica*," which is the scientific name of the most important coffee species. However, it is credited to the Arabs of Yemen for spreading the coffee culture to the rest of the world (Pimenta, 2003). They held a monopoly on coffee for a long time and kept the secret of its cultivation and processing. Coffee was transported along the Coffee Route, a trade network that extended from the Middle East to North Africa, India, and eventually to Europe. Coffee reached Europe in the late 17th century, initially in the city of Venice, Italy, and then spread to other parts of the continent. Coffeehouses became popular venues for intellectual and social gatherings. Over time, coffee spread to other tropical regions worldwide, such as Central America, Africa, and Asia. Each region developed its own varieties and cultivation methods, resulting in the diversity of coffee flavors we know today. Coffee's arrival in Brazil occurred around 1727 when it was brought by Father Francisco Mello Palheta from French Guiana (Ukers, 1922). Initially, coffee plantations in Brazil were established in the state of Pará and later in Maranhão. Years later, the cultivation of this crop spread to other states such as Minas Gerais, Rio de Janeiro, Bahia, São Paulo, and Paraná (Ferrão, 2004; Matiello et al., 2008). Coffee adapted well to the Brazilian tropical climate and quickly gained importance in the national economy.

In recent years, the coffee market has gained significant prominence due to its development and production. South America stands out in coffee production for the year/harvest, with a total production of 88.2 million 60 kg bags in 2020. In 2020, the estimated global coffee production was 175,347 million 60 kg bags, with consumption reaching 167,670

million 60 kg bags. Brazil excelled in the production and export of this agricultural commodity, producing approximately 69 million 60 kg bags (year/harvest). Following Brazil in production rankings, notable countries include Vietnam (29 million 60 kg bags), Colombia (14.3 million 60 kg bags), and Indonesia (12.1 million 60 kg bags). The respective production and global consumption figures are presented in Figure 1. The lowest year/harvest production in 2020 was prominent in the African continent, with an estimated total production of 18.5 million 60 kg bags (ICO, 2022).

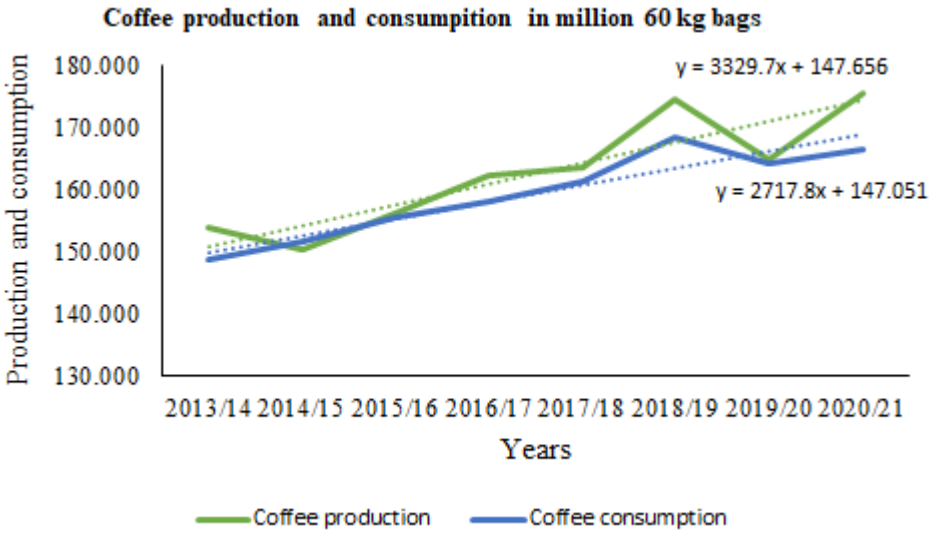


Figure 1. Estimation of coffee production and consumption in millions of 60 kg bags (ICO, 2022).

The Brazilian states that stood out in production in 2020 were Minas Gerais (34.6 million 60 kg bags), Espírito Santo (13.9 million 60 kg bags), São Paulo (6.1 million 60 kg bags), and Bahia (3.9 million 60 kg bags) (CONAB, 2022). The price of coffee beans reached its highest value in 10 years, around 204.29 cents per pound (ICO, 2022).In the last 50 years, up to 2015, coffee consumption increased by approximately 1.9%. (Lee et al., 2015). Global consumption in 2022 was estimated at 166.34 million 60 kg bags. The United States was listed as the largest consumer of coffee, with 26.1 million 60 kg bags, followed by Brazil with 21.9 million 60 kg bags. In terms of daily cup consumption, approximately two billion cups are consumed worldwide, totaling a relatively high annual consumption volume (about 10 million tons of coffee) (BCA, 2021; ICO, 2022).

Being a traditional beverage consumed worldwide, coffee plays a significant role in the Brazilian economy, as well as in other countries (Bermejo et al., 2013; Debatiani et al., 2018).

Due to high production and daily consumption, the coffee market has been growing in parallel with consumer preferences for high-quality products. Currently, coffee is produced and marketed under a variety of production structures, meaning modifications in processes (Ufer et al., 2019).

Specifically, it is widely known that domestic consumption of this product has been increasing over the years due to greater awareness of coffee quality and even due to the restructuring efforts by regulatory bodies (SCA - Special Coffee Association, COB - Brazilian Official Classification; ABIC - Brazilian Coffee Industry Association, and other international organizations) concerning product quality. Different coffee-based products are available in the market, with the top five relevant to consumption being fresh ground coffee, instant coffee, instant coffee blends, fresh ground coffee capsules, and standard decaffeinated instant coffee (Gosalvitr et al., 2023). Coffee production is on the rise, with a growing focus on specialty and sustainable coffee. The trend is for single-origin, high-quality coffee to be more appreciated in the future, along with increased consumption in emerging countries and the use of technology in coffee production and preparation.

4. Principles of coffee quality and processing

The quality of coffee is characterized by the combination of various factors. Among the relevant factors in the complexity of the beverage are the processes related to agriculture, processing method, roasting, and grinding of the beans, the methods used in preparing the beverage, as well as consumer preferences (Fig. 2).

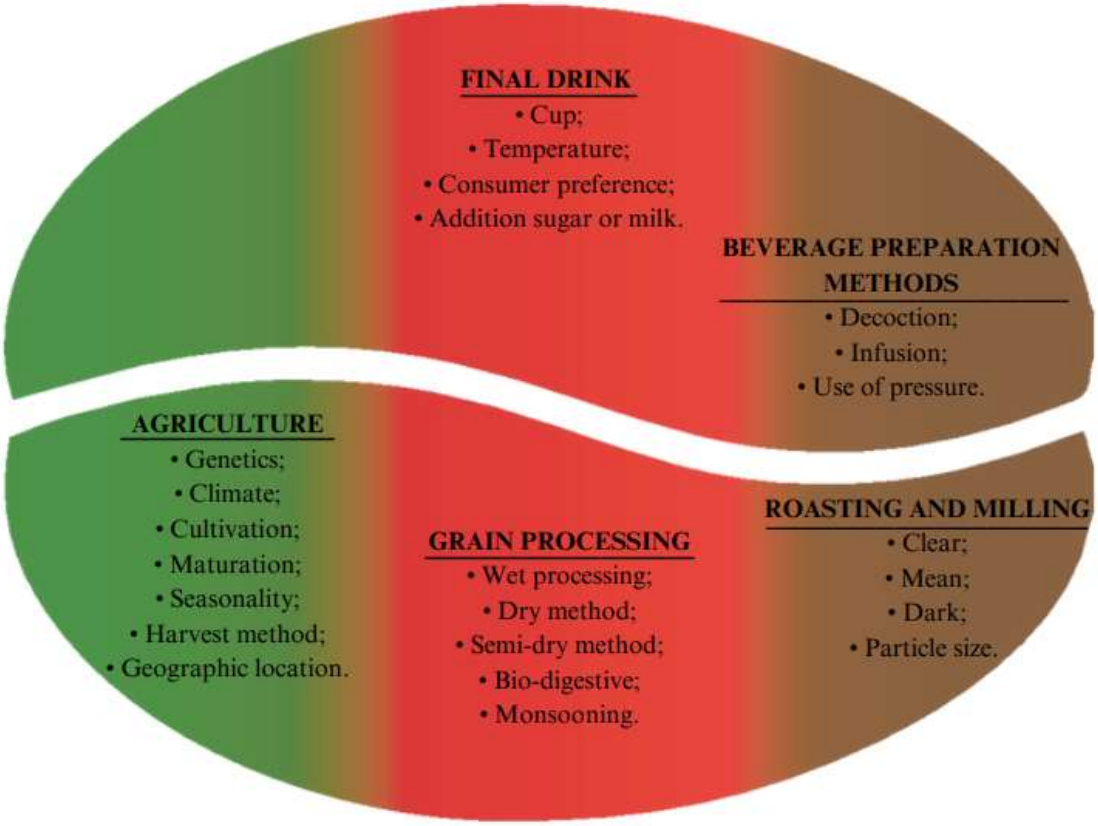


Figure 2. Principles of cultivation, processing, and preparation methods that influence the final quality of coffee beverage.

Specifically, among the agricultural factors related to beverage quality, the ripeness of coffee beans, the harvesting method, seasonality, geographical location, climate, cultivation method, and genetic makeup of the beans stand out (Pereira et al., 2021; Poltronieri & Rossi, 2016; Worku et al., 2023).

The composition of coffee beans is highly complex and variable, which is why it is necessary to harvest the beans at an early stage of ripening to ensure uniformity in terms of chemical and sensory characteristics (Ferreira et al., 2023; Poltronieri & Rossi, 2016; Vale et al., 2019). Another intriguing factor that has been the subject of various studies is the location of coffee plantations. In particular, the altitude of cultivation has been used as a reference for the potential quality of the final beverage (Pereira et al., 2021). It is reported that the altitude of coffee plantations has a direct impact on the beverage, related to factors like temperature, humidity, and sunlight exposure. However, studies on the effect of altitude on coffee quality have produced conflicting results. According to some researchers, higher altitudes yield higher-quality coffee. Ribeiro et al. (2016), in a study using *C. arabica* variety Bourbon Amarelo, compared plantations at 1000 and 1200 meters, and coffee cultivated at 1200 meters was characterized as higher quality, attributed to higher concentrations of trigonelline and

chlorogenic acids (3-CQA) in the coffee. On the other hand, Muschler et al. (2001) claimed that growing coffee at lower altitudes (700 meters above sea level) with shading over most of the plantation can favor the final quality of the beverage. Additionally, the study evaluated *C. arabica* varieties Caturra and Catimor 5175 and found that shading leads to uniform ripening of coffee beans, resulting in higher quality. It is believed that geographical origin plays a significant role in the quality and chemical composition of coffee beans (Worku et al., 2023).

Intrinsically, the region's climate is another influential characteristic in coffee production and quality. It is reported that high temperatures and irregular rainfall indirectly affect coffee production and, consequently, the final beverage because these environmental factors can promote the spread and increase of pests and diseases in coffee plants. These factors can disrupt the flowering process and bean development, resulting in lower-quality coffee and reduced productivity (Magrach & Ghazoul, 2015; Mukherjee et al., 2012). As reported to Ayal et al. (2023), coffee growing regions experience significant climatic variability throughout the year, and it is likely that plantations may be affected in the future, leading to decreased production of this commodity and economic losses.

Another relevant factor in the production of specialty coffees is the use of shading systems in conjunction with other plant species. This consortium provides lower temperature variations during the day and night, significantly inhibits weed growth, and reduces soil erosion (Hairiah et al., 2006; Meylan et al., 2017). The shading system often integrates with the soil, contributing to greater nutrient availability, as well as favoring biodiversity. However, it is believed that the yield in bags is lower compared to coffee plants with more direct sunlight exposure (Meylan et al., 2017; Steiman et al., 2011).

Directly related to climate, we have the genetics of coffee beans (the species or variety) (Pereira et al., 2021). Among the most popular and appreciated species are *C. arabica* and *C. canephora* (Fig. 3), both having distinct characteristics regarding quality due to their chemical composition (Chindapam et al., 2019; Febrianto & Zhu, 2023). *C. arabica* is the most cultivated species, with 44 chromosomes, and is known for its fine and exquisite aromas, characterized as mild and pleasant coffee, making it the most consumed and preferred by consumers. Additionally, *C. arabica* represents 70% of the world's production, and due to its stable yields, some studies indicate that this species requires altitudes of at least 700 meters for optimal cultivation conditions (Batista et al., 2016; Dong et al., 2015). *C. arabica* is characterized by higher concentrations of carbohydrates (50-60%), lipids (< 2%) and proteins (10-15%), and lower caffeine content between 0.9% and 1.3% (Poisson et al., 2017). *C. canephora* has 22 chromosomes and is considered lower quality compared to *C. arabica* due to its higher caffeine

content (1.6 to 2.5%) and soluble solids (1.2-1.5%). *C. canephora* also has a unique and distinctive flavor due to its bitterness and astringency, as well as being characterized by low acidity, making it suitable for instant coffee preparation (Chindapam et al., 2019; Dong et al., 2015; Hall et al., 2022; Poisson et al., 2017). The cultivation conditions for this species are favored at lower altitudes (Girma et al., 2020; Park et al., 2023).

Figure 3. Representation of the shape of *Coffea arabica* and *Coffea canephora* species.

The genetics of the fruit is closely linked to cultivars and species, thereby influencing the final quality of the beverage (Hall et al., 2022; Pereira et al., 2021; Scholz et al., 2018). The most cultivated varieties in Brazil are Catuaí and Mundo Novo, which originated from a natural hybridization between the Red Bourbon and Sumatra cultivars. In turn, the hybridization between Mundo Novo and Yellow Caturra resulted in the Catuaí Amarelo and Catuaí Vermelho cultivars. Intending to optimize the vegetative vigor of the Catuaí Amarelo cultivar, the backcrossing of this variety with Mundo Novo resulted in the Rubi, Ouro Amarelo, Travessia, Ouro Verde, Topázio, and Ouro Bronze cultivars. Each variety has a specific relationship with the quality of the beans and consequently the final beverage (Kitzberger et al., 2013).

Another factor affecting the final quality of coffee is the harvesting process, and as mentioned earlier, this process should be carried out at the ideal stage of ripeness (the cherries). Harvesting can be done in three different ways: manual, semi-mechanized, and mechanized (Poltronieri & Rossi, 2016; Vale et al., 2019). In the most common method (manual), it is reported that beans exhibit higher quality compared to semi-mechanized and mechanized methods, but it comes with the disadvantage of higher labor costs and a more time-consuming harvesting process (Bertone et al., 2016; Ramos et al., 2017; Veloso et al., 2020).

After the pre-harvest process, coffee beans undergo processing. Coffee can be processed in three different ways: dry, semi-dry, and wet processing (Cortés-Macías et al., 2023; Pereira

et al., 2019; Saloko et al., 2019). The advantages and disadvantages of the type of processing used are listed in Table 1 (Cassimiro et al., 2022; Cassimiro et al., 2023; Ferreira et al., 2023; Matiello & Santinato, 2010; Pereira et al., 2015; Pereira et al., 2021; Ribeiro et al., 2016; Widodo et al., 2023; Worku et al., 2018).

In the dry processing (Fig. 4), fruits at different stages of ripeness are preferably separated, and then they are placed on cement platforms, where they remain for approximately 3 weeks or until the moisture content reaches 12%. This is why coffee from this process is called "platform" coffee. If faster drying is needed, the beans can be subjected to mechanical dryers after exposure to the sun. This type of processing is commonly used for most *C. arabica* in Brazil, Yemen, and Ethiopia, and generally for nearly all *C. canephora* (Pereira et al., 2019; Poltronieri & Rossi, 2016). Dry processing can result in coffees with more complex and fruity flavors due to drying the beans with the skin and pulp intact. However, the beverage quality can be more variable due to exposure to the environment and risks of unwanted fermentation. In terms of cost-effectiveness, dry processing is generally more economical as it requires fewer processing steps and less water. This can reduce production costs and make coffee more affordable in terms of price.

Table 1. Comparative analysis of coffee processing methods: Positive and negative Aspects.

Processing methods	Positive points	Negative points
Dry processing	• The dry process (natural) is typically associated with certain characteristics, such as low acidity, exotic flavors, and a richer body profile. On the other hand, full-washed processing tends to exhibit cleaner, lighter, and slightly fruity attributes; • The resulting coffee tends to have a lighter and softer body with a higher level of acidity; • In these processing systems, high levels of glucose and fructose are present, which result from the low sugar metabolism occurring in more aerobic conditions; • It is an environmentally-friendly practice with minimal implementation and operating costs.	• This processing method carries significant risks to the quality as the coffee beans are dried at varying stages of maturation and different water contents, which can result in fruits with various abnormalities; • The harvest peak in some regions, such as in many Latin American countries, coincides with the rainy season, making it challenging to dry the coffee, thus impacting the final quality of the product; • Due to their need for large areas, these methods tend to result in low drying rates, especially when on-farm drying capacity is limited.
Semi-dry processing	• These processing systems offer the advantage of significantly reducing both the yard area needed and the drying time required; • Fermentation tanks are not necessary for this process; • Microbial growth can be facilitated by the nutrient-rich content present in coffee pulp and wastewater from fruit demucilage, which are the primary residues generated during coffee processing. Consequently, these residues hold the potential for utilization in various bioprocesses.	• Eliminating the bark and mucilage is essential as they provide suitable environments for the growth of microorganisms. By removing them, the occurrence of harmful fermentations that could negatively impact the final product's quality can be prevented; • The primary processes, including cleaning, float separation, and pulping, are fundamental steps in coffee processing and can strongly influence the sensory qualities of final coffee products.

Wet processing	• This technique finds its primary application in Arabica coffee processing, where coffee cherries are harvested and then mechanically stripped of their outer peel and pulp. As a result, the beans retain the mucilage firmly attached to them; • One of the key benefits of this method is its cost-effectiveness due to the minimal infrastructure investment required. It entails the use of a tank, typically constructed from cement, which keeps the expenses relatively low; • During this process, fermentation takes place concurrently with the germination process, leading to a notable increase in the abundance of amino acids; • The submerged process offers the advantage of facilitating homogenization and accelerating mucilage removal, as most of the components involved are soluble; • By regulating the aeration rate, it becomes feasible to control both the aerobic and anaerobic phases' duration during the process; • The submerged process produces coffee with differentiated composition and sensory characteristics when compared to dry and semi-dry processed coffee.	• Employing the submerged process results in elevated water activity while gradually reducing the availability of oxygen; • Soaking coffee in water for 36-40 hours as part of the wet processing method leads to a reduction in caffeine content. This decrease is primarily attributed to conventional and enzymatic processing, which helps minimize the caffeine content; • More expensive method when contrasted with wet processing, necessitating the utilization of water; • This processing method is more suitable for countries with lower temperatures, as the coffee covered in mucilage needs to dry quickly to prevent fermentation. In areas with high humidity, the beans may be affected due to increased fungal development, making it a more regionally dependent approach.

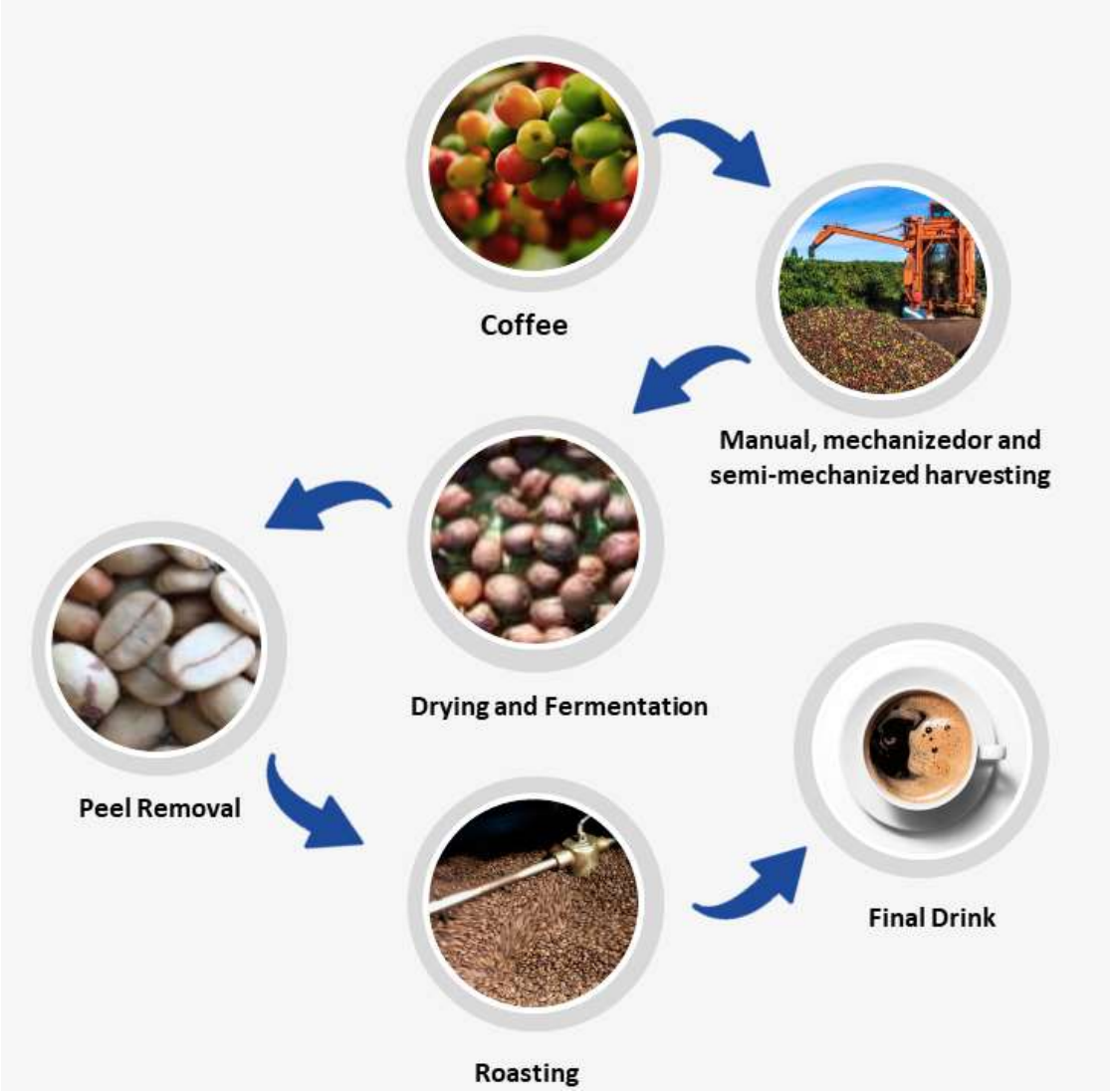


Figure 4. Schematic representation of coffee processing by the dry method.

In the wet processing of coffee (Fig. 5), beans go through a washing process, and floating beans are selected, which will be processed separately; in this process, beans are peeled, depulped, or demucilaged from the fruit (Cortés-Macías et al., 2023; Febrianto & Zhu, 2023; Ferreira et al., 2023). Wet processing of coffee originated out of practical necessity rather than as an alternative to modifying coffee flavor. As *C. arabica*, native to subtropical climates, began to be grown in tropical areas, intense fermentative processes were observed in cherry fruits immediately after harvesting, which had an impact on the final product's quality (Ferreira et al., 2023; Poltronieri & Rossi, 2016). To prevent this type of fermentation, the removal of the mesocarp, rich in sugars, began to be performed. Thus, fermentation in this process aims to facilitate the removal of the mucilage layer from the seed (Mahingsapun et al., 2022; Pereira et al., 2015). Wet processing is generally considered the method that provides a more consistent

and typically more refined beverage quality. This is because the coffee's skin and pulp are removed before drying, resulting in a cleaner and brighter drink. The method allows for better control of fermentation and coffee flavor.

Figure 5. Schematic representation of coffee processing by the wet method.

In the semi-dry processing (or pulped natural) (Fig. 6), for the separation of coffee beans from the fruit, they go through the pulping process, where some or most of the mucilage is mechanically removed, and it is considered the least common form of processing (Cortés-Macías et al., 2023; Poltronieri & Rossi, 2016). The beans are dried in the open air, which can take from 10 to 15 days, depending on climatic conditions, and the process is considered complete when the bean moisture content is between 10 and 12%. The amount of mucilage removed depends on the characteristics of the machine used (Ferreira et al., 2023; Widodo et al., 2023).

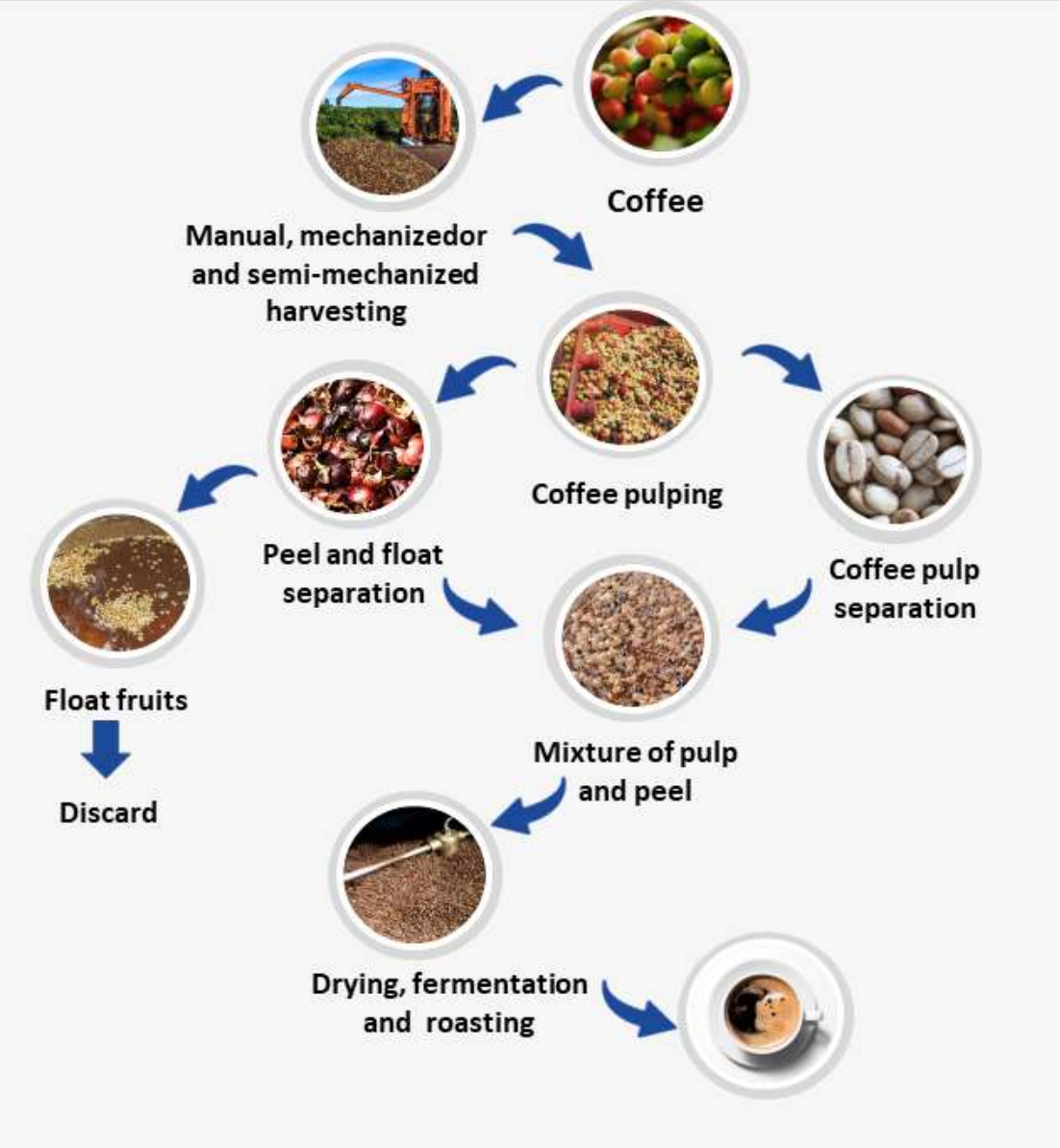


Figure 6. Schematic representation of coffee processing by the semi-dry method.

Coffee produced through the digestive process of animals is known for its unique characteristics in the beverage, resulting from spontaneous fermentation that occurs within the animal's digestive system (Fig. 7). This type of coffee is recognized by the ingestion of ripe coffee cherries by two animals: the Jacu (*Penelope superciliaris*), a bird, and the Civet (*Paradoxurus hermaphroditus*), a mammal (Raveendran & Murthy, 2022). The Jacu produces the well-known "Jacu Bird Coffee," originating from Brazil, particularly the Atlantic rainforest, and is found in greater numbers on farms in the state of Espírito Santo, Brazil. "Kopi Luwak" coffee is produced by the Civet, a mammal native to Africa and Asia with nocturnal habits and sharp vision and sense of smell to locate and subsequently ingest fully ripe coffee cherries (cherries). After fermentation with enzymatic action in their digestive systems, the beans are expelled along with feces, cleaned, and processed for consumption. Both animals result in high-

quality coffee with higher prices in the market (Febrianto & Zhu, 2023; Febrina et al., 2021; Jumhawan et al., 2016; Marcone, 2004; Raveendran & Murthy, 2022).

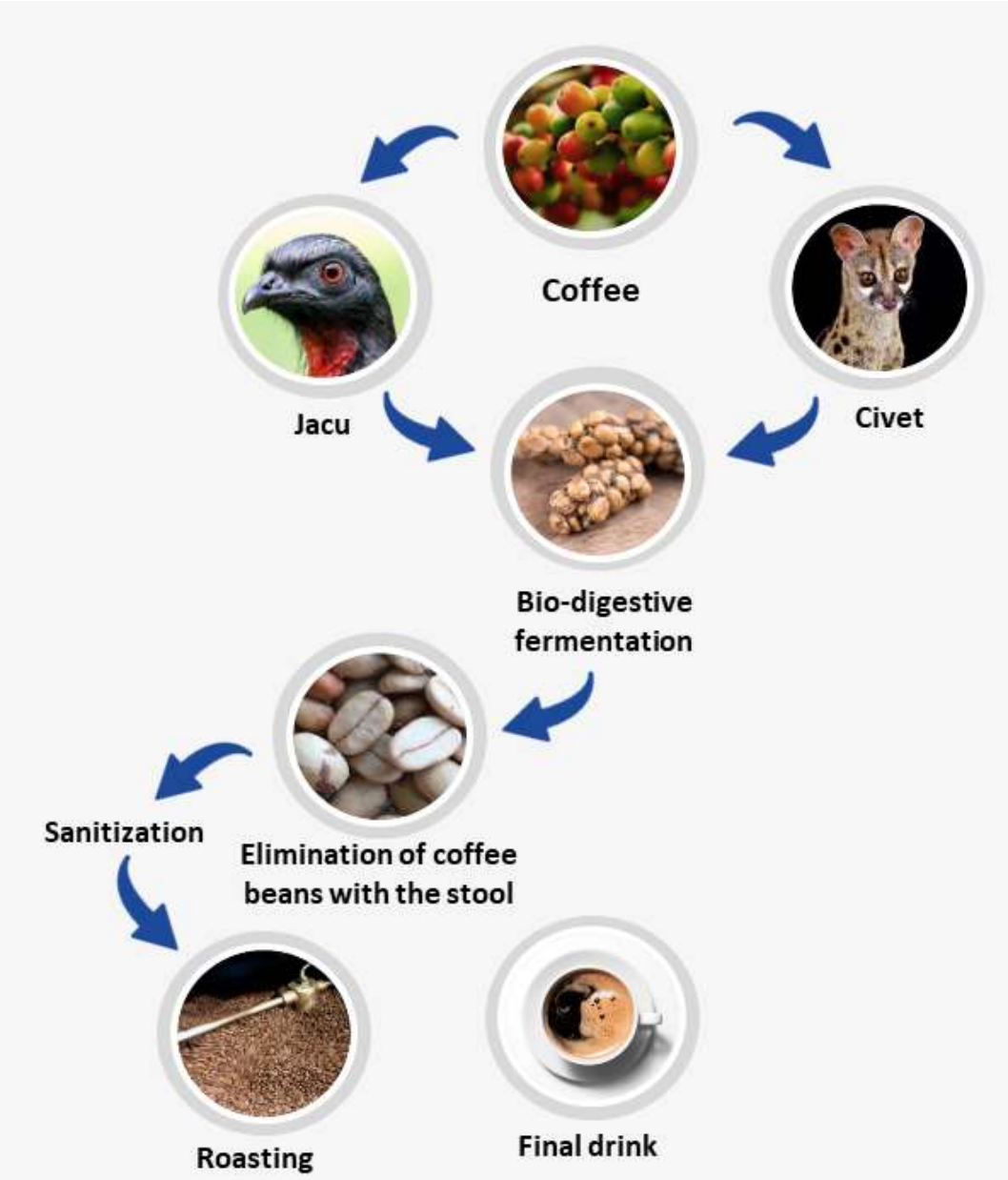


Figure 7. Schematic representation of coffee processing through the animal bio-digestive system.

The processing method employed for coffee defines changes in the components of the bean, which are closely related to the final quality of the beverage. After harvesting and processing, the obtained beans are roasted, which imparts flavor, aroma, and the typical color of coffee (Poltronieri & Rossi, 2016).

5. Roasting process

Roasting coffee is an essential process in creating the unique flavors and aromas found in the final beverage. This process can be divided into several stages that occur sequentially and contribute to the transformation of green coffee beans into ready-to-consume roasted beans (Baggenstoss et al., 2008; Cortés-Macías et al., 2023; Sruthi et al., 2021).

Initially, coffee beans undergo meticulous preparation, involving selection, cleaning, and classification based on criteria such as size and quality. Subsequently, the beans are subjected to drying to reduce the moisture content, with 12% moisture content being an essential parameter. This process is crucial to ensure even roasting and to prevent issues such as fungal development (Poltronieri & Rossi, 2016; Sruthi et al., 2021).

After drying, the beans are placed in the roaster, where they are exposed to high temperatures, typically ranging from 160 °C to 240 °C. In the industrial-scale coffee roasting sector, it's common to find fluidized bed or semi-fluidized bed roasters widely adopted. In conventional fluidized bed roasters, coffee beans are suspended in a bed of hot air, allowing for even heat distribution. This is essential to ensure a consistent roast and prevent beans from burning. The fluidized bed is maintained through a combination of airflow and mechanical movement. In semi-fluidized bed roasters, there are intermediate features between fluidized bed roasters and traditional drum roasters. In this method, coffee beans are partially suspended in the hot air, while a portion of them rests on a fixed bed. This enables greater control over the roasting process and is suitable for producing specific roast profiles. These roasters operate using hot air flow and also utilize a heated surface (Sruthi et al., 2021). A notable improvement in this technology is the ability to monitor the temperature of coffee beans during the roasting process, as well as the possibility to create temperature gradients. These innovations allow for the creation of customized roast profiles tailored to the specific characteristics of different bean types, ensuring a pleasing final taste (Freitas et al., 2023; Sruthi et al., 2021; Tocia et al., 2020).

During roasting, a series of chemical reactions occur, causing physical and chemical changes in the beans (Freitas et al., 2023; Poltronieri & Rossi, 2016). The first indication of this process is the first crack, which occurs when the beans start to expand, releasing steam and carbon dioxide. This event is accompanied by a popping sound and the release of light smoke. The first crack marks the beginning of the transition from green coffee beans to roasted (Milani et al., 2017).

As roasting progresses, the Maillard reaction and caramelization reactions take place. These reactions involve the interaction of sugars and amino acids present in the beans, resulting in the formation of compounds responsible for providing the complex flavors and aromas characteristic of coffee (Aguiar et al., 2016; Freitas et al., 2023; Strezov & Evans 2005). These

reactions are essential to develop a wide range of desirable sensory characteristics in the final beverage, ranging from fruity and floral notes to chocolate, caramel, and nutty flavors (Sruthi et al., 2021).

In some darker roasts, a second crack can occur. In this phase, less audible than the first crack, the beans continue to expand, and there is additional release of steam and carbon dioxide (Silva et al., 2023). After reaching the desired roast level, coffee beans are rapidly cooled to halt the roasting process (Grzelczyk et al., 2022). Specifically, the roasting process is a crucial step in coffee processing, and during this dry heating process, the Maillard reaction, caramelization reaction, and oxidation of phenolic compounds occur, contributing to the development of coffee's sensory properties such as aroma, flavor, and color (Aguiar et al., 2016; Freitas et al., 2023; Sruthi et al., 2021). However, it's important to note that roasting can also lead to the degradation of essential coffee components, such as proteins, polysaccharides, caffeine, trigonelline, and chlorogenic acids, as well as the formation of the compound 5-hydroxymethylfurfural (5-HMF) (Chaichi et al., 2015; Lopes et al., 2020). 5-HMF is a furanic aldehyde resulting from the thermal decomposition of sugars through the Maillard or caramelization reaction, and post-harvest methods can vary its concentration (Acquaticci et al., 2023; Chaichi et al., 2015; Cortés-Macías et al., 2023). The concentration of HMF (5-Hydroxymethylfurfural) in roasted coffee can vary widely depending on various factors, including the type of coffee, roasting method, roasting time, and storage conditions. In general, the concentration of HMF in roasted coffee can range from a few milligrams per gram (mg/g) to nearly undetectable levels. The importance of this compound in coffee is related to aspects of flavor and aroma, as an indicator of roasting quality, storage potential, and health.

Studies indicate that roasting affects the antioxidant and anti-inflammatory properties of coffee, with a direct correlation to the roast level and the compounds present in the beans after roasting (Freitas et al., 2023; Wang et al., 2022). The antioxidant compounds found in roasted coffee include chlorogenic acid, caffeine, melanoidins, ascorbic acid, ferulic acid, quinides, and catechins Roasting conditions can vary, with different roast levels (light, medium, and dark) primarily determined by temperature (160-240 °C) and roasting time variation (8-25 min), aiming to achieve the desired final product profile (Freitas et al., 2023; Nóbrega et al., 2023; Park et al., 2023; Sruthi et al., 2021; Strezov & Evans 2005). It is important to highlight that high temperatures during roasting promote significant changes in the chemical composition and physical properties of coffee (Sruthi et al., 2021). The most common temperature ranges during the roasting process vary between 160 °C and 240 °C, with roasting at 210 °C for a maximum heat exposure time of 14 minutes being more common. This range of temperatures

and roasting times can significantly influence the resulting flavor profile of the coffee. (Freitas et al., 2023; Park et al., 2023; Sruthi et al., 2021).

The coffee roasting process begins with the drying phase, in which free water is easily evaporated, and the temperature of coffee beans exceeds 100 °C. In the early stages of roasting, free amino acids and reducing sugars are rapidly consumed in the Maillard reaction, with significant degradation of sucrose also occurring. As the temperature exceeds 160 °C, caramelization becomes more prominent, resulting in the complete depletion of sucrose, which is present in 4 to 8 % of coffee beans (Aguiar et al., 2016; Strezov & Evans 2005). From the first crack of coffee beans, which occurs due to pressure generated by water and carbon dioxide inside them, pyrolysis reactions begin. This moment marks the development of the coffee's aromatic profile and corresponds to light to medium roast levels (Silva et al., 2023).

As roasting continues, the reactions intensify with increasing temperature, resulting in an increase in the specific volume of coffee and a gradual darkening of its color (Freitas et al., 2023). With the occurrence of the second crack, high-temperature roasting levels are achieved, producing dark roasted coffee (Baggenstoss et al., 2008). At this point, coffee oil migrates to the surface, creating a shiny appearance. These changes mentioned above occur when coffee beans are exposed to high temperatures in the range of 200-240 °C (Sruthi et al., 2021). The time-temperature combination in coffee roasting is determined based on the roaster's preferences and the desired flavor profile. Roasting temperature affects the intensity and speed of chemical reactions, while roasting time influences flavor complexity. The roast profile is the specific combination of temperature and time throughout the roasting process, and roasters adjust it to achieve the desired flavor. The roast curve is a graph that represents temperature changes over time. Finding the ideal combination is a critical part of roasting, balancing flavor and coffee characteristics. Figure 8 displays the various coffees and their respective levels of roasting: light, medium, and dark.

Figure 8. Coffee roasting levels: Light (**A**); medium (**B**); and dark (**C**).

6. Coffee chemistry

The chemistry of coffee is a fascinating field that involves a multitude of compounds and reactions contributing to the unique sensory characteristics of this beloved beverage enjoyed worldwide. By delving into the chemistry of coffee, it becomes possible to better understand the processes that occur from the cultivation of beans to the moment they are prepared for consumption (Hall et al., 2022).

Coffee beans are rich in chemical compounds, with caffeine being one of the most well-known and studied (Nóbrega et al., 2023). Caffeine is a natural stimulant of the central nervous system and is present in coffee in concentrations that vary depending on the type of bean, origin, and preparation method (Angeloni et al., 2019; Campbell & Young, 2017). Studies show that excessive caffeine consumption can lead to undesirable health effects such as increased heart rate, feelings of anxiety, tremors, gastrointestinal disturbances, and sleep difficulties (Angeloni et al., 2019; Bae et al., 2014). Moderate consumption of caffeine in coffee can bring benefits such as increased attention, improved physical performance, provides antioxidants, potential reduction in the risk of chronic diseases, positive impact on mood, temporary metabolism boost, and relief from headaches in some people. For this reason, some consumers prefer to opt for decaffeinated instant coffee to avoid or limit the intake of this stimulating substance (Brasil, 2005; Nóbrega et al., 2023). In addition to caffeine, coffee contains a wide range of other compounds, including chlorogenic acids, trigonelline, sugars, lipids, amino acids, minerals, and vitamins (Folwarczna et al., 2016; Freitas et al., 2023; Lopes et al., 2020; Munyendo et al., 2021; Viencz et al., 2023).

During the roasting process, the chemistry composition of coffee undergoes significant transformations. The choice of roast level also affects the chemistry and characteristics of the coffee. Coffee beans roasted to lighter levels tend to retain more acidic compounds, resulting in a brighter and more acidic beverage. Conversely, coffee beans roasted to darker levels tend to have more bitter flavors and fewer acids due to the degradation of some compounds during more intense roasting (Anisa et al., 2017; Morais et al., 2008; Stiefel et al., 2022).

Another important aspect of coffee chemistry is the extraction process during beverage preparation. The hot water used in brewing extracts soluble compounds from coffee beans, including carbohydrates, acids, and aromatic compounds. Proper extraction of desirable compounds results in a balanced and flavorful beverage, while inadequate or excessive

extraction can lead to under-extracted or over-extracted coffee, respectively (Angeloni et al., 2019; Kang et al., 2018).

Coffee chemistry can also be influenced by preparation methods. For instance, the pressure used in espresso machines affects the extraction of soluble compounds and the formation of crema, a layer of oils and gases that imparts unique texture and aroma to the beverage. On the other hand, filtration methods such as paper filters remove some oils and sediments, resulting in a cleaner and less intense brew (Angeloni et al., 2019; Kang et al., 2022; Oliveira et al., 2005).

In addition to its sensory characteristics, the chemistry composition of coffee has also been studied for its potential health benefits. Research suggests that compounds like antioxidants found in coffee may have protective effects against diseases such as type 2 diabetes, cardiovascular diseases, and some types of cancer (Poole et al., 2017; Wang et al., 2022; Zhi et al., 2022). However, it's important to note that coffee consumption should be balanced and individualized, taking into account factors such as caffeine sensitivity and specific health conditions (Poole et al., 2017).

Coffee is a beverage that contains various organic acids, each with its own functionality and contribution to the final flavor. Among the organic acids found in coffee, chlorogenic acid, quinic acid, oxalic acid, acetic acid, citric acid, succinic acid, and propionic acid are notable (Cordoba et al., 2020; Rune et al., 2023; Yeager et al., 2021).

Chlorogenic acid is one of the primary acids in coffee and plays a significant role in protecting against free radicals due to its antioxidant properties. Additionally, this acid contributes to the distinctive flavor and aroma of coffee (Clifford, 2000; Lopes et al., 2020; Munyendo et al., 2021; Vilas-boas et al., 2020). Quinic acid, another organic acid found in coffee, contributes to the beverage's bitter taste. This acid is formed during the roasting process of coffee beans, and its concentration can vary depending on the roasting time and temperature (Aree 2019; Freitas et al., 2023). Oxalic acid, although present in smaller quantities, can also be found in coffee. This acid can influence taste perception by adding a slight acidity to the beverage, as well as imparting a caramelized flavor (Yeager et al., 2021). Acetic acid is a volatile organic acid that contributes to the coffee's aromas. When present in appropriate concentrations, it can add vinegar-like notes to the final flavor of the drink (Kalschne et al., 2018; Xu et al., 2019; Yeager et al., 2021). Citric acid, on the other hand, contributes to the coffee's acidic and citrusy flavor. It also plays a role in regulating pH during coffee extraction, influencing the overall acidity of the beverage. Succinic acid is a minor organic acid found in coffee. Its specific functionality in the drink is still being investigated, but it is known to

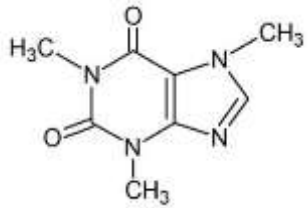
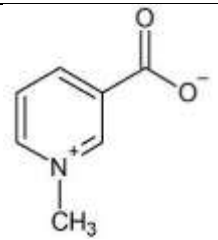
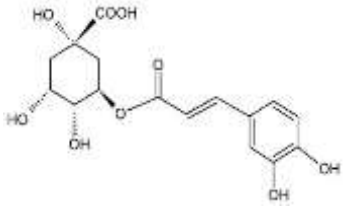
contribute to the overall sensory profile of coffee. Propionic acid is found in very small quantities in coffee. Although its specific function in the final beverage is not fully understood, it is known to contribute to the general sensory characteristics of coffee, often leading to a herbaceous flavor (Kalschne et al., 2018).

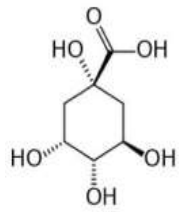
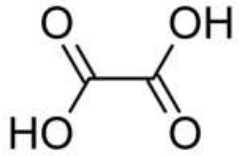
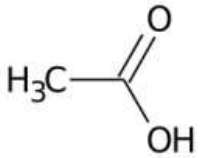
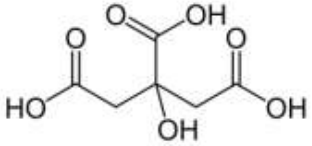
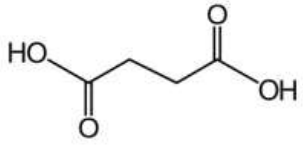
Each of these organic acids contributes uniquely to the taste, aroma, and sensory characteristics of coffee (Yeager et al., 2021). The combination and interaction of these acids result in the complexity of flavors enjoyed by consumers. Although further scientific research is needed for a better characterization of acid compositions and the role of acids in coffee, acidity is an intrinsic element in the evaluation by experts, especially in the context of the specialty coffee industry (Rune et al., 2023). It's worth noting that the concentration and proportion of organic acids can vary depending on factors such as coffee type, processing method, roasting time and temperature, as well as the brewing method (Yeager et al., 2021).

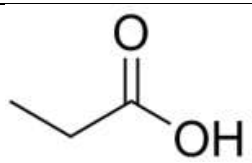
In summary, the organic acids present in coffee play distinct roles in the composition and final flavor of the beverage (Balzer, 2008; Cordoba et al., 2020; Yeager et al., 2021). Each of them contributes to the complexity and diversity of flavors that make coffee a highly appreciated beverage worldwide (Wang et al., 2021). In addition to acids, another compound present in relatively high quantities in coffee is the alkaloid trigonelline (Folwarczna et al., 2016).

Trigonelline is an alkaloid found in various plants, including coffee. It is produced through the enzymatic methylation of nicotinic acid. In coffee, trigonelline is present in similar amounts to caffeine (Mehari et al., 2016). During the roasting process of coffee, trigonelline undergoes demethylation, resulting in the formation of nicotinic acid, which is known as niacin, a B-complex vitamin (Santos & Rangel, 2015). Niacin plays important roles in energy metabolism, nervous system function, and the health of skin, hair, and eyes. It's worth noting that the quantity of trigonelline and niacin can vary depending on the type of coffee and the roasting process, but coffee is considered a significant dietary source of niacin, among other beneficial compounds (Folwarczna et al., 2016; Hirakawa et al., 2005; Santos & Rangel, 2015).

Table 2 presents data on the respective quantities of these compounds in different coffee samples. In summary, the chemistry of coffee encompasses a variety of compounds and reactions that contribute to the unique flavors, aromas, and characteristics of this sought-after beverage. In recent years, the coffee market has gained significant prominence due to its development and production, as well as the pleasure of consumption, emotions, and health benefits associated with the presence of certain chemical compounds.

Chemical compounds	Chemical structure	Specie	Main results (Quantities found)	Reference
Caffeine		*Coffea arabica*	9.4 - 110.0 mg/g^{-1}	(Worku et al., 2023)
		Coffea arabica	10.0 - 25.0 g/kg^{-1}	(Cortés-Macías et al., 2023)
		Coffea arabica	13.93 - 20.88 mg/g	(Girma et al., 2020)
		Coffea arabica	6.07 - 9.19 g/kg	(Cassimiro et al., 2022)
		Coffea arabica	0.80 - 1.42 mg/mL	(Córdoba et al., 2021)
Trigonelline		*Coffea arabica*	5.03 - 8.92 g/kg	(Cassimiro et al., 2022)
		Coffea arabica	8.14 - 11.84 g/kg^{-1}	(Cortés-Macías et al., 2023)
		Coffea arabica	0.46 - 0.48 mg/g	(Córdoba et al., 2021)
		Coffea arabica	0.94 - 5.76 mg/g	(Freitas et al., 2023)
		Coffea canephora	1.27 - 9.72 mg/g	(Freitas et al., 2023)
Chlorogenic acids (5-CQA)		*Coffea arabica*	26.2 - 30.5 mg/g^{-1}	(Worku et al., 2023)
		Coffea arabica	10.8 -13.4 g/kg^{-1}	(Cortés-Macías et al., 2023)
		Coffea arabica	8.56 - 16.21 mg/g	(Girma et al., 2020)
		Coffea arabica	10.0 - 16.26 g/kg	(Cassimiro et al., 2022)
		Coffea arabica	0.004 - 0.78 mg/mL	(Córdoba et al., 2021)

Quinic acid		*Coffea canephora*	0 - 84 mg/mL	(Rodrigues et al., 2007)
		Coffea arabica	0.032 - 0.731 mg/mL	(Rune et al., 2023)
		Coffea arabica	6.7 - 8.5 mg/g	(Jham et al., 2002)
Oxalic acid		*Coffea arabica*	0 - 0.9 mg/g	(Jham et al., 2002)
		Coffea canephora	0.01 - 0.05 mg/g	(Prakash et al., 2022)
Acetic acid		*Coffea arabica*	0.86 - 23.41 g/kg	(Cassimiro et al., 2022)
		Coffea arabica	1.55 - 1.85 mg/g	(Pereira et al., 2015)
		Coffea arabica	0.19 - 0.32 mg/mL	(Córdoba et al., 2021)
		Coffea arabica	123.64 - 158.89 ug/g	(Wang et al., 2021)
		Coffea canephora	296 - 1309 mg/mL	(Rodrigues et al., 2007)
Citric acid		*Coffea arabica*	1.08 - 8.64 g/kg	(Cassimiro et al., 2022)
		Coffea arabica	3.0 - 3.45 mg/g	(Pereira et al., 2015)
		Coffea arabica	65 - 495 mg/mL	(Rodrigues et al., 2007)
		Coffea canephora	329 - 399 mg/mL	(Rodrigues et al., 2007)
Succinic acid		*Coffea canephora*	0.05 - 0.12 g/kg	(Cassimiro et al., 2023)
		Coffea arabica	143 - 1402 mg/mL	(Rodrigues et al., 2007)
		Coffea canephora	286 - 1429 mg/mL	(Rodrigues et al., 2007)

		Coffea arabica	0 - 3.3 mg/g	(Jham et al., 2002)
Propionic acid		*Coffea arabica*	4.66 - 8.09 ug/g	(Wang et al., 2021)

7. Final considerations

The quality of coffee is influenced by several stages, including agriculture, processing methods, roasting, grinding, and fermentation techniques. Quality-related factors in agriculture encompass grain ripeness, harvesting method, seasonality, geographic location, climate, cultivation practices, and genetic characteristics. Coffee's composition is intricate and variable, so harvesting at the early ripening stage is essential to ensure homogeneity and specific chemical and sensory attributes. The cultivation altitude also affects coffee quality, although there is conflicting research on the ideal altitude. Regional climate profoundly impacts coffee production, where high temperatures and irregular rainfall can compromise quality. Shade-grown methods can be beneficial in improving quality but may reduce overall yield. Genetic factors, such as species or variety, also play a critical role in determining coffee quality. Manual harvesting is considered the most suitable for preserving quality, despite being more time-consuming and costly. Additionally, the processing method employed significantly influences coffee's chemical composition. Roasting plays a fundamental role in developing coffee's flavors and aromas, involving Maillard reactions and caramelization processes. The degree of roasting and preparation techniques also influence beverage characteristics. Coffee contains various chemical compounds, including caffeine, chlorogenic acids, trigonelline, sugars, lipids, amino acids, minerals, and vitamins. Coffee chemistry can offer health benefits, although consumption should be moderate and personalized. In summary, coffee quality is the result of a complex interplay of factors ranging from cultivation to preparation, with chemistry playing a fundamental role in crafting the distinct sensory attributes of this globally cherished beverage. The review provided offers a valuable scientific contribution to the field of coffee production and food science. By synthesizing and analyzing a wide range of factors that affect coffee quality, from cultivation to preparation, it provides a comprehensive view of the challenges and opportunities associated with this industry. Delving into the complex interplay of elements such as bean ripeness, cultivation practices, chemical composition, and roasting processes, the review offers a solid foundation for researchers, producers, and coffee enthusiasts to understand the underlying mechanisms that influence the flavor and quality of the beverage. Furthermore, by highlighting the importance of factors like manual harvesting and processing methods, the review provides practical insights to enhance the production of high-quality coffee. Ultimately, this work contributes to the advancement of coffee science, enabling the continuous

improvement of cultivation and production techniques, as well as the development of new approaches to enhance the coffee experience for enthusiasts worldwide.

References

Acquaticci, L., Angeloni, S., Cela, N., Galgano, F., Vittori, S., Caprioli, G., Condelli, N. (2023). Impact of coffee species, post-harvesting treatments and roasting conditions on coffee quality and safety related compounds. *Food Control*, *149*, article 109714. https://doi.org/10.1016/j.foodcont.2023.109714

Aguiar, J., Estevinho, B. N., Santos, L. (2016). Microencapsulation of natural antioxidants for food application - The specific case of coffee antioxidants - A review. *Trends in Food Science & Technology*, *58*, 21-39. https://doi.org/10.1016/j.tifs.2016.10.012

Angeloni, G., Guerrini, L., Masella, P., Bellumori, M., Daluiso, S., Parenti, A., Innocenti, M. (2019). What kind of coffee do you drink? An investigation on effects of eight different extraction methods. *Food Research International*, *116*, 1327-1335. https://doi.org/10.1016/j.foodres.2018.10.022

Anisa, A., Solomon, W. K., Solomon, A. (2017). Optimization of roasting time and temperature for brewed hararghe coffee (*Coffea arabica* L.) using central composite design. *International Food Research Journal*, *24*(6), 2285-2294.

Aree, T. (2019). Understanding structures and thermodynamics of β-cyclodextrin encapsulation of chlorogenic, caffeic and quinic acids: Implications for enriching antioxidant capacity and masking bitterness in coffee. *Food Chemistry*, *293*, 550-560. https://doi.org/10.1016/j.foodchem.2019.04.084

Ayal, D. Y., Nure, A., Tesfaye, B., Ture, K., Zeleke, T. T. (2023). An appraisal on the determinants of adaptation responses to the impacts of climate variability on coffee Production: Implication to household food security in Nensebo Woreda, Ethiopia. *Climate Services*, *30*, article 100383. https://doi.org/10.1016/j.cliser.2023.100383

Bae, J. H., Park, J. H., Im, S. S., Song, D. K. (2014). Coffee and health. *Integrative Medicine Research*, *3*(4), 189-191. https://doi.org/10.1016/j.imr.2014.08.002

Baggenstoss, J., Poisson, L., Kaegi, R., Perren, R., Escher, F. (2008). Coffee roasting and aroma formation: application of different time-temperature conditions. *Journal of Agricultural and Food Chemistry*, *56*(14), 5836-5846. https://doi.org/10.1021/jf800327j

Balzer, H. H. (2008). Acids in coffee. In *Coffee: Recent developments*, ed. Ronald Clarke, and O. G. Vitzthum, 18-32. Hoboken, NJ, USA: John Wiley & Sons.

Batista, L. R., de Souza, S. C., Batista, C. S., Schwan, R. F. (2016). Coffee: types and production. *Encyclopedia of Food and Health*, 244-251. https://doi.org/10.1016/B978-0-12-384947-2.00184-7

BCA - British Coffee Association. Coffee Facts. (2021). Available from: https://www.britishcoffeeassociation.org/coffee-in-the-uk/coffee-facts.

Bermejo, D. V., Luna, P., Manic, M. S., Najdanovic-Visak, V., Reglero, G.,Fornari, T. (2013). Extraction of caffeine from natural matter using a biorenewable agrochemical solvent. *Food and Bioproducts Processing*, *91*, 303-309. https://doi.org/10.1016/j.fbp.2012.11.007

Bertone, E., Venturello, A., Giraudo, A., Pellegrino, G., Geobaldo, F. J. F. C. (2016). Simultaneous determination by NIR spectroscopy of the roasting degree and Arabica/Robusta ratio in roasted and ground coffee. *Food Control*, *59*, 683-689. https://doi.org/10.1016/j.foodcont.2015.06.055

BRASIL. Agência Nacional de Vigilância Sanitária. Resolução RDC n° 277, de 22 de setembro de 2005 https://www.gov.br/agricultura/pt-br/assuntos/inspecao/produtos-vegetal/legislacao-1/biblioteca-de-normas-vinhos-e-bebidas/resolucao-rdc-no-277-de-22-de-setembro-de-2005.pdf/view (accessed 24 february 2023).

Campbell, R., Young, S. P. (2017). Central nervous system stimulants: basic pharmacology and relevance to anaesthesia and critical care. *Anaesthesia and Intensive Care Medicine*, *19*(1), 20–24. https://doi.org/10.1016/j.mpaic.2017.10.008

Cassimiro, D. M. J., Batista, N, N., Fonseca, H. C., Naves, J. A. O., Coelho, J. M., Bernardes, P. C., Dias, D. R., Schwan, R. F. (2023). Wet fermentation of *Coffea canephora* by lactic acid bacteria and yeasts using the self-induced anaerobic fermentation (SIAF) method enhances the coffee quality. *Food Microbiology*, *110*, article 104161. https://doi.org/10.1016/j.fm.2022.104161

Cassimiro, D. M. J., Batista, N. N., Fonseca, H. C., Naves, J. A. O., Dias, D. R., Schwan, R. F. (2022). Coinoculation of lactic acid bacteria and yeasts increases the quality of wet fermented Arabica coffee. *International Journal of Food Microbiology*, *369*, article 109627. https://doi.org/10.1016/j.ijfoodmicro.2022.109627

Chaichi, M., Ghasemzadeh-Mohammadi, V., Hashemi, M., Mohammadi, A. (2015). Furanic compounds and furfural in different coffee products by headspace liquid-phase micro-extraction followed by gas chromatography–mass spectrometry: Survey and effect of brewing procedures. *Food Additives & Contaminants*, *8*(1), 73-80. https://doi.org/10.1080/19393210.2014.981601

Chindapan, N., Soydok, S., Devahastin, S. (2019). Roasting Kinetics and Chemical Composition Changes of Robusta Coffee Beans During Hot Air and Superheated Steam Roasting. *Journal of Food Science*, *0*, 1-11. https://doi.org/10.1111/1750-3841.14422

Clifford, M. N. (2000). Chlorogenic acids and other cinnamates - nature, occurrence, dietary burden, absorption and metabolism. *Journal of the Science of Food and Agriculture*, *80*(7), 1033-1043. https://doi.org/10.1002/(SICI)1097-0010(20000515)80:7<1033::AID-JSFA595>3.0.CO;2-T

CONAB – COMPANHIA NACIONAL DE ABASTECIMENTO. (2022). Available from: https://www.conab.gov.br.

Córdoba, N., Fernandez-Alduenda, M., Moreno, F. L., Ruiz, Y. (2020). Coffee extraction: A review of parameters and their influence on the physicochemical characteristics and flavour of coffee brews. *Trends in Food Science & Technology*, *96*, 45-60. https://doi.org/10.1016/j.tifs.2019.12.004

Córdoba, N., Moreno, F. L., Osorio, C., Velásquez, S., Ruiz, Y. (2021). Chemical and sensory evaluation of cold brew coffees using different roasting profiles and brewing methods. *Food Research International*, *141*, article 110141. https://doi.org/10.1016/j.foodres.2021.110141

Cortés-Macías, E. T., López, C. F., Gentile, P., Girón-Hernández, J., López, A. F. (2023). Impact of post-harvest treatments on physicochemical and sensory characteristics of coffee beans in Huila, Colombia. *Postharvest Biology and Technology*, *187*, article 111852. https://doi.org/10.1016/j.postharvbio.2022.111852

Debastiani, R., Eliete, C., Maciel, M., Sobrosa, V., Amaral, L., Lucia, M., Ferraz, J. (2019). Elemental analysis of Brazilian coffee with ion beam techniques: From ground coffee to the final beverage. *Food Research International (Ottawa ont,)*, *119*, 297-304. https://doi.org/10.1016/j.foodres.2019.02.007

Febrianto, N. A., Zhu, F. (2023). Coffee bean processing: Emerging methods and their effects on chemical, biological and sensory properties. *Food Chemistry*, *412*, article 135489. https://doi.org/10.1016/j.foodchem.2023.135489

Febrina, L., Happyana, N., Maolana, Y. (2021). Metabolite profiles and antidiabetic activity of the green beans of Luwak (civet) coffees. *Food Chemistry*, *355*, article 129496. https://doi.org/10.1016/j.foodchem.2021.129496

Ferrão, A. M. A. (2004). Arquitetura do café. Editora da Unicamp, 296, 47-74. Available from:https://loja.editoraunicamp.com.br/arquitetura-urbanismo-epaisagismo/arquitetura-do-cafe-ed--2-386/p

Ferreira, L. J. C., Gomes, M. S., Maciel, L., Oliveira, L. M., Santos, L. D. (2023). Coffee fermentation process: A review. *Food Research International*, *169*, article 112793. https://doi.org/10.1016/j.foodres.2023.112793

Folwarczna, J., Janas, A., Pytlik, M., Cegieła, U., Śliwiński, L., Krivošíková, Z., Štefíková, K., Gajdoš, M. (2016). Effects of trigonelline, an alkaloid present in coffee, on diabetes-induced disorders in the rat skeletal system. *Nutrients*, *8*(3), 133. https://doi.org/10.3390/nu8030133

Freitas, V. V., Rodrigues, L. L. B., Castro, G. A. D., dos Santos, M. H., Vidigal, M. C. T. R., Fernandes, S. A., Stringheta, P. C. (2023). Impact of different roasting conditions on the chemical composition, antioxidant activities, and color of *Coffea canephora* and *Coffea arabica* L. samples. *Heliyon*, *9*(9), article e19580. https://doi.org/10.1016/j.heliyon.2023.e19580

Girma, B., Gure, A., Wedajo, F. (2020). Influence of altitude on caffeine, 5-caffeoylquinic acid, and nicotinic acid contents of arabica coffee varieties. *Journal of Chemistry*, *2020*, 1-7. https://doi.org/10.1155/2020/3904761. Article ID 3904761

Gosalvitr, P., Cuéllar-Franca, R. M., Smith, R., Azapagic, A. (2023). An environmental and economic sustainability assessment of coffee production in the UK. *Chemical Engineering Journal*, *465*, article 14793. https://doi.org/10.1016/j.cej.2023.142793

Grzelczyk, J., Fiurasek, P., Kakkar, A., Grazyna, B. (2022). Evaluation of the thermal stability of bioactive compounds in coffee beans and their fractions modified in the roasting process. *Food Chemistry*, *387*, article 132888. https://doi.org/10.1016/j.foodchem.2022.132888

Hairiah, K., Sulistyani, H., Suprayogo, D., Purnomosidhi, P., Widodo, R. H., Van Noordwijk, M. (2006). Litter layer residence time in forest and coffee agroforestry systems in Sumberjaya, West Lampung. *Forest ecology and management*, *224*(1-2), 45-57. https://doi.org/10.1016/j.foreco.2005.12.007

Hall, R. D., Trevisan, F., de Vos, R. C. (2022). Coffee berry and green bean chemistry–Opportunities for improving cup quality and crop circularity. *Food Research International*, *151*, article 110825. https://doi.org/10.1016/j.foodres.2021.110825

Hirakawa, N., Okauchi, R., Miura, Y., Yagasaki, K. (2005). Anti-invasive activity of niacin and trigonelline against cancer cells. *Bioscience, biotechnology, and biochemistry*, *69*(3), 653-658. https://doi.org/10.1271/bbb.69.653

ICO – International Coffee Association. (2022). Available from: http://www.ico.org/prices/new-consumption-table.pdf.

Jumhawan, U., Putri, S. P., Bamba, T., Fukusaki, E. (2016). Quantification of coffee blends for authentication of Asian palm civet coffee (Kopi Luwak) via metabolomics: A proof of concept.

Journal of Bioscience and Bioengineering, *122*(1), 79-84. https://doi.org/10.1016/j.jbiosc.2015.12.008

Kalschne, D. L., Viegas, M. C. De Conti, A. J., Corso, M. P., Benassi, M. T. (2018). Steam pressure treatment of defective *Coffea canephora* beans improves the volatile profile and sensory acceptance of roasted coffee blends. *Food Research International*, *105*, 393-402. https://doi.org/10.1016/j.foodres.2017.11.017

Kang, G. W., Piao, Z., Ko, J. Y. (2022). Effects of water types and roasting points on consumer liking and emotional responses toward coffee. *Food Quality and Preference*, *101*, article 104631. https://doi.org/10.1016/j.foodqual.2022.104631

Kitzberger, C. S. G., Scholz, M. B. S., Pereira, L. F. P., Vieira, L. G. E., Sera, T., Silva, J. B. G., Benassi, M. T. (2013). Diterpenes in green and roasted coffee of *Coffea arabica* cultivars growing in the same edapho-climatic conditions. *Journal of Food Composition and Analysis*, *30*, 52-57. https://doi.org/10.1016/j.jfca.2013.01.007

Lee, L. W., Cheong, M. W., Curran, P., Yu, B., Liu, S. Q. (2015). Coffee fermentation and flavor - An intricate and delicate relationship. *Food chemistry*, *185*, 182-191. https://doi.org/10.1016/j.foodchem.2015.03.124

Lopes, G. R., Passos, C. P., Rodrigues, C., Teixeira, J. A., Coimbra, M. A. (2020). Impact of microwave-assisted extraction on roasted coffee carbohydrates, caffeine, chlorogenic acids and coloured compounds. *Food Research International*, *129*, article 108864. https://doi.org/10.1016/j.foodres.2019.108864

Magrach, A., Ghazoul, J. (2015). Climate and pest-driven geographic shifts in global coffee production: Implications for forest cover, biodiversity and carbon storage. *PloS one*, *10*(7), e0133071. https://doi.org/10.1371/journal.pone.0133071

Mahingsapun, R., Tantayotai, P., Panyachanakul, T. (2022). Enhancement of Arabica coffee quality with selected potential microbial starter culture under controlled fermentation in wet process. *Food Bioscience*, *48*, article 101819. https://doi.org/10.1016/j.fbio.2022.101819

Marcone, F. M. (2004). Composition and properties of Indonesian palm civet coffee (Kopi Luwak) and Ethiopian civet coffee. *Food Research International*, *37*, 901-912. https://doi.org/10.1016/j.foodres.2004.05.008

Matiello, J.B., Santinato, R. (2010). Harvesting, Processing and Quality of Coffee. Coffee Culture in Brazil: *Manual of Recommendations*, 7, 471-526. Available from: https://biblioteca.incaper.es.gov.br

Mehari, B., Redi-Abshiro, M., Chandravanshi, B. S., Atlabachew, M., Combrinck, S., McCrindle, R. (2016). Simultaneous determination of alkaloids in green coffee beans from Ethiopia: Chemometric evaluation of geographical origin. *Food analytical methods*, *9*, 1627-1637. https://doi.org/10.1007/s12161-015-0340-2

Meylan, L., Gary, C., Allinne, C., Ortiz, J., Jackson, L., Rica, C. (2017). Evaluating the effect of shade trees on provision of ecosystem services in intensively managed coffee plantations. *Agriculture, Ecosystems and Environment*, *245*, 32-42. https://doi.org/10.1016/j.agee.2017.05.005

Milani, M., Montorsi, L., Terzi, S. (2017). Numerical analysis of the heat recovery efficiency for the post- combustion flue gas treatment in a coffee roaster plant. *Energy*, *141*, 729-743. https://doi.org/10.1016/j.energy.2017.09.098

Morais, S. A. L., Aquino, F. J. T., Chang, R., Nascimento, E. A., Oliveira, G. S., Santos, N. C. (2008). Chemical analysis of arabica coffee (*Coffea arabica*) and defective beans submitted to different degrees of roasting. *Coffee Science*, *2*(2), 97-111. Available from: http://www.coffeescience.ufla.br/index.php/Coffeescience/article/view/50. Acesso em: 8 jul. 2023.

Munyendo, L. M., Njoroge, D. M., Owaga, E. E., Mugendi, B. (2021). Coffee phytochemicals and post-harvest handling - A complex and delicate balance. *Journal of Food Composition and Analysis*, *102*, article 103995. https://doi.org/10.1016/j.jfca.2021.103995

Muschler, R. G. (2001). Shade improves coffee quality in a sub-optimal coffee-zone of Costa Rica. *Agroforestry Systems*, *51*(2), 131-139. https://doi.org/10.1023/A:1010603320653

Nóbrega. R. O., daSilva., S. F., Fernandes, D. D. S., Lyra, W. S., deAraújo, T. K. L., Diniz, P. H. G. D., Araújo, M. C. U. (2023). Classification of instant coffees based on caffeine content and roasting degree using NIR spectrometry and multivariate analysis. *Microchemical Journal*, *190*, article 108624. https://doi.org/10.1016/j.microc.2023.108624

Oliveira, A. L de., Cruz, P. M., Eberlin, M. N., Cabral, F. A. (2005). Brazilian roasted coffee oil obtained by mechanical expelling: compositional analysis by GC-MS. *Food Science and Technology*, *25*(4), 677-682. https://doi.org/10.1590/S0101-20612005000400009

Park, J. B., Peters, R., Novotny, J. A. (2023). Impact of roasting on javamide-I/-II in Arabica and Robusta coffee beans. *Food Chemistry*, *412*, article 135586. https://doi.org/10.1016/j.foodchem.2023.135586

Pereira, G. V. M., Neto, D. P. C, Júnior, A. I. M., Vásquez, Z. S., Medeiros, A. B., Vandenberghe, L. P., Soccol, C. R. (2019). Exploring the impacts of postharvest processing on

the aroma formation of coffee beans - A review. *Food chemistry*, *272*, 441-452. https://doi.org/10.5327/Z1679443520190350

Pereira, G. V. M., Neto, E., Soccol, V. T., Medeiros, A. B. P., Woiciechowski, A. L., Soccol, C. R. (2015). Conducting starter culture-controlled fermentations of coffee beans during on-farm wet processing: Growth, metabolic analyses and sensorial effects. *Food Research International*, *75*, 348-356. https://doi.org/10.1016/j.foodres.2015.06.027

Pereira, L. L., Júnior, D. B., de Sousa, L. H. B. P., dos Santos, W. G., Cardoso, W. S., Guarçoni, R. C., ten Caten, C. S. (2021). Relationship Between Coffee Processing and Fermentation. Quality Determinants In Coffee Production, 255-301. https://doi.org/10.1007/978-3-030-54437-9

Pimenta, C. J. Qualidade de café. Lavras: UFLA, 2003. 304p.

Poisson, L., Blank, I., Dunkel, A., & Hofmann, T. (2017). The chemistry of roasting: Decoding flavor formation. In B. Folmer (Ed.), the craft and science of coffee (pp. 273–309). London: Academic Press.

Poltronieri, P., Rossi, F. (2016). Challenges in Specialty Coffee Processing and Quality Assurance. *Challenges*, 7, 19. https://doi.org/10.3390/challe7020019

Poole, R., Kennedy, O. J., Roderick, P., Fallowfield, J. A., Hayes, P. C., Parkes, J. (2017) Coffee consumption and health: umbrella review of meta-analyses of multiple health outcomes. *BMJ*, *359*. https://doi.org/10.1136/bmj.j5024

Prakash, I., Shankar, S. R., Sneha, H. P., Kumar, P., Om, H., Basavaraj, K., Murthy, P. S. (2022). Metabolomics and volatile fingerprint of yeast fermented robusta coffee: A value added coffee. *LWT- Food Science and Technology*, *154*, article 112717. https://doi.org/10.1016/j.lwt.2021.112717

Ramos, P. J., Prieto, F. A., Montoya, E. C., Oliveros, C. E. (2017). Automatic fruit count on coffee branches using computer vision. *Computers and Electronics in Agriculture*, *137*, 9-22. https://doi.org/10.1016/j.compag.2017.03.010

Raveendran, A., Murthy, P. S. (2022). New trends in specialty coffees-“the digested coffees”. *Critical Reviews in Food Science and Nutrition*, *62*(17), 4622-4628. https://doi.org/10.1080/10408398.2021.1877111

Ribeiro, D. E., Borem, F. M., Cirillo, M. A., Prado, M. V. B., Ferraz, V. P., Alves, H. M. R., Taveira, J. D. S. (2016). Interaction of genotype, environment and processing in the chemical composition expression and sensorial quality of Arabica coffee. *African Journal of Agricultural Research*, *11*(27), 2412-2422. https://doi.org/10.5897/AJAR2016.10832

Rodrigues, C. I., Marta, L., Maia, R., Miranda, M., Ribeirinho, M., Máguas, C. (2007). Application of solid-phase extraction to brewed coffee caffeine and organic acid determination by UV/HPLC. *Journal of Food Composition and Analysis*, *20*, 440-448. https://doi.org/10.1016/j.jfca.2006.08.005

Rune, C. J. B., Giacalone, D., Steen, I., Duelund, L., Munchow, M., Clausen, M. P. (2023). Acids in brewed coffees: Chemical composition and sensory threshold. *Current Research in Food Science*, *6*, article 100485. https://doi.org/10.1016/j.crfs.2023.100485

Saloko, S., Sulastri, Y., Murad, M., Rinjani, M. A. (2019). The effects of temperature and roasting time on the quality of ground Robusta coffee (*Coffea robusta*) using Gene Café roaster. In *AIP Conference Proceedings*, *2199*(1). https://doi.org/10.1063/1.5141310

Santos, J. R., Rangel, A. O. S. S. (2015). Development of a chromatographic low pressure flow injection system using amperometric detection: Application to the analysis of niacin in coffee. *Food Chemistry*, *187*, 152-158. https://doi.org/10.1016/j.foodchem.2015.04.093

Scholz, M. B. S., Kitzberger, C. S. G., Prudêncio, S. H., Silva, R. S. S. F. (2018). The typicity of coffees from different terroirs determined by groups of physico-chemical and sensory variables and multiple factor analysis. *Food Research International*, *114*, 72-80. https://doi.org/10.1016/j.foodres.2018.07.058

Silva, M. Q. M., Valente, I. M., Almeida, P. J., Santos, J. R. (2023). Carbon dioxide spectrophotometric determination in whole roasted coffee beans using a total analysis system after super-modified simplex optimization. *Journal of Food Composition and Analysis*, *115*, article 104978. https://doi.org/10.1016/j.jfca.2022.104978

Sruthi, N. U., Premjit, Y., Pandiselvam, R., Kothakota, A., Ramesh, V. (2021). An overview of conventional and emerging techniques of roasting: Effect on food bioactive signatures. *Food Chemistry*, *348*, article 129088. https://doi.org/10.1016/j.foodchem.2021.129088

Steiman, S., Idol, T., Bittenbender, H. C., Gautz, L. (2011). Shade coffee in Hawai‘i–Exploring some aspects of quality, growth, yield, and nutrition. *Scientia Horticulturae*, *128*(2), 152-158. https://doi.org/10.1016/j.scienta.2011.01.011

Stiefel, C., Lindemann, B., Morlock, G. E. (2022). Non-target bioactive compound profiles of coffee roasts and preparations. *Food Chemistry*, *391*, article 133263. https://doi.org/10.1016/j.foodchem.2022.133263

Strezov, V., Evans, T. J. (2005). Thermal analysis of the reactions and kinetics of green coffee during roasting. *International Journal of Food Properties*, *8*(1), 101-111. https://doi.org/10.1081/JFP-200048060

Toci, A. T., Azevedo, D. A., Farah, A. (2020). Effect of roasting speed on the volatile composition of coffees with different cup quality. *Food Research International*, *137*, article 109546. https://doi.org/10.1016/j.foodres.2020.109546

Vale, A. S., Pereira, G. V. M., de Carvalho, D. P. N., Rodrigues, C., Pagnoncelli, M. G. B., Soccol, C. R. (2019). Effect of co-inoculation with *Pichia fermentans* and *Pediococcus acidilactici* on metabolite produced during fermentation and volatile composition of coffee beans. *Fermentation*, *5*(3), 67. https://doi.org/10.3390/fermentation5030067

Velloso, N. S., Magalhães, R. R., Santos, F. L., Santos, A. A. R. (2020). Modal properties of coffee plants via numerical simulation. *Computers and Electronics in Agriculture, 175*, article 105552. https://doi.org/10.1016/j.compag.2020.105552

Viencz, T., Bonfanti, L., Barros, R., Anast, E., Ramalho, R., Benassi, M. D. T. (2023). Caffeine, trigonelline, chlorogenic acids, melanoidins, and diterpenes contents of Coffea canephora coffees produced in the Amazon. *Journal of Food Composition and Analysis*, *117*, article 105140. https://doi.org/10.1016/j.jfca.2023.105140

Vilas-boas, A. A., Oliveira, A., Jesus, D., Rodrigues, C., Figueira, C., Gomes, A. (2020). Chlorogenic acids composition and the impact of in vitro gastrointestinal digestion on espresso coffee from single-dose capsule. *Food Research International*, *134*, article 109223. https://doi.org/10.1016/j.foodres.2020.109223

Ukers, W. H. (1922). All About Coffee. Inter-American Copyright Union. By Burr Pirnting House. First Edition

Wang, X., Wang, Y., Hu, G., Hong, D., Guo, T., Li, J., Li, Z., Qiu, M. (2022). Review on factors affecting coffee volatiles: From seed to cup. *Journal of the Science of Food and Agriculture*, *102*(4), 1341-1352. https://doi.org/10.1002/jsfa.11647

Wang, Y., Wang, X., Hu, G., Hong, D., Bai, X., Guo, T., Zuo, T., Li. J. Qiu, M. (2021). Chemical ingredients characterization basing on ^{1}HNMR and SHS-GC/MS in twelve cultivars of *Coffea arabica* roasted beans. *Food Research International*, *147*, article 110544. https://doi.org/10.1016/j.foodres.2021.110544

Widodo, P. B., Yulianto, M. E., Ariyanto, H. D., Paramita, V. (2023). Materials Today : Proceedings Efficacy of natural and full washed post-harvest processing variations on arabica coffee characteristics. *Materials Today: Proceedings*, (xxxx). https://doi.org/10.1016/j.matpr.2023.02.376

Worku, M., Astatkie, T., Boeckx, P. (2023). Quality and biochemical composition of Ethiopian coffee varied with growing region and locality. *Journal of Food Composition and Analysis*, *115*, article 105015. https://doi.org/10.1016/j.jfca.2022.105015

Worku, M., Meulenaer, B. De, Duchateau, L., Boeckx, P. (2018). Effect of altitude on biochemical composition and quality of green arabica coffee beans can be affected by shade and postharvest processing method. *Food Research International*, *105*, 278-285. https://doi.org/10.1016/j.foodres.2017.11.016

Yeager, S. E., Batali, M. E., Guinard, J. X., Ristenpart, W. D. (2021). Acids in coffee: A review of sensory measurements and meta-analysis of chemical composition. *Critical Reviews in Food Science and Nutrition*, *1*, 1-27. https://doi.org/10.1080/10408398.2021.1957767

Zhi, M., Chan, A., Liu, S. (2022). Coffee brews as food matrices for delivering probiotics: Opportunities, challenges, and potential health benefits. *Trends in Food Science & Technology*, *119*, 227-242. https://doi.org/10.1016/j.tifs.2021.11.030

Artigo 2*

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Impact of different roasting conditions on the chemical composition, antioxidant activities, and color of *Coffea canephora* and *Coffea arabica L.* samples

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Abstract

This work aimed to evaluate the physicochemical changes during the roasting process of Robusta and Arabica coffee. The highest content of total phenolics was detected in roasted coffee at temperatures of 135 °C/20.20 min, 210 °C/9.02 min, 210 °C/11.01 min, and 220 °C/13.47 min for both species. Robusta coffee showed greater antioxidant activity compared to Arabica coffee, except for the profiles at 230 °C/17.43 min and 275 °C/7.46 min that did not differ between samples by the DPPH and FRAP methods. For Arabica coffee, the antioxidant activity was independent of the roasting profile used. Robusta coffee presented higher values of the indexes b* (intensity of yellow vs blue), c* (chroma) and hue, being characterized as lighter and with greater chroma and hue. The highest levels of caffeoylquinic acid **(**5-CQA) were observed in Robusta coffee. Arabica coffee had lower trigonelline values. Caffeic acid and hydroxymethylfurfural were identified only in Robusta coffee. However, the results provided solid knowledge for the design of general properties and chemical compounds generated from binomials of roasting time and temperature that are little used in the world market.

Keywords: Antioxidant activity; Phenolics totals; Coffee beans; Roasting; Food Science.

1. Introduction

Coffee is a drink of vast popularity and appreciated worldwide. The Brazilian coffee production, initially estimated for the 2023 harvest, was estimated at 54.94 million bags of 60 kg, of which 37.43 million bags are of the coffee especies *Coffea arabica* and 17.5 million bags of *Coffea canephora* (robusta and conilon). The Brazilian states with the largest coffee production are Minas Gerais, Espírito Santo, São Paulo and Bahia [1]. The most cultivated species are *C. arabica* and *C. canephora* (robusta), robust being considered of inferior quality when compared to arabica coffee because it has a more bitter and astringent taste [2].

Coffee is the second most important beverage after water, with an estimated annual consumption of approximately 500 billion cups [3][4]. Most coffee drinkers do not drink the beverage for health-related reasons. However, coffee has a variety of antioxidant compounds and numerous types of functional phenolic compounds that play a protective role against various diseases. The main phenolic compounds present in coffee are chlorogenic (CGA), caffeic and ferulic acids [5] [6] [7]. Antioxidants have been the subject of growing interest due to their ability to inhibit oxidative reactions and their role in food preservation. Total phenolics, a diverse class of bioactive compounds of plant origin, are widely recognized for their potent antioxidant potential and ability to eliminate free radicals [8]. In addition to providing functionality, the sensory profile (fragrance/aroma and flavor) is strongly enhanced and influenced by the coffee beans roasting process. In this process, the time-temperature binomial is considered a relevant parameter in obtaining a drink with different flavor and aroma profiles [9] [10].

During the roasting process, modification and/or generation and release of various chemical compounds occur through Maillard reactions, Strecker degradation, caramelization and other chemical reactions. These reactions are responsible for the desired physicochemical and sensory attributes in the coffee beverage, such as flavor, aroma and color, but also the formation of undesirable compounds (Hidroximetilfurfural (HMF), acrylamide and others) [11] [12].

During coffee roasting, it is essential to control the temperature and interrupt the process at the right time to obtain a product with good sensory and physicochemical properties. The degree of roasting of the coffee bean is determined by the habit and preference of the consumer. The roasting conditions usually employed are close to the temperature and time of 200-210 °C/8-12 min [13] [14]. In this context, it is necessary to explore other time and temperature binomials to predict the impact on the chemical composition and antioxidant properties of

coffee through the use of unusual temperatures for coffee processing. The study of different roasting profiles is important because it can generate data that will help in the implementation of new roasting indices that can benefit the chemical composition as well as the final quality of the product. Some studies have already evaluated the effect of different time/temperature binomials on the phenolic composition and antioxidant activities of coffee varieties [5] [6] [15]. However, in the present study, the binomials used were different from previous studies, using a wide temperature range. Therefore, this study aimed to evaluate colorimetric indices, chemical composition, antioxidant activity, and total phenolics in Robusta and Arabica coffees, alternating the binomial time and temperature.

2. Materials and methods

2.1. Materials

All reagents met the quality norms required for analytical grade reagents. Folin–Ciocalteu's phenol reagent (FCR), acetic acid, caffeic acid, chlorogenic acid, gallic acid (>98%), 6-hydroxy-2578-tet-ramethylchroman-2-carboxylic acid (Trolox), 2,2-diphenyl-1-picrylhydrazyl (DPPH), Triphenyltetrazolium chloride (TPTZ), caffeine, trigonelline and 5-hidroxymethylfurfural were purchased from Sigma-Aldrich (St. Louis, MO, USA). Ethyl acetate (≥99,7%), methanol (≥99.9%) were purchased from Chromasolv (Shanghai, China). Ethyl alcohol ((≥99.5%), sodium carbonate, ferric chloride and sodium were purchased from Êxodo Científica (Sumaré, SP, Brasil).

2.2.Coffee samples

Coffee samples (*Coffea arabica Catúai variety* and *Coffea canephora Pierre variety*), dry processed, June-July/2020 crop, were supplied from coffee farms in the São Geraldo city, located in Zona da Mata Mineira, Minas Gerais, Brazil.

2.3. Coffee roasting process

The coffee beans were roasted using a Probat drum roaster (Probat-Werke). Each roast profile was performed only once. Then, the samples of roasted and ground coffee beans were individually packaged in an odor-free closed hermetic package and transported to the

Laboratory of Natural Dyes and Bioactive Compounds of the Federal University of Viçosa Food Technology Department and kept in storage at 5°C for further analysis. Six different roasting profiles were obtained by varying the roasting temperature and time. Five of the roasting profiles were created to obtain standard roasting [Underdeveloped (T1): 135 °C/20.20 min; Light (T2): 210 °C/9.02 min; Dark (T3): 220 °C/13.47 min; Baked (T4): 230 °C/17.43 min; and Scorched (T5): 275 °C/7.46 min)], while the control was the standard procedure commonly used in coffee roasting (T6: 210 °C/11.01 min) (Table 1) [16]. The choice of roasting defects was based reflecting a consensual configuration of pre-existing and applied roasting in the market, the most common being T6: 210 °C/11.01 min (standard).

Table 1. Roasting profile with respective time/temperature binomial.

Roasting profile	Roasting Temperature (°C)	Start time: 1° CRACK (min)	Total roasting time (min)
T1	135	2.16	20.20
T2	210	0.13	9.02
T3	220	4.55	13.47
T4	230	6.20	17.43
T5	275	1.56	7.46
T6	210	2.38	11.01

2.4. Determination of color

The roasted coffee color was determined using a Colorquest XE Colorimeter (Hunter Lab, Reston, VA), with direct reading of the indexes values L* (brightness), a* (intensity of red vs green), and b* (intensity of yellow vs blue). The hue (h*) and chroma (c*) indexes were calculated from the values of a* and b*, according to equations 1 and 2, respectively [17].

$$h^* = \arctan\left(\frac{b^*}{a^*}\right) \qquad (1)$$

$$c^* = \sqrt{a^{*2} + b^{*2}} \qquad (2)$$

2.5. Total phenolic content

The quantification of total phenolic compounds was performed according to the method described by [18]. The results were expressed in gallic acid equivalent/g of coffee.

2.6. Determination of antioxidant activity

The scavenging activity on DPPH radicals was determined according to the method described by [19] and the Ferric Reducing Antioxidant Power (FRAP) according to the method of [20].

2.7. Analysis of caffeine, caffeoylquinic acid (5-CQA), trigonelline, caffeic acid and HMF contents in roasted and ground coffee

Caffeic acid, caffeoylquinic acid, caffeine, trigonelline, and hydroxymethylfurfural were determined in roasted coffee samples according to the methodology adapted by [21]. Analyzes were performed by high performance liquid chromatography (HPLC) on a Thermo Scientific Accela LC system (diode array detector (DAD), autoinjector, and Accela pump) (Thermo Fisher Scientific, Austin, TX). The column used for the separation was the reverse phase Lichrospher 100 RP-18 (250 x 4.6 mm, with a particle size of 5 µm and 10 nm pore) (Merck, Germany). The mobile phase consisted of water (A) and methanol (B), with elution in isocratic mode of 0 - 6 min (90% A and 10% B), gradient mode of 6 - 7 min (90 - 80% A and 10 - 20% B), isocratic mode of 7 - 23 min (80% A and 20%), gradient 23 - 24 min (80 - 0% A and 20 - 100% B), 24 - 25 min (0 - 90 % A and 100 – 10% B) and ending with isocratic mode of 25 – 26 min (90% A and 10% B). The flow was 1 mL/min, and the injection volume was 1 µL (partial loop), with a temperature of 25 °C for the injector and 40 °C for the column. Peaks were detected at wavelengths of 272 nm. Caffeine, caffeoylquinic acid (5-CQA), trigonelline, caffeic acid, and HMF were identified by standards injection and calibration curve.

2.8. Statistical analysis

All analyses were performed in 3 repetitions. The data was expressed as mean ± standard deviation. One-way analysis of variance (ANOVA) in a factorial design was used. A 2-factor factorial design was used (2x6), with the first factor being the coffee species (Robusta and Arabica) and the second factor the roasting profiles (Table 1), totaling 12 treatments. Differences in means were compared using Tukey’s post hoc test. All analyses adopted a

significance level of 5 % and were performed using the R software (R Core Team, Vienna, Austria). Principal component analysis (PCA) based on the correlation matrix was conducted to differentiate the color indexes using the R program (R Core Team, Vienna, Austria).

3. Results and Discussion

3.1. Analysis of color

The coffee bean color is related to the beverage quality and is an important factor in the product value. Changing the degree of temperature applied in the roasting process allows obtaining information on changes in coffee bean color, which is intrinsically related to the Maillard reaction. The color changes result from the formation of some Maillard reaction products that can impart functionality and appearance to roasted coffee beans [22] [23]. The quantitative color evaluation of the roasted and ground coffee beans was reasoned on the indexes value L*, a *, b *, C*, and hue (Table 2).

Regarding the L* indexes values, significant differences ($p<0.05$) were observed between the two species and corresponding roasting conditions, except for roasting performed at 275 °C/7.46 min, which presented values equal for Robusta and Arabica coffees. Robusta coffee samples were significantly lighter. The Arabica coffee samples had a darker color, and the samples roasted at lower temperatures had lower values of the L* index. Robusta coffee samples had higher a* values than Arabica coffee, except for roasting at 230 °C/17.43 min, in which the values did not differ from each other. As for the b* index, the Robusta coffee samples showed significantly higher values ($p<0.05$) for all the roasts applied. The values of the indexes h* and C* of Arabica coffee in the different roasting conditions used were significantly lower than those of Robusta, characterizing the samples of Robusta coffee with higher values of chroma and hue, respectively.

According to [24] depending on the roasting intensity used, roasted and ground coffee may have a brownish, yellow, lighter, or stronger color. At average temperature (210 °C) can present a reddish brown color and high temperature (>220 °C) darker color brown. In the present study, Robusta coffee showed greater luminosity and higher chroma and hue values than Arabica coffee. [25] reported lower luminosity values for Arabica coffee mixed with Robusta when compared to pure Robusta.

Table 2. Average attributes color of *canephora* (Robusta) and *arabica* coffee variety Catúai samples.

Samples	Roasting Profiles					
	135 °C/20.20 min	210 °C/9.02 min	220 °C/13.47 min	230 °C/17.43 min	275 °C/7.46 min	210 °C/11.01 min
L* (brightness)						
C. canephora	37.26 ± 0.78^{Aab}	36.76 ± 0.38^{Aab}	38.32 ± 1.64^{Aa}	37.96 ± 2.27^{Aab}	34.15 ± 2.92^{Ab}	37.36 ± 2.14^{Aab}
C. arábica	24.25 ± 1.24^{Bb}	24.97 ± 0.37^{Bb}	26.12 ± 0.60^{Bb}	35.28 ± 0.80^{Ba}	31.60 ± 1.75^{Aa}	25.52 ± 1.38^{Bb}
a*(intensity of red vs green)						
C. canephora	26.10 ± 0.42^{Aa}	25.66 ± 0.46^{Aa}	26.12 ± 0.83^{Aa}	25.29 ± 0.92^{Aa}	22.50 ± 0.18^{Ab}	25.56 ± 0.82^{Aa}
C. arábica	4.96 ± 0.63^{Bd}	7.99 ± 0.87^{Bc}	11.93 ± 1.71^{Bb}	24.55 ± 0.50^{Aa}	11.38 ± 0.40^{Bb}	12.38 ± 1.60^{Bb}
b* (intensity of yellow vs blue)						
C. canephora	23.08 ± 1.05^{Ab}	22.38 ± 0.65^{Ab}	26.56 ± 0.68^{Aa}	26.53 ± 0.65^{Aa}	15.36 ± 0.44^{Ac}	21.56 ± 1.22^{Ab}
C. arábica	0.81 ± 0.27^{Be}	2.18 ± 0.41^{Bde}	4.18 ± 1.02^{Bcd}	19.57 ± 1.36^{Ba}	10.14 ± 0.84^{Bb}	4.49 ± 0.92^{Bc}
h* (hue)						
C. canephora	41.48 ± 0.87^{Ab}	41.09 ± 0.32^{Ab}	45.47 ± 1.17^{Aa}	46.38 ± 1.37^{Aa}	41.65 ± 0.63^{Ac}	40.12 ± 1.52^{Ab}
C. arábica	9.11 ± 1.93^{Bb}	15.14 ± 1.21^{Bc}	19.16 ± 1.71^{Bb}	38.52 ± 1.41^{Ba}	34.31 ± 1.34^{Ba}	19.81 ± 1.43^{Bb}
c* (chroma)						
C. canephora	34.85 ± 1.81^{Aabc}	34.04 ± 1.00^{Abc}	37.25 ± 0.77^{Aa}	36.66 ± 0.77^{Aab}	27.25 ± 0.72^{Ad}	33.45 ± 0.37^{Ac}
C. arábica	5.02 ± 0.66^{Bd}	8.29 ± 0.94^{Bc}	12.65 ± 1.96^{Bb}	31.41 ± 1.24^{Ba}	15.24 ± 0.86^{Bb}	13.17 ± 1.81^{Bb}

Means followed by the same lowercase letters in the row and uppercase letters in the column do not differ by Tukey's test (p>0,05).

The data obtained in the color evaluation of the roasted coffees were also analyzed by PCA (Fig. 1), commonly used to interpret the correlation between the color indexes of roasted Robusta and Arabica coffee beans. Data matrices for PCA study were set up configuring that every line was equivalent to a sample (coffee species) and each column to a color principle. The first two principal components (PCs) explained 52.4% and 46% of the data variance, respectively, with both components accumulating 98.37% of the variation. From the sample's spatial dispersion, it is possible to identify four distinct groups, separated by quadrant: 230 °C/17.43 min (PC1 positive, PC2 positive); 220°C/13.47 min (PC1 negative, PC2 positive); 135°C/20.20 min, 210°C/9.02 min and 210°C/11.01 min (PC1 negative, PC2 negative); 275 °C/7.46 min (PC1 positive, PC2 negative). The first component allowed the division between darker and lighter samples, being mainly affected by luminosity values.

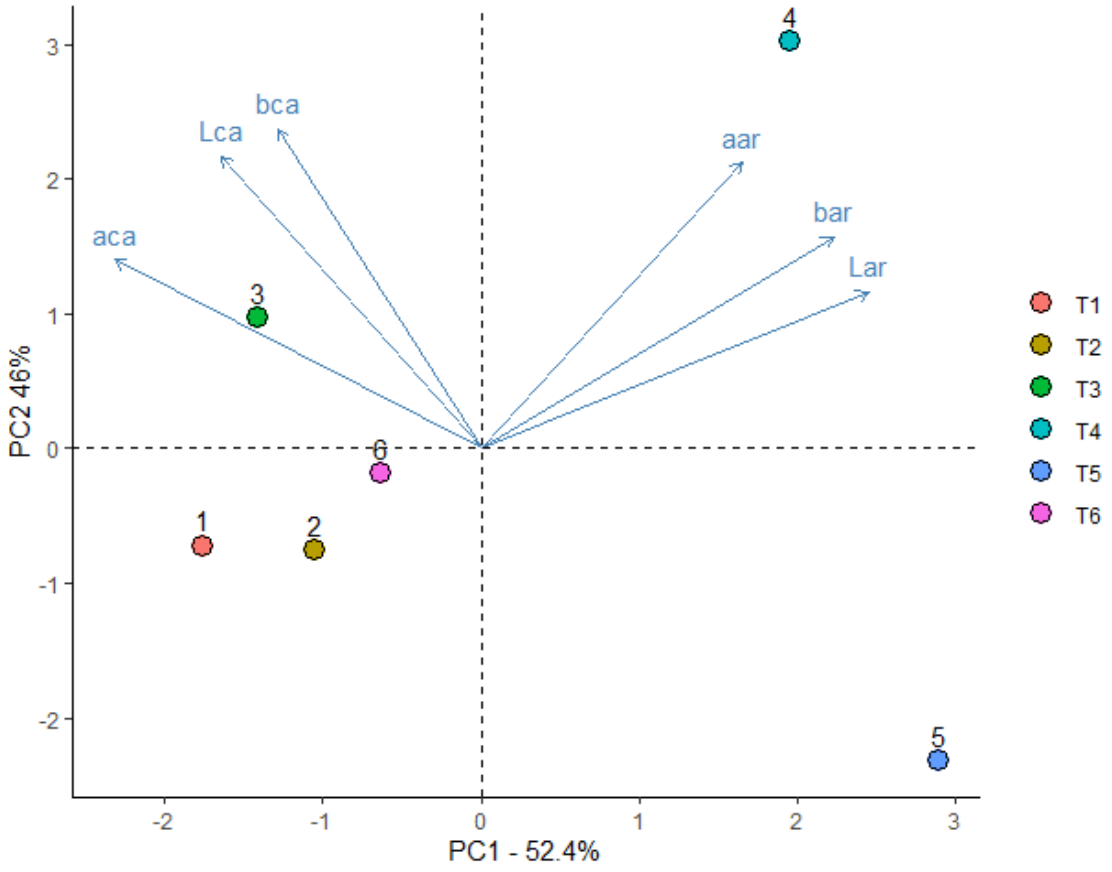

Figure 1. Scatter plot of Principal Component Analysis (PCA) scores of $L^*a^*b^*$ color indexes for Robusta and Arabica coffee samples after different roasting treatments (PC1 vs. PC2).

The color of coffee beans varies between light brown and dark brown due to the pyrolysis of organic compounds and the formation of melanoidins [26]. The decreases in L*

values and increases in a* and b* values after greater exposure of the coffee beans to the roasting process (increased time and temperature) may be due to the development of dark pigments through non-enzymatic browning and degradation of phospholipids, as well as thermal total phenolics oxidation [27] [28].

3.2. Phenolic Content and Antioxidant activity

Different roasting conditions result in different final product quality, that, different colors, flavors, aroma, and acidity [29]. Futhermore, the chemical coffee bean properties depend on other factors such as species and geographic location [30] [31] [32] [33] [29]. Different roasting profiles in two coffee species were evaluated in this study. The results of the impact of these conditions on the TPC and antioxidant activities by the DPPH and FRAP methods are introduced in Fig. 2.

The TPC ranged from 12.31 to 52.47 mg GAE/g for Robusta and 11.52 to 21.47 mg GAE/g for Arabica. The highest values of TPC were detected in roasted coffee at temperatures of 135 °C/20.20 min, 210 °C/9.02 min, 210°C/ 11.01 min and 220 °C/13.47 min for both species. The TPC contents of Robusta coffee were significantly higher than those of Arabica coffee ($p<0.05$), except for roasts at 230 °C/17.43 min and 275 °C/7.46 min. The results also indicated a significant decrease in TPC when roasting profiles at higher temperatures of 230 °C/17.43 min and 275 °C/7.46 min were used. Long roasting times at low temperatures result in little exposure to heat and oxygen and less total phenolic content decrease [34].

The results of the DPPH method (Fig. 2) revealed that the Robusta coffee exhibited greater antioxidant activity when low or standard temperatures in the roasting process were used. Comparing the antioxidant properties determined in the DPPH assay within each coffee species, it was observed that the highest Robusta coffee samples antioxidant activity was provided by treatments at 135 °C/20.20 min, 210 °C/9.02 min, and 210 °C/11.01 min, followed by 220 °C/13.47 min. The methods at 230 °C/17.43 min and 275 °C/7.46 min were the ones that provided samples with lower antioxidant activity, which complies with the TPC. Arabica coffee did not show significant differences ($p>0.05$) in antioxidant activity by the DPPH method among the pre-established roasts. A higher antioxidant activity was also observed in robusta coffee samples compared to Arabica coffee in different roasting profiles, except for treatments at 230 °C / 17.43 min and 275 °C / 7.46 min that showed the same antioxidant activity for both species. Similar results were found by [35] (roasting at 203-205 °C / 11-13

min), indicating that the coffee antioxidant properties are affected by the species and roasting, with Robusta coffee being the one with higher antioxidant activity.

The ferric reducing antioxidant power (FRAP) of each roasted coffee sample was also evaluated and the results are pictured in Fig. 2. The ferric reducing power oscillated from 547.28-666.83 µmol FSE/g and 838,02-3150.62 µmol FSE/g for Arabica and Robusta samples, respectively. Robusta coffee showed greater antioxidant activity in coffees roasted at 135 °C/20.20 min, 210 °C/9.02 min, 220 °C/13.47 min and 220 °C/11.01 min. For Arabica coffee no significant differences ($p>0.05$) were observed in the samples antioxidant activity. Therefore, after roasting, Robusta samples showed significantly higher antioxidant activity values (FRAP) compared to Arabica samples, except for samples roasted at 230 °C/17.43 min and at 275 °C/7.46 min. The higher antioxidant activity in Robusta coffee can be attributed to its caffeine content, which is an alkaloid and has antioxidant properties, whose content can be changed along the roasting standard [36].

The causes of changes in antioxidant activity in coffee beans subjected to different roasting temperatures are associated with chlorogenic acid degradation and the development of products from the advanced glycation [15]. Following the Maillard reaction during the coffee bean roasting process, non-covalent interactions between the phenolic compounds and the reaction products (melanoidins) occur and cause the complexes production that have varying degrees of antioxidant activity [37].

The roasting process impact on the antioxidant properties was verified in several studies, which revealed an increase in the antioxidant activity when using roasts at low temperatures and a subtraction in the antioxidant activity when using roasts at high temperatures [15] [38]. The present study, Robusta coffee showed significantly higher antioxidant activity values (DPPH and FRAP) in treatments using roasts at lower temperatures (<210 °C) and significantly lower activities when roasting at high temperatures.

It is noteworthy that several methodologies are used in the characterization of antioxidant activity in foods, with no single, standardized and universal method in the process of performing the analysis. To determine the antioxidant activity, the ideal is to use at least two evaluation methods, with the DPPH, FRAP and total phenolic methods widely applied in the determination, as seen in the related work [39] [40].

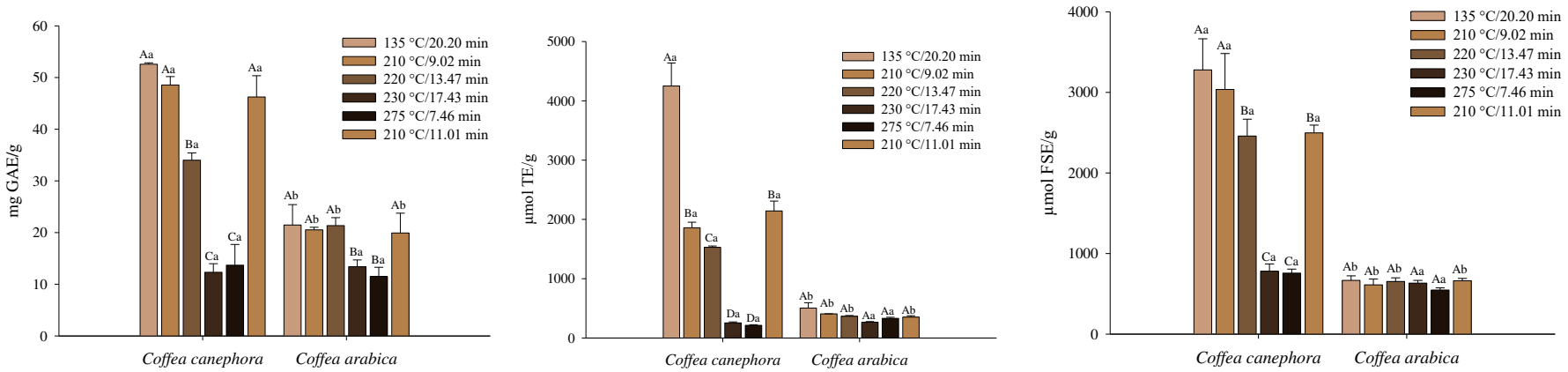

Figure 2. Total phenolic content (TPC) (A); DPPH radical scavenging activity (B); Ferric Reducing Antioxidant Power (FRAP) (C) of two coffee species after different roasting treatments. Lowercase letters represent Tukey's test at 5% probability between species and uppercase letters between treatments for the same species.

3.3. Caffeine, caffeoylquinic acid (5-CQA), trigonelline, caffeic acid, and HMF in roast and ground coffee

Aiming to evaluate whether the applied roasting process affected the caffeine, 5-CQA, trigonelline, caffeic acid, and HMF concentration, the analysis was carried out in HPLC.

Caffeine contents in roasted and ground coffee samples varied in a wide range from 9.27 mg/g to 33.29 mg/g in Robusta coffee and from 5.55 mg/g to 10.15 mg/g in coffee Arabica, with the highest content found in roasting at 135 °C/20.20 min for Robusta and at 220 °C/13.47 min for Arabica. (Table 3). The presence of caffeine in the roasts may be due to the compound thermostability and the loss of mass of thermolabile compounds due to the roasting temperature applied [41]. The presence of caffeine in the samples may be due to the compound thermostability and the loss of mass of thermolabile compounds due to the roasting temperature applied [41]. Notably, this compound's thermal resistance was predominantly higher in almost all treatments in relation to caffeic acids and 5-CQA, as well as trigonelline and HMF, under the pre-established roasting conditions (Table 3). As reported, the coffee samples caffeine content in both species was in agreement with the ranges reported in the literature [42] [21], with higher values in Robusta coffee.

The highest levels of 5-CQA were observed in Robusta coffee at roasting profiles of 135 °C/20.20 min, 210 °C/11.01 min, and 210 °C/9.02 min, with average values of 17, 27, 15.03, and 17.67 mg/g, respectively. The results also indicated that there was a significant decrease ($p<0.05$) of 5-CQA at higher temperatures of 220 °C/13.47 min, 230 °C/17.43 min, and 275° C/7.46 min (Table 3). Concentrations of 5-CQA decrease drastically when more severe roast conditions (between 180-200 °C) are used in the process of obtaining the roasted coffee powder, with Robusta coffee being the species with a slightly higher amount of chlorogenic acids (CQAs) [43].

Table 3. Caffeine, caffeoylquinic acid (5-CQA), trigonelline, caffeic acid and hydroxymethylfurfural (HMF) (mg/g) content in *canephora* (Robusta) and *arabica* coffee variety Catúai affected by different degrees of roasting.

Samples	135 °C/20.20 min	210 °C/9.02 min	220 °C/13.47 min	230 °C/17.43 min	275 °C/7.46 min	210 °C/11.01 min
Caffeine						
C. canephora	33.29 ± 0.50^{Aa}	31.16 ± 2.29^{Aa}	19.27 ± 2.24^{Ab}	12.40 ± 1.63^{Abc}	9.27 ± 0.10^{Ac}	30.19 ± 2.28^{Aa}
C. arábica	5.55 ± 2.09^{Ba}	6.71 ± 1.95^{Ba}	10.15 ± 2.18^{Ba}	6.19 ± 1.18^{Ba}	9.33 ± 0.12^{Aa}	7.19 ± 0.37^{Ba}
5-CQA						
C. canephora	17.27 ± 0.19^{Aa}	17.67 ± 1.5^{Aa}	10.26 ± 2.15^{Ab}	3.50 ± 0.08^{Ac}	0.93 ± 0.05^{Ac}	15.03 ± 1.15^{Aab}
C. arábica	6.03 ± 2.05^{Bab}	7.08 ± 1.92^{Bab}	8.85 ± 1.13^{Aa}	2.13 ± 0.98^{Ab}	3.07 ± 1.58^{Aab}	6.11 ± 1.06^{Bab}
Trigonelline						
C. canephora	9.11 ± 0.12^{Aa}	9.72 ± 0.75^{Aa}	6.47 ± 0.41^{Ab}	4.36 ± 0.07^{Ab}	1.27 ± 0.03^{Ac}	5.34 ± 0.06^{Ab}
C. arábica	5.02 ± 1.39^{Bab}	3.95 ± 0.00^{Bab}	5.73 ± 0.00^{Aa}	2.59 ± 0.82^{Bbc}	0.94 ± 0.02^{Ac}	5.58 ± 0.39^{Aa}
Caffeic acid						
C. canephora	0.08 ± 0.02^{Ab}	0.55 ± 0.11^{Aa}	0.00 ± 0.00^{Ab}	0.00 ± 0.00^{Ab}	0.00 ± 0.00^{Ab}	0.42 ± 0.02^{Aa}
C. arábica	0.00 ± 0.00^{Aa}	0.00 ± 0.00^{Ba}	0.00 ± 0.00^{Aa}	0.00 ± 0.00^{Aa}	0.00 ± 0.00^{Aa}	0.00 ± 0.00^{Ba}
HMF						
C. canephora	0.27 ± 0.22	0.06 ± 0.05	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.02 ± 0.01
C. arábica	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00

Means followed by the same lowercase letters in the row and uppercase letters in the column do not differ by Tukey's test ($p>0,05$).

In the present study, Robusta coffee had a higher trigonelline content in almost all roasting profiles, with the highest levels found in coffees roasted at mild temperatures, especially in roasting profiles 135 °C/20.20 min and 210 °C/9.02 min, with values of 9.11 and 9.72 mg/g, respectively. Arabica coffee had lower trigonelline content (Table 3). The local climate, species, temperature, and roasting time can perform an important role in trigonelline content [44], which possibly explains the higher trigonelline content in Robusta coffee. Caffeic acid is a hydroxycinnamic compound that partially originates from the hydrolysis of caffeoylquinic and dicaffeoylquinic acids of roasting technique [36] and is found in low levels. Minimum contents of this compound were found in the analyzed Robusta coffee samples. In Arabica coffee samples, the compound was not found (Table 3). It was verified the absence of HMF in the Arabica coffee used in this study in all roasting profiles and a minimum amount of this compound in Robusta coffee, showing the ability of this compound to decompose quickly. These results indicated that the coffee species and temperatures employed did not interfere with the concentration of HMF, thus resulting in a non-significant interaction. The HMF degradation could have occurred from the reaction between the furan compound and the amino acid decomposition products or compact with sugar alcohols and nitrogen-free polymer to trigger flavor compounds and melanoidins [45].

For the analysis of composition and caffeine, trigonelline, 5-CQA, caffeic acid, and HMF levels, in order to investigate the correlation between the studied parameters, the statistical method known as Principal Component Analysis (PCA) was employed. This procedure allowed for a graphical evaluation of the variable values' dispersions with respect to component 1 and component 2 through a visual representation on the PCA score plot (Fig. 3).

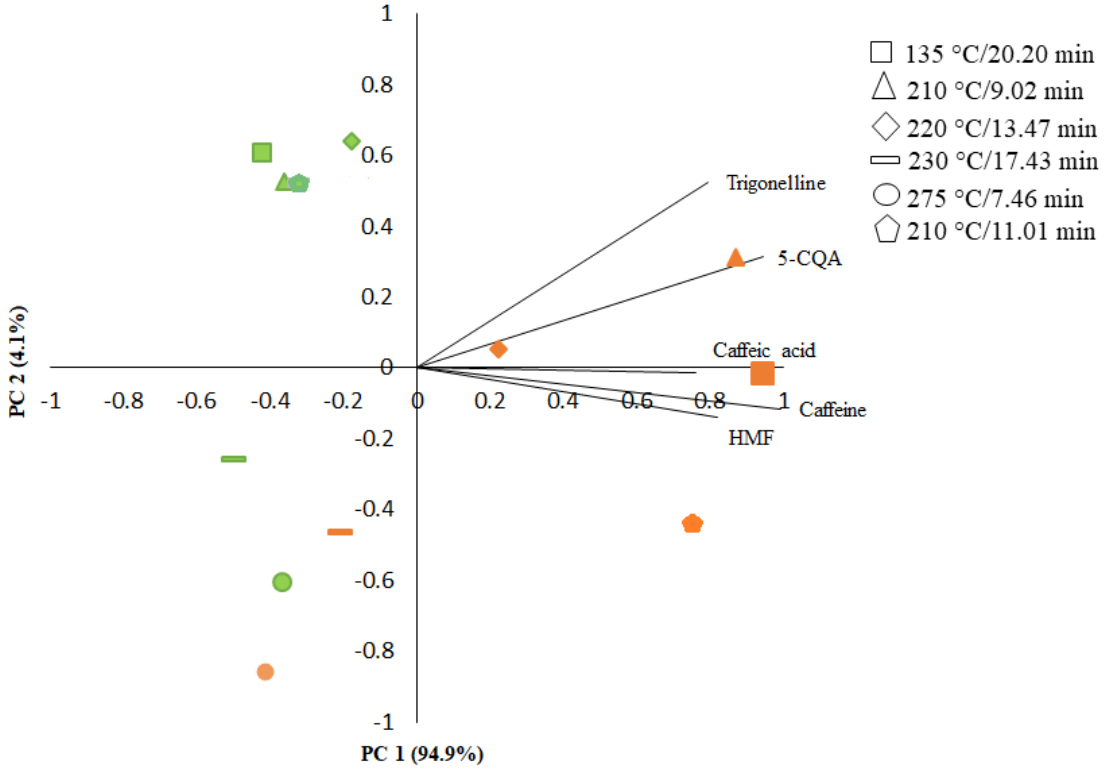

Figure 3. Scatter plot of Principal Component Analysis (PCA) scores of chemical compounds for Robusta and Arabica coffee samples after different roasting treatments (PC1 vs. PC2).

Figure 3 illustrates the PCA score plot, where the samples are represented in a two-dimensional space formed by two axes or coordinate components. In this context, samples that cluster closely to these components possibly share similar chemical concentrations. It was observed that the first principal component (PC1) was able to explain 94.9 % of the variation present in the data, while the second principal component (PC2) explained only 4.1 % of the variation. This finding reinforces the representativeness of the analysis performed.

Consequently, it was observed that the analyzed chemical compounds presented higher concentrations in Robusta coffee. Additionally, it is noteworthy that temperature played a relevant role in altering the concentrations of the chemical compounds, with roasting at 275 °C/7.46 min being the most drastic condition for the reduction of these compounds.

These results underscore the importance of PCA as a valuable tool in investigating the chemical composition and variations of components in different coffee samples, providing a more comprehensive and precise understanding of the factors influencing the quality and chemical profile of this globally cherished beverage.

4. Conclusion

The present study investigated the physicochemical changes during the roasting process of Robusta and Arabica coffees. In general, TPC gradually reduced with the addition of temperature and roasting time for both species. Robusta coffee showed higher antioxidant capacity than arabica coffee samples, except for profiles 230 °C/17.43 and 275 °C/7.46 min, in which both samples showed equivalent antioxidant capacity in all methods applied. Robusta coffee samples were characterized as lighter and with higher chroma and hue values. The thermal resistance of caffeine was higher than that of chlorogenic (5-CQA) and caffeic acids. Robusta coffee samples in all roasting profiles showed higher values of trigonelline content. In Arabica coffee, the absence of HMF was verified in all roasting profiles. The results showed that different roasting profiles directly influence the physicochemical characteristics and antioxidant properties of coffee.

References

[1] CONAB, COMPANHIA NACIONAL DE ABASTECIMENTO, https://www.conab.gov.br. (2020). Access: 29 mar. 2019.

[2] X. Wang, L.-T. Lim, Y. Fu, Review of Analytical Methods to Detect Adulteration in Coffee, J. AOAC Int. 103 (2020) 295–305. https://doi.org/10.1093/jaocint/qsz019.

[3] H.O. Agunbiade, T.N. Fagbemi, T.A. Aderinola, Antioxidant properties of beverages from graded mixture of green/roasted coffee and hibiscus sabdariffa calyx flours, Appl. Food Res. 2 (2022) 100163. https://doi.org/10.1016/j.afres.2022.100163.

[4] H. Endeshaw, A. Belay, Optimization of the roasting conditions to lower acrylamide content and improve the nutrient composition and antioxidant properties of Coffea arabica, PLoS One. 15 (2020) e0237265. https://doi.org/10.1371/journal.pone.0237265.

[5] A.E. Muñoz, S.S. Hernández, A.R. Tolosa, S.P. Burillo, M. Olalla Herrera, Evaluation of differences in the antioxidant capacity and phenolic compounds of green and roasted coffee and their relationship with sensory properties., LWT. 128 (2020) 109457. https://doi.org/10.1016/j.lwt.2020.109457.

[6] Y.-C. Liao, T. Kim, J.L. Silva, W.-Y. Hu, B.-Y. Chen, Effects of roasting degrees on phenolic compounds and antioxidant activity in coffee beans from different geographic origins, LWT. 168 (2022) 113965. https://doi.org/10.1016/j.lwt.2022.113965.

[7] S. Pastoriza, J.A. Rufián-Henares, Contribution of melanoidins to the antioxidant

capacity of the Spanish diet, Food Chem. 164 (2014) 438–445. https://doi.org/10.1016/j.foodchem.2014.04.118.

[8] A. Ahmad, N. Mahmood, M. Hussain, U. Aiman, S.H. Al-Mijalli, M.A. Raza, E. Al Jbawi, Improvement in oxidative stability and quality characteristics of functional chicken meat product supplemented with aqueous coriander extract, Int. J. Food Prop. 26 (2023) 855–865. https://doi.org/10.1080/10942912.2023.2189086.

[9] C. Liu, N. Yang, Q. Yang, C. Ayed, R. Linforth, I.D. Fisk, Enhancing Robusta coffee aroma by modifying flavour precursors in the green coffee bean, Food Chem. 281 (2019) 8–17. https://doi.org/10.1016/j.foodchem.2018.12.080.

[10] C. Liu, Q. Yang, R. Linforth, I.D. Fisk, N. Yang, Modifying Robusta coffee aroma by green bean chemical pre-treatment, Food Chem. 272 (2019) 251–257. https://doi.org/10.1016/j.foodchem.2018.07.226.

[11] J. Aguiar, B.N. Estevinho, L. Santos, Microencapsulation of natural antioxidants for food application – The specific case of coffee antioxidants – A review, Trends Food Sci. Technol. 58 (2016) 21–39. https://doi.org/10.1016/j.tifs.2016.10.012.

[12] D.R. Seninde, E. Chambers, Coffee Flavor: A Review, Beverages. 6 (2020) 44. https://doi.org/10.3390/beverages6030044.

[13] J.V. Malaquias, S.M.C. Celestino, M.F.F. Xavier, Optimization of the roasting conditions of arabica coffee cultivated in the cerrado area of Brazil, Brazilian J. Food Technol. 21 (2018). https://doi.org/10.1590/1981-6723.16216.

[14] E. Nakilcioglu-tas, S. Otles, Physical characterization of Arabica ground coffee with different roasting degrees, An. Acad. Bras. Cienc. 91 (2019). https://doi.org/10.1590/0001-3765201920180191.

[15] F.M. Mehaya, A.A. Mohammad, Thermostability of bioactive compounds during roasting process of coffee beans, Heliyon. 6 (2020) e05508. https://doi.org/10.1016/j.heliyon.2020.e05508.

[16] D. Giacalone, T.K. Degn, N. Yang, C. Liu, I. Fisk, M. Münchow, Common roasting defects in coffee: Aroma composition, sensory characterization and consumer perception, Food Qual. Prefer. 71 (2019) 463–474. https://doi.org/10.1016/j.foodqual.2018.03.009.

[17] J. de C.G. Rocha, F.A.R. de Barros, Í.T. Perrone, K.W.C. Viana, G.M. Tavares, R. Stephani, P.C. Stringheta, Microencapsulation by atomization of the mixture of phenolic extracts, Powder Technol. 343 (2019) 317–325. https://doi.org/10.1016/j.powtec.2018.11.040.

[18] V.L.& R.J.A.J. Singleton, Colorimetry of Total Phenolics with Phosphomolybdic-Phosphotungstic Acid Reagents, Am. J. Enol. Vitic. 16 (1965) 144–158.

[19] D.-O. Kim, K.W. Lee, H.J. Lee, C.Y. Lee, Vitamin C Equivalent Antioxidant Capacity (VCEAC) of Phenolic Phytochemicals, J. Agric. Food Chem. 50 (2002) 3713–3717. https://doi.org/10.1021/jf020071c.

[20] M.. V.J.. C.S.. M.D. Boroski, Antioxidantes: Princípios e Métodos Analíticos, 1st ed., appris, n.d.

[21] J.A. Vignoli, M.C. Viegas, D.G. Bassoli, M. de T. Benassi, Roasting process affects differently the bioactive compounds and the antioxidant activity of arabica and robusta coffees, Food Res. Int. 61 (2014) 279–285. https://doi.org/10.1016/j.foodres.2013.06.006.

[22] W. Dong, R. Hu, Z. Chu, J. Zhao, L. Tan, Effect of different drying techniques on bioactive components, fatty acid composition, and volatile profile of robusta coffee beans, Food Chem. 234 (2017) 121–130. https://doi.org/10.1016/j.foodchem.2017.04.156.

[23] A.T. Toci, A. Farah, Volatile fingerprint of Brazilian defective coffee seeds: corroboration of potential marker compounds and identification of new low quality indicators, Food Chem. 153 (2014) 298–314. https://doi.org/10.1016/j.foodchem.2013.12.040.

[24] N.C. Bicho, A.E. Leitão, J.C. Ramalho, F.C. Lidon, Use of colour parameters for roasted coffee assessment, Food Sci. Technol. 32 (2012) 436–442. https://doi.org/10.1590/S0101-20612012005000068.

[25] P. Wongsa, N. Khampa, S. Horadee, J. Chaiwarith, N. Rattanapanone, Quality and bioactive compounds of blends of Arabica and Robusta spray-dried coffee, Food Chem. 283 (2019) 579–587. https://doi.org/10.1016/j.foodchem.2019.01.088.

[26] M.C.. P.M.P. Cid, Coffee: analysis and composition, Encycl. Food Heal. (2016) 225–23.

[27] G. Budryn, E. Nebesny, A. Podsędek, D. Żyżelewicz, M. Materska, S. Jankowski, B. Janda, Effect of different extraction methods on the recovery of chlorogenic acids, caffeine and Maillard reaction products in coffee beans, Eur. Food Res. Technol. 228 (2009) 913–922. https://doi.org/10.1007/s00217-008-1004-x.

[28] A. Patras, N.P. Brunton, C. O'Donnell, B.K. Tiwari, Effect of thermal processing on anthocyanin stability in foods; mechanisms and kinetics of degradation, Trends Food Sci. Technol. 21 (2010) 3–11. https://doi.org/10.1016/j.tifs.2009.07.004.

[29] M. Zhu, Y. Long, Y. Ma, Y. Chen, Q. Yu, J. Xie, B. Li, J. Tian, Comparison of chemical

and fatty acid composition of green coffee bean (Coffea arabica L.) from different geographical origins, LWT. 140 (2021) 110802. https://doi.org/10.1016/j.lwt.2020.110802.

[30] E. Bertone, A. Venturello, A. Giraudo, G. Pellegrino, F. Geobaldo, Simultaneous determination by NIR spectroscopy of the roasting degree and Arabica/Robusta ratio in roasted and ground coffee, Food Control. 59 (2016) 683–689. https://doi.org/10.1016/j.foodcont.2015.06.055.

[31] Z. Sandoval, F. Prieto, J. Betancur, Digital Image Processing for Classification of Coffee Cherries, in: 2010 IEEE Electron. Robot. Automot. Mech. Conf., IEEE, 2010: pp. 417–421. https://doi.org/10.1109/CERMA.2010.54.

[32] C. Zheng, D.-W. Sun, L. Zheng, Recent developments and applications of image features for food quality evaluation and inspection – a review, Trends Food Sci. Technol. 17 (2006) 642–655. https://doi.org/10.1016/j.tifs.2006.06.005.

[33] D. Wu, D.-W. Sun, Colour measurements by computer vision for food quality control – A review, Trends Food Sci. Technol. 29 (2013) 5–20. https://doi.org/10.1016/j.tifs.2012.08.004.

[34] T.M. Kieu Tran, T. Kirkman, M. Nguyen, Q. Van Vuong, Effects of drying on physical properties, phenolic compounds and antioxidant capacity of Robusta wet coffee pulp (Coffea canephora), Heliyon. 6 (2020) e04498. https://doi.org/10.1016/j.heliyon.2020.e04498.

[35] S. Andueza, C. Cid, M. Cristina Nicoli, Comparison of antioxidant and pro-oxidant activity in coffee beverages prepared with conventional and “Torrefacto” coffee, LWT - Food Sci. Technol. 37 (2004) 893–897. https://doi.org/10.1016/j.lwt.2004.04.004.

[36] J.A. Vignoli, D.G. Bassoli, M.T. Benassi, Antioxidant activity, polyphenols, caffeine and melanoidins in soluble coffee: The influence of processing conditions and raw material, Food Chem. 124 (2011) 863–868. https://doi.org/10.1016/j.foodchem.2010.07.008.

[37] K.L. Wolfe, R.H. Liu, Cellular Antioxidant Activity (CAA) Assay for Assessing Antioxidants, Foods, and Dietary Supplements, J. Agric. Food Chem. 55 (2007) 8896–8907. https://doi.org/10.1021/jf0715166.

[38] J. Pokorná, P.R. Venskutonis, V. Kraujalyte, P. Kraujalis, P. Dvorák, B. Tremlová, V. Kopriva, M. Oštádalová, Comparison of different methods of antioxidant activity evaluation of green and roast C. Arabica and C. Robusta coffee beans, Acta Aliment. 44 (2015) 454–460. https://doi.org/10.1556/066.2015.44.0017.

[39] N.N. Batista, D.P. de Andrade, C.L. Ramos, D.R. Dias, R.F. Schwan, Antioxidant capacity of cocoa beans and chocolate assessed by FTIR, Food Res. Int. 90 (2016) 313–319. https://doi.org/10.1016/j.foodres.2016.10.028.

[40] A.P.P. Bressani, N.N. Batista, G. Ferreira, S.J. Martinez, J.B.P. Simão, D.R. Dias, R.F. Schwan, Characterization of bioactive, chemical, and sensory compounds from fermented coffees with different yeasts species, Food Res. Int. 150 (2021) 110755. https://doi.org/10.1016/j.foodres.2021.110755.

[41] T.W.M. Crozier, A. Stalmach, M.E.J. Lean, A. Crozier, Espresso coffees, caffeine and chlorogenic acid intake: potential health implications, Food Funct. 3 (2012) 30–33. https://doi.org/10.1039/C1FO10240K.

[42] Farah. A., Coffee constituents, Coffee: Emerging health effects and disease prevention, Wiley-Blackwell, Oxford, 2012.

[43] A. Farah, T. de Paulis, L.C. Trugo, P.R. Martin, Effect of Roasting on the Formation of Chlorogenic Acid Lactones in Coffee, J. Agric. Food Chem. 53 (2005) 1505–1513. https://doi.org/10.1021/jf048701t.

[44] M. Murkovic, M.-A. Bornik, Formation of 5-hydroxymethyl-2-furfural (HMF) and 5-hydroxymethyl-2-furoic acid during roasting of coffee, Mol. Nutr. Food Res. 51 (2007) 390–394. https://doi.org/10.1002/mnfr.200600251.

[45] D. Rigo, D. Polidoro, A. Perosa, M. Selva, Diversified upgrading of HMF via acetylation, aldol condensation, carboxymethylation, vinylation and reductive amination reactions, Mol. Catal. 514 (2021) 111838. https://doi.org/10.1016/j.mcat.2021.111838.

Artigo 3*

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Post-harvest roasting conditions: evaluation of carbohydrate, organic acid, and melanoidin composition and their levels in *Coffea canephora* and *Coffea arabica*

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Graphical abstract

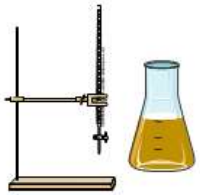
C. canephora and *C. arabica*

Roasting

Milling

Sample preparation

Extract preparation

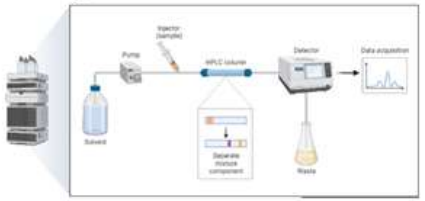


Titratable acidity

Moisture

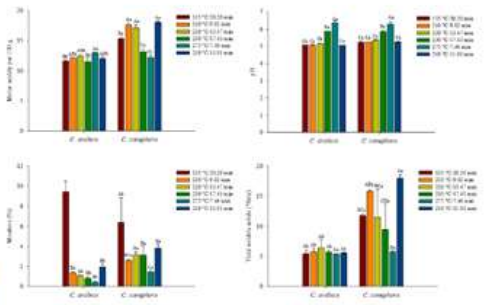
pH

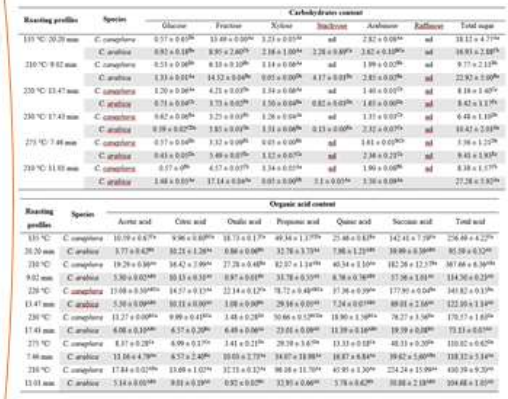
Total solids

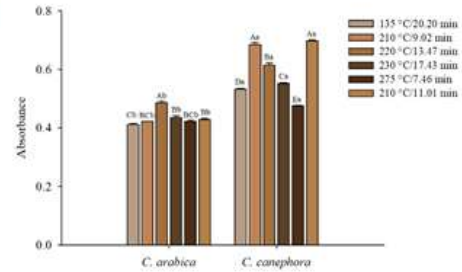


HPLC

Melanoidins (Abs_{420})







Abstract

The post-harvest techniques used to process coffee beans have a significant impact on their physicochemical characteristics. Furthermore, the roasting stage plays a fundamental role in transforming the composition of the beans. Therefore, this study investigated the influence of different roasting time and temperature profiles on the physicochemical characteristics, sugar and organic acid concentrations, and melanoidins of coffee beans (*C. canephora* and *C. arabica*). The results showed that both the roasting profiles and coffee species strongly influenced all the parameters investigated, especially sugar concentrations, organic acids, and melanoidins. Results related to sugars, organic acids, and melanoidins showed connections with different roasting profiles. Succinic acid was the organic compound with the highest concentrations, with the highest concentration observed in *C. canephora* at 210 °C/11.01 min (224.24 mg/g), with the highest concentrations of organic acids found in this same roasting profile and species (430.39 mg/g). Fructose was the sugar with the highest concentration, particularly in the 210 °C/11.01 min roast, which exhibited 17.14 mg/g. The highest melanoidin content was also found in this same roasting profile and species. Expanding on this perspective, all evaluations of concentrations and physicochemical properties proved capable of distinguishing between the species and roasting processes employed. Ultimately, post-harvest roasting procedures emerged as the determinants of the characteristic chemical profile differences between *C. canephora* and *C. arabica*.

Keywords: Acids; Sugars; Arabica Coffee; Robusta Coffee; Melanoidins; Coffee Chemistry.

1. Introduction

Coffee belongs to the Coffea gender, a genus with over 80 species belonging to the *Rubiaceae* family. Among the many species, the most well-known are robusta (*Coffea canephora*) and arabica (*Coffea arabica*). Both species are traded worldwide and represent a total of 99 % of coffee production, highlighting their potential in the global economy (Farah, 2012; Jayakumar et al., 2017; Jeszka-Skowron et al., 2016; Klól et al., 2020). Due to stable and high yields, coffee has become one of the main cultivars with the highest production in Brazil, with global consumption estimated at over 163,141 thousand 60 kg bags in 2020/2021 (USDA, 2021; USDA, 2021). It is essential to study coffee as consumers are increasingly willing to invest in coffees with pleasant and unique sensory characteristics (Gatti & Croijmans 2022; Hazebroek et al., 2023).

The flavor of coffee depends on the composition and levels of soluble sugars and organic acids, with variations in both resulting in different characteristics in the final product (Borém et al., 2016; Ribeiro et al., 2018). The sugars sucrose, fructose, and glucose are the most abundant in coffee berries (Bressani et al., 2018; Mussato et al., 2011). The main organic acids present are lactic, quinic, tartaric, acetic, citric, and others (Ribeiro et al., 2018; Yeager et al., 2021). The effect of fruit composition is complex, and the key compounds responsible for coffee acidity are non-volatile organic acids and low molecular weight organic acids, both contributing to the liveliness of the beverage, primarily influencing the characteristic flavor and aroma of the product (Cardoso et al., 2021; Borém et al., 2016; Ginz et al., 2000; Vitzthum et al., 1975). The formation of these compounds is evident from the early stages of grain maturation, followed by processing, beneficiation, post-harvest handling, roasting, and product infusion, with these processes being relevant to the sweetness and acidity of the final drink (Avelino et al., 2005).

However, a significant puzzle still remains regarding the intricate compositions of sugars, organic acids, and melanoidins in coffee beans, as well as their variations among different coffee species and how these components are impacted by the roasting process. This study aims not only to unravel these mysteries but also to provide a reference framework for understanding the concentrations of sugars and organic acids in C. canephora and C. arabica coffee varieties by subjecting the raw material to various temperature and time conditions during the post-harvest roasting process.

2. Materials e methods

2.1. Materials

The *Coffea arabica* variety Catuaí and *Coffea canephora* variety Pierre were harvested at the stage of ripeness considered ideal on properties in the city of São Geraldo, located in the Southeastern region of Minas Gerais, Brazil.

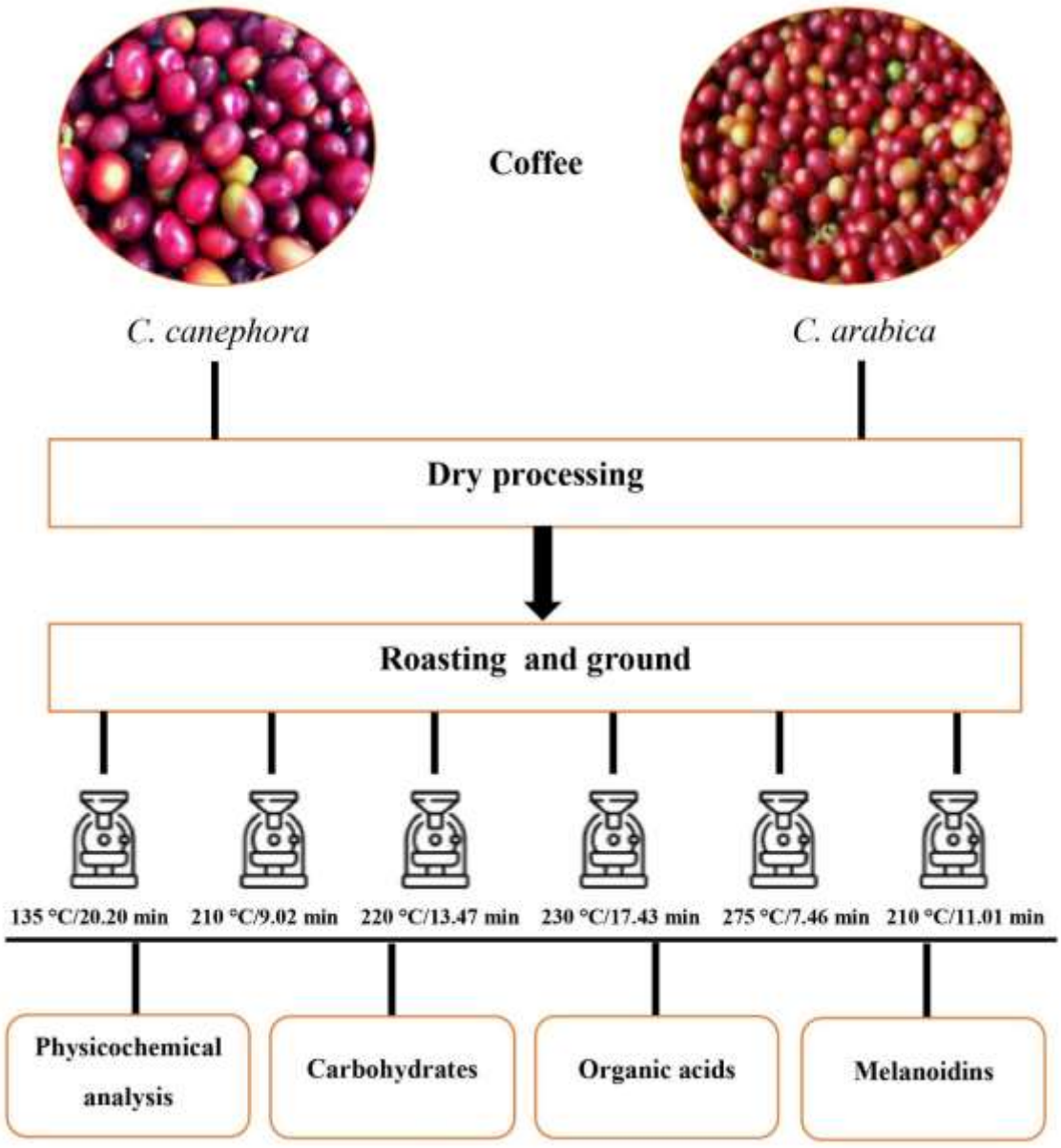


Figure 1. Experimental design.

For the processing of the beans, a Probat drum roaster (Probat-Werke) (Fig. 1) was used. After this process, the samples were individually packaged in airtight, odor-free packaging, transported to the Natural Dyes and Bioactive Compounds Laboratory (LacBio) at the Department of Food Technology of the Federal University of Viçosa (UFV), and stored at 5 °C for subsequent analysis. Different roasting profiles were obtained by varying temperature and time (Table 1). The selection of temperatures was guided by specific criteria. Initially, a review of the existing scientific literature was conducted to identify gaps and inconsistencies in preexisting studies. The approach covered a spectrum ranging from lower temperatures to substantially higher ones, aiming for a comprehensive understanding of the effects on coffee. Additionally, relevant chemical transition thresholds for compounds present in coffee were considered, as well as temperatures that might have practical relevance from an industry perspective. Meteorological data for the region at the time of harvest are presented (Table 2) (INMET, 2023).

Table 1. Roasting profile with respective time/temperature binomial.

Roasting profile	Roasting Temperature (°C)	Start time: 1° CRACK (min)	Total roasting time (min)
T1	135	2.16	20.20
T2	210	0.13	9.02
T3	220	4.55	13.47
T4	230	6.20	17.43
T5	275	1.56	7.46
T6	210	2.38	11.01

Table 2. Meteorological data for the region in the month of July in the coffee harvest region.

Metereological data	**Value**
Accumulated Precipitation	26.3 mm
Maximum temperature	22.4 °C
Average temperature Relative	16.4 °C
Minimum temperature	11.3 °C
Relative humidity	80.8 %
ATM pressure	1029.9mb

2.2. Reagentes

Acetic acid, citric acid, isovaleric acid, lactic acid, malic acid, oxalic acid, propionic acid, quinic acid, succinic acid, and tartaric acid standards, as well as arabinose, stachyose, fructose, glucose, xylose, raffinose, and HPLC-grade acetonitrile (CH_3CN-HPLC gradient), and phosphoric acid (H_3PO_4 85%) were obtained from Sigma-Aldrich (St. Louis, MO, USA). Sodium hydroxide (NaOH) was purchased from Synth (Diadema, Brazil).

2.3. Preparation of the extract

The coffee extracts were obtained through solid-liquid extraction using 100 °C ultrapure water. Five grams of each coffee powder sample were weighed and diluted in 20 mL of ultrapure water. Subsequently, the mixtures were centrifuged at 10,000 x g for 10 min (Silva et al., 2008). The extracts were immediately cooled and filtered through a 0.2 μm cellulose acetate filter for chromatographic analysis.

2.4. Titratable acidity, pH, moisture, and soluble solids

The acidity was determined by titration with 0.1 N NaOH. The results were expressed in mL of 0.1 N NaOH per 100 g of the sample. The pH was measured using a DM-20 pH meter (Digimed, São Paulo, Brazil). Moisture content was determined by the standard oven method at 105 °C for 24 hours. The soluble solids content was determined using a digital refractometer AR200 (Leica, São Paulo, Brazil) according to the technique described by AOAC (1990).

2.5. Analysis of carbohydrate variation

The monomers of sugars were quantified using High-Performance Liquid Chromatography (HPLC). This process was carried out on the Shimadzu CBM-20A/20Alite chromatograph equipped with a RID-20A refractive index detector (Shimadzu).

The quantification of monomeric sugars was performed using the BioRad Aminex7 HPX87H column. The flow rate was set at 0.6 mL/min, and the oven temperature was adjusted to 45 °C. Elution was done isocratically using a 0.005 mol/L sulfuric acid solution, following the protocol established by Alyammahi et al., (2023), known for enabling the separation and detection of sugars by refractive index.

The calibration curves obtained for the sugars showed a linearity range between concentrations of 0.1 g/L to 10 g/L. The equations for the calibration curves were as follows: arabinose: y = 111245x + 1495.2, with R^2 = 0.9999; stachyose: y = 126912x + 103425, with R^2 = 0.9848; fructose: y = 120753x + 11839, with R^2 = 0.9973; glucose: y = 138289x + 814.48, with R^2 = 0.9979; and xylose: y = 112158x + 5632.1, with R^2 = 0.9997; raffinose: y = 114705x + 202955, with R^2 = 0.9333. These standards served as references for quantifying the sugars present in the study sample.

2.6. Analysis of organic acid variation by UPLC

The analyses were performed using High-Performance Liquid Chromatography (HPLC) on a Thermo Scientific Accela LC system (with a Diode Array Detector (DAD), auto-injector, and Accela pump) (Thermo Fisher Scientific, Austin, TX). The column used for separation was the Lichrospher 100 RP-18 reverse-phase column (250 x 4.6 mm, with a particle size of 5 µm and a pore size of 10 nm) (Merck, Germany). The mobile phase consisted of water acidified with 0.1 % phosphoric acid. The flow rate was 600 µL/min, and the injection volume was 2 µL (partial loop), with a temperature of 25 °C for the injector and 50 °C for the column. Peaks were detected at a wavelength of 210 nm. Peak identification was done by comparing the retention time in the chromatogram and the ultraviolet spectra to those of separately injected standards. The concentration of oxalic acid, quinic acid, acetic acid, citric acid, succinic acid, and propionic acid was calculated based on the area of each peak at 210 nm using a calibration curve. The calibration curves obtained for oxalic acid, quinic acid, acetic acid, citric acid, succinic acid, and propionic acid showed a linear range between concentrations of 100 mg/L and 8000 mg/L. The equations for the calibration curves were as follows: oxalic acid: y = 3203.5x + 435068, with R^2 = 0.9905; quinic acid: y = 178.69x - 26232, with R^2 = 0.9923; acetic acid: y = 212.19x + 15254, with R^2 = 0.9990; citric acid: y = 438.65x + 46680, with R^2 = 0.9990; succinic acid: y = 92.684x + 11416, with R^2 = 0.9980; and propionic acid: y = 201.56x + 14884, with R^2 = 0.9988.

2.7. Melanoidins

200 µL of coffee extracts were diluted in 4 mL of distilled water. The darkened compounds were quantified by measuring the absorbance at 420 nm (UV-M51, Bel Photonics, Monza, Italy) (Ludwig et al., 2013).

2.8. Statistical analysis

The experimental design adopted was completely randomized in a double factorial scheme (2x6), with the first factor being coffee species and the second factor being roasting profiles. The data were analyzed by analysis of variance (ANOVA), and the means of three replicates were subjected to the Tukey test at a 5 % probability level. The statistical analysis was conducted using the R program (R Core Team, Vienna, Austria). Principal component analysis (PCA) based on the Pearson correlation matrix was performed to observe differences between the coffee samples using the R program (R Core Team, Vienna, Austria).

3. Results and discussion

3.1. Acidity, pH, moisture, and soluble solids

The values of acidity, pH, moisture, and soluble solids found for roasted and ground coffee samples at different temperature levels are presented in Figure 2.

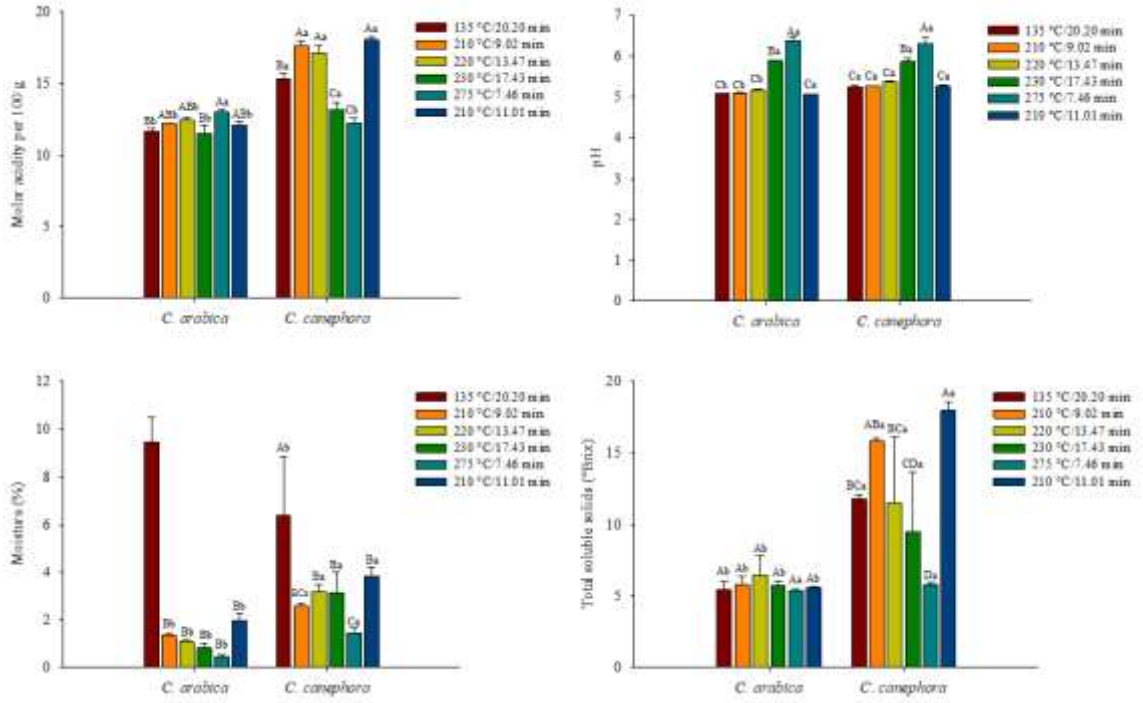


Figure 2. Physicalchemical characteristics of *canephora* (Robusta) and *arabica* coffee variety Catúai affected by different degrees of roasting. Means followed by the same lowercase letters within different species and the same roasting profiles, and uppercase letters within the same species and all roasting profiles do not differ according to Tukey's test ($p > 0.05$).

The acidity in *C. arabica* showed lower values compared to *C. canephora*, except at the roasting temperature of 275 °C /7.46 min. Coffee acidity is a relevant parameter in determining the characteristic flavor of the final product, along with other attributes such as sweetness, bitterness, and saltiness (Dong et al., 2017; Kim et al., 2021). The acidity of roasted coffee depends on the species and variety, although they contain comparable amounts of carboxylic acids (Park et al., 2019; Park et al., 2023). Furthermore, the roasting process tends to increase the concentration of volatile acids, as the degradation of sugars occurs in this process, and it is reported that the concentration of volatile acids is higher at temperatures close to the standard method (210 °C) and decreases with increasing temperature due to the breakdown of chlorogenic acids (Badmos et al., 2019). This phenomenon was observed in *C. canephora*, which showed higher acidity values at roasting profiles of 210 °C/9.02 min, 210 °C/11.01 min, and 220 °C/17.43 min.

In relation to the pH results in the analyzed coffee species, no significant difference was observed ($p>0.05$) between the roasting temperatures of 230 °C/17.43 min and 275 °C/7.46 min for *C. canephora* and *C. arabica*, respectively, in which both exhibited higher values.The pH value for *C. canephora* ranged from 5.25 to 6.30, while for *C. arabica*, it ranged from 5.08 to

6.38 (Fig. 2). With an increase in roasting temperature and the consequent degradation of acids, it is evident that lower pH values are obtained. It is worth noting that the average pH of Brazilian coffee is 5.0 (Brollo et al., 2008). Additionally, the intensity of acidity varies between the *C. arabica* and *C. canephora* species, with *C. canephora* having higher acidity (Babova et al., 2016). The low pH may be related to the use of mild roasting temperatures, but other conditions, besides the degree of roasting, can also modify pH, such as different preparation methods for the same coffee samples (Cordoba et al., 2021; Rune et al., 2023).

When considering the effect of roasting temperature on the percentage of moisture, this parameter did not show a significant effect ($p>0.05$) with an increase in roasting temperature from profiles of 210 °C/9.02 min to 275 °C/7.46 min for the *C. arabica* species. Comparing the two species, *C. canephora* had a higher moisture percentage ($p<0.05$), ranging from 3.82 % to 1.44 %, while *C. arabica* ranged from 1.95% to 0.46%. When the temperature of 135 °C/20.20 min was applied, *C. canephora* and *C. arabica* had 6.36 % and 9.45 % moisture, respectively, with *C. arabica* significantly wetter at this temperature/time (Fig. 2). During roasting, coffee beans lose 14 % to 20 % of their mass due to a decrease in moisture content and changes in their carbohydrate, oil, and protein composition (Belitz et al., 2009). The roasting process of food materials is favorable for providing a crispy texture through chemical modifications, including reducing moisture content, which can lead to a crisper and more fragile structure (Mosayebi et al., 2018). However, coffee subjected to the roasting process has a highly hygroscopic matrix, quickly adsorbing water when interacting with its environment during storage, and this process can result in changes in the freshness of the coffee. Nevertheless, with an increase in roasting temperature, coffee becomes less hygroscopic (Collazos-Escobar et al., 2022; Iaccheri et al., 2015).

The soluble solids content represents the concentration of sugars, organic acids, and other minor constituents (Clifford et al., 1979). In this study, the concentrations of soluble solids in *C. arabica* ranged from 5.36 to 6.43 °Brix, but no significant difference ($p>0.05$) was observed between roasting profiles. The concentrations of soluble solids in *C. canephora* ranged from 5.76 to 17.96 °Brix. The highest concentration was found in the roasting profile at 210 °C/11.01 min, and the lowest concentration was in the profile at 275 °C/7.46 min. As observed, the concentrations of soluble solids decreased with higher roasting temperatures due to the loss of chemical constituents during the roasting process at high temperatures (Murthy et al., 2019).

3.2. Composition of carbohydrates

The compositions of carbohydrates in the *C. canephora* and *C. arabica* species subjected to different roasting profiles were determined using HPLC. Raffinose sugar was not identified in any roasting profile (Table 4). Glucose, fructose, xylose, stachyose, and arabinose were quantified in the different roasting profiles. Fructose was the sugar with the highest concentration among the sugars, ranging from 3.73 mg/g to 17.14 mg/g for *C. arabica* and 3.25 mg/g to 13.49 mg/g for *C. canephora*. Regarding the species and the same roasting levels, *C. canephora* showed higher concentrations compared to *C. arabica* in the 135 °C/20.20 min and 220 °C/13.47 min roasting profiles, with concentrations of 13.49 mg/g and 4.21 mg/g, respectively, while the other roasting profiles favored *C. arabica* in terms of concentration. The highest concentration of fructose was found in the standard roasting profile at 210 °C/11.01 min, with a concentration of 17.14 mg/g. The elevated concentration of fructose is due to the thermal hydrolysis of sucrose, which is reduced to glucose and fructose during the application of high temperatures (Chindapan et al., 2019).

When analyzing the impact of roasting temperature, it was observed that the amount of fructose present in coffee beans was higher when milder temperatures were used. This can be explained by the fact that, at these temperatures, the loss of moisture is lower compared to higher temperatures (Fig. 2). This gradual rate of moisture loss at lower temperatures likely allowed for the thermal hydrolysis of sucrose into glucose and fructose to occur (Chindapan et al., 2019). It's worth noting that the longer exposure time, even when applying the 135 °C/20.20 min roasting profile to *C. arabica*, resulted in significantly lower quantities ($p<0.05$) compared to the 210 °C/11.01 min and 210 °C/9.02 min roasting profiles. Meanwhile, in *C. canephora*, a decrease in fructose concentration was observed with increasing temperature, regardless of the roasting exposure time.

Table 3. Carbohydrates content of *canephora* (Robusta) and *arabica* coffee variety Catúai affected by different degrees of roasting.

Roasting profiles	Species	Carbohydrates content						
		Glucose	Fructose	Xylose	Stachyose	Arabinose	Raffinose	Total sugar
135 °C/ 20.20 min	*C. canephora*	0.57 ± 0.65^{Bb}	13.49 ± 0.00^{Aa}	1.23 ± 0.05^{Ab}	nd	2.82 ± 0.08^{Aa}	nd	18.12 ± 4.77^{Aa}
	C. arabica	0.92 ± 0.18^{Ba}	8.95 ± 2.60^{Cb}	2.16 ± 1.00^{Aa}	2.28 ± 0.89^{Ca}	2.62 ± 0.10^{BCa}	nd	16.93 ± 2.88^{Cb}
210 °C/ 9.02 min	*C. canephora*	0.53 ± 0.06^{Bb}	6.10 ± 0.10^{Bb}	1.14 ± 0.06^{Aa}	nd	1.99 ± 0.02^{Bb}	nd	9.77 ± 2.11^{Bb}
	C. arabica	1.33 ± 0.01^{Aa}	14.52 ± 0.04^{Ba}	0.05 ± 0.00^{Db}	4.17 ± 0.01^{Ba}	2.85 ± 0.02^{Ba}	nd	22.92 ± 5.00^{Ba}
220 °C/ 13.47 min	*C. canephora*	1.20 ± 0.06^{Aa}	4.21 ± 0.03^{Da}	1.34 ± 0.06^{Aa}	nd	1.40 ± 0.01^{Cb}	nd	8.16 ± 1.40^{Ca}
	C. Arabica	0.71 ± 0.04^{Cb}	3.73 ± 0.02^{Fb}	1.50 ± 0.04^{Ba}	0.82 ± 0.03^{Da}	1.65 ± 0.00^{Da}	nd	8.42 ± 1.17^{Fa}
230 °C/ 17.43 min	*C. canephora*	0.62 ± 0.06^{Ba}	3.25 ± 0.03^{Eb}	1.26 ± 0.04^{Ab}	nd	1.35 ± 0.03^{Cb}	nd	6.48 ± 1.10^{Db}
	C. Arabica	0.59 ± 0.02^{CDa}	5.85 ± 0.01^{Da}	1.51 ± 0.06^{Ba}	0.13 ± 0.00^{Ea}	2.32 ± 0.07^{Ca}	nd	10.42 ± 2.01^{Da}
275 °C/ 7.46 min	*C. canephora*	0.57 ± 0.04^{Bb}	3.32 ± 0.09^{Eb}	0.05 ± 0.00^{Bb}	nd	1.61 ± 0.01^{BCb}	nd	5.56 ± 1.21^{Db}
	C. arabica	0.43 ± 0.05^{Da}	5.49 ± 0.07^{Ea}	1.12 ± 0.07^{Ca}	nd	2.36 ± 0.21^{Ca}	nd	9.41 ± 1.93^{Ea}
210 °C/ 11.01 min	*C. canephora*	0.57 ± 0^{Bb}	4.57 ± 0.05^{Cb}	1.34 ± 0.05^{Aa}	nd	1.90 ± 0.08^{Bb}	nd	8.38 ± 1.57^{Cb}
	C. arabica	1.48 ± 0.05^{Aa}	17.14 ± 0.04^{Aa}	0.05 ± 0.00^{Db}	5.1 ± 0.05^{Aa}	3.50 ± 0.09^{Aa}	nd	27.28 ± 5.92^{Aa}

Means followed by the same lowercase letters in the row and uppercase letters in the column for each compound do not differ by Tukey's test ($p>0.05$).

nd: no detect.

C. arabica showed significantly higher levels of glucose in almost all roasting profiles compared to *C. canephora* ($p<0.05$), except in the 220 °C/17.43 min roasting profile, where *C. canephora* had a higher concentration. It is worth noting that in the 230 °C/17.43 min roasting profile, no significant differences were observed between the two species. In the case of *C. canephora*, only the 220 °C/17.43 min roasting profile showed a higher concentration of glucose compared to *C. arabica*, recording a concentration of 1.20 mg/g. When analyzing the species individually among the various roasting profiles, *C. canephora* exhibited its highest concentration in the mentioned roasting profile (220 °C/17.43 min), while *C. arabica* showed its highest concentrations in the 210 °C/9.02 min and 210 °C/11.01 min roasting profiles. This suggests that at temperatures in this range, the preservation and concentration of glucose are maximized (Table 3). These results significantly differ from a substantial body of previous studies that pointed to a higher concentration of glucose compared to fructose in coffee after the roasting process (Ajandouz et al., 2001; Brands & Van Boekel, 2001; Chindapan et al., 2019). The discrepancy between these results is noteworthy, with the evidence at hand showing that glucose was more susceptible to thermal degradation.

Arabinose is a constituent derived from arabinogalactan, a polysaccharide found in the plant cell wall matrix, coexisting with proteins in the configuration known as arabinogalactan proteins (Poisson et al., 2017). Higher concentrations of arabinose were observed in *C. canephora* in the 135 °C/20.20 min roasting profile and in *C. arabica* in the 210 °C/11.01 min roasting profile compared to the other roasting profiles. Between the two species in the same roasting profiles, statistically significant differences ($p<0.05$) were identified in the following roasting profiles: 210 °C/9.02 min, 220 °C/17.43 min, 230 °C/17.43 min, 275 °C/7.46 min, and 210 °C/11.01 min, with *C. arabica* standing out for higher arabinose concentration. The only roasting profile that did not show significant differences ($p>0.05$) was the 135 °C/20.20 min, where concentrations were 2.82 mg/g for *C. canephora* and 2.62 mg/g for *C. arabica*. It is recognized that the roasting process causes depolymerization of arabinogalactan protein structures and thermal hydrolysis of arabinogalactan, resulting in the release of free arabinose, which plays an essential role in the mechanisms responsible for the formation of melanoidins and various acids, including formic, acetic, and lactic acids (Chindapan et al., 2019; Moreira et al., 2013).

Xylose concentrations ranged from 0.05 mg/g to 1.34 mg/g for *C. canephora* and from 0.05 mg/g to 2.16 mg/g for *C. arabica*. For *C. canephora*, statistically significant differences ($p<0.05$) were identified, with the minimum concentration of xylose in the 275 °C/7.46 min roasting profile. For *C. arabica,* significant differences ($p<0.05$) were also observed, with the

135 °C/20.20 min roasting profile exhibiting the maximum xylose concentration, while the 210 °C/9.02 min and 210 °C/11.01 min temperatures had the lowest xylose concentration. This monosaccharide is widely recognized for its role in xylitol production and has gained attention as a low-calorie sweetener. This characteristic has sparked significant interest due to its potential functionality in the context of human health, notably its ability to mitigate glycemic levels (Bae et al., 2011; Moon et al., 2012).

The presence of stachyose was observed in almost all *C. arabica* roasting profiles, except for the process conducted at 275 °C/7.46 min. The highest concentration of stachyose, reaching 5.1 mg/g, was recorded in the 210°C/11.01 min roasting profile. On the other hand, the analysis of different roasting profiles applied to *C. canephora* did not reveal any detectable traces of stachyose. The absence of detection of certain sugar concentrations, such as stachyose, in *C. canephora*, may be attributed to the hypothesis that the accumulation of this specific sugar occurs transiently and in limited quantities in the endosperm during the early stages of fruit development (Santos et al., 2011). Stachyose, being a less common disaccharide compared to sucrose in many plant species, may be subject to distinct metabolic pathways or a temporary storage profile in *C. canephora*. For a comprehensive understanding of these biochemical processes and sugar accumulation, it is essential to consider the specific mechanisms governing carbohydrate metabolism in this species. Further studies could elucidate the precise dynamics of sugar accumulation in *C. canephora*, including stachyose. Stachyose, a sugar from the raffinose oligosaccharide family, also imparts sweetness to fruits (Wu et al., 2023).

The predominant concentration of sugars proved to be of greater importance in the analysis of roasting profiles, notably in the 210 °C/11.01 min range, which corresponds to the standard roasting method for *C. arabica*. In the case of *C. canephora*, the most pronounced concentration of sugars stood out in the roasting profile at 135 °C/20.20 min. When comparing the same roasting profiles between the two species, it was found that *C. canephora* exhibited a higher concentration than *C. arabica* in the 135 °C/20.20 min roasting profile. Among the various roasting profiles investigated, there were no significant differences ($p>0.05$) in samples subjected to roasting at 220 °C/17.43 min (Table 3).

In the broader context, considering the remaining roasting profiles, *C. arabica* exhibited higher concentration levels when compared to *C. canephora*. Given the fundamental role of sugars as precursors in generating the aromatic profile of coffee, through the complex interactions of the Maillard reaction and caramelization process (Chindapan et al., 2019; Poisson et al., 2017) variations in the concentrations of fructose, glucose, xylose, stachyose,

and arabinose, as influenced by roasting temperatures, can play an important role in increasing the proportions of aromatic compounds, thereby benefiting the final product's quality.

3.3. Composition of organic acids

The compositions of organic acids in the *C. canephora* and *C. arabica* species subjected to different roasting profiles were determined using HPLC. Lactic, malic, tartaric, and isovaleric acids were not identified (Table 4). Among the organic acids present in samples of the coffee species *C. canephora* and *C. arabica*, succinic acid was the compound with the highest concentrations. The highest concentration of this acid was found in *C. canephora* at 210 °C/11.01 min (standard roasting method), with a content of 224.24 mg/g. The other roastings with the use of higher temperatures revealed that the concentrations of this acid significantly decreased, as in *C. canephora*, reaching a concentration of 48.33 mg/g in the 275 °C/7.46 min roasting. The concentrations of this acid were significantly lower ($p<0.05$) in *C. arabica*, except in the 275 °C/7.46 min roasting (Table 4). Succinic acid is formed in coffee through the degradation of malic and citric acids (Balzer, 2008).

Acetic acid is a natural metabolic compound that occurs as an intermediate substance in plant metabolism. This compound is undesirable in some products as it imparts an unpleasant taste and a vinegar-like aroma when formed in excess. However, in coffee, it can contribute to a sweet flavor (Kalschne et al., 2018; Xu et al., 2019; Yeager et al., 2021). *C. arabica* showed low concentrations of acetic acid, with no significant differences ($p>0.05$) between the roasting profiles. The highest concentrations were found in *C. canephora* (8.37 mg/g to 19.29 mg/g), with significantly higher concentrations ($p<0.05$) compared to *C. arabica*, except in the 275 °C/7.46 min roasting (Table 4). *C. arabica* subjected to roasting has lower amounts of acetic acid compared to *C. canephora*, due to higher levels of chemical compounds in *C. canephora* (Yeager et al., 2021).

Table 4. Organic acid content of *canephora* (Robusta) and *arabica* coffee variety Catúai affected by different degrees of roasting.

Roasting profiles	Species	Organic acid content						
		Acetic acid	Citric acid	Oxalic acid	Propionic acid	Quinic acid	Succinic acid	Total acid
135 °C/ 20.20 min	*C. canephora*	10.59 ± 0.67^{Ca}	9.96 ± 0.80^{BCa}	18.73 ± 0.17^{Ca}	49.34 ± 1.37^{CDa}	25.46 ± 0.83^{Ba}	142.41 ± 7.59^{Ca}	256.49 ± 4.22^{Ca}
	C. arabica	3.77 ± 0.42^{Bb}	10.21 ± 1.26^{Aa}	0.86 ± 0.06^{Bb}	32.78 ± 3.73^{Aa}	7.98 ± 1.21^{Abb}	39.99 ± 0.39^{ABb}	95.59 ± 0.52^{Ab}
210 °C/ 9.02 min	*C. canephora*	19.29 ± 0.86^{Aa}	16.42 ± 2.99^{Aa}	27.28 ± 0.48^{Ba}	82.07 ± 1.14^{Aba}	40.34 ± 1.10^{Aa}	182.26 ± 12.57^{Ba}	367.66 ± 6.36^{ABa}
	C. arabica	5.30 ± 0.02^{Abb}	10.13 ± 0.31^{Ab}	0.97 ± 0.01^{Bb}	33.78 ± 0.55^{Ab}	6.76 ± 0.76^{ABb}	57.56 ± 1.01^{Ab}	114.50 ± 0.23^{Ab}
220 °C/ 13.47 min	*C. canephora*	15.08 ± 0.30^{ABCa}	14.57 ± 0.15^{Aa}	22.14 ± 0.12^{Ca}	78.72 ± 0.48^{ABCa}	37.36 ± 0.39^{Aa}	177.95 ± 0.04^{Ba}	345.82 ± 0.15^{Ba}
	C. arabica	5.50 ± 0.09^{ABb}	10.11 ± 0.00^{Ab}	1.08 ± 0.00^{Bb}	29.16 ± 0.05^{Ab}	7.24 ± 0.07^{ABb}	69.01 ± 2.16^{Ab}	122.10 ± 1.14^{Ab}
230 °C/ 17.43 min	*C. canephora*	11.27 ± 0.00^{BCa}	9.99 ± 0.41^{BCa}	3.48 ± 0.28^{Db}	50.66 ± 0.52^{BCDa}	18.90 ± 1.56^{BCa}	76.27 ± 3.56^{Da}	170.57 ± 1.63^{Da}
	C. arabica	6.08 ± 0,10^{Abb}	6.57 ± 0.20^{Ba}	6.49 ± 0.06^{Aa}	23.01 ± 0.09^{Ab}	11.39 ± 0.16^{Abb}	19.59 ± 0,08^{Bb}	73.13 ± 0.07^{Ab}
275 °C/ 7.46 min	*C. canephora*	8.37 ± 0.28^{Ca}	6.99 ± 0.17^{Ca}	3.41 ± 0.21^{Db}	29.59 ± 3.67^{Da}	13.33 ± 0.18^{Ca}	48.33 ± 0.20^{Da}	110.02 ± 0.62^{Da}
	C. arabica	11.16 ± 4.79^{Aa}	6.57 ± 2.40^{Ba}	10.03 ± 2.73^{Aa}	34.07 ± 18.98^{Aa}	16.87 ± 6.84^{Aa}	39.62 ± 5,60^{ABa}	118.32 ± 5.14^{Aa}
210 °C/ 11.01 min	*C. canephora*	17.84 ± 0.02^{Aba}	13.69 ± 1.02^{Aa}	32.51 ± 0.32^{Aa}	96.16 ± 11.70^{Aa}	45.95 ± 1.30^{Aa}	224.24 ± 15.99^{Aa}	430.39 ± 9.20^{Aa}
	C. arabica	5.14 ± 0.01^{Abb}	9.01 ± 0.19^{Ab}	0.92 ± 0.02^{Bb}	32.95 ± 0.66^{Ab}	5.78 ± 0.62^{Bb}	50.88 ± 2.18^{ABb}	104.68 ± 1.05^{Ab}

Means followed by the same lowercase letters in the row and uppercase letters in the column for each compound do not differ by Tukey's test ($p>0.05$).

The increase in roasting temperature decreased the concentration of citric acid in *C. arabica*. Green *C. arabica* beans have a higher concentration of citric acid compared to green *C. canephora* beans. However, when coffee is roasted, roasted *C. arabica* beans have a lower concentration of citric acid compared to roasted *C. canephora* (Yeager et al., 2021). In this study, the concentration of citric acid was higher in *C. canephora* in the roasting profiles at 210 °C/9.02 min, 220 °C/17.43 min, and 210 °C/11.01 min (Table 4). Citric acid contributes to herbaceous and citrus sensory perceptions, and this sensory profile was observed using the critical sensory approach by the temporal dominance of sensation (TDS) method. Additionally, the microbiota present in coffee beans during natural fermentation can impact higher levels of citric acid and provide coffees with high taste scores using the international coffee quality standardization method (trained Q-grader certified tasters) (Evangelista et al., 2015; Ribeiro et al., 2018).

C. canephora showed a higher concentration of propionic acid in almost all roasting profiles, with the highest concentrations found in the roasting profiles at 210 °C/9.02 min, 210 °C/11.01 min, and 220 °C/17.43 min (Table 4). *C. arabica* did not show significant differences ($p>0.05$) between the roasting profiles. Propionic acid is an organic acid with oily, liquid properties and a pungent aroma. High concentrations of propionic acid can lead to negative taste preferences due to the pronounced herbaceous and vegetal flavors (Kalschne et al., 2018).

Regarding oxalic acid, there was a wide variation in concentrations among the species and analyzed roasting profiles, with higher concentrations of the acid in *C. canephora* in almost all roasting profiles, except at higher temperatures (230 °C/17.43 min and 275 °C/7.46 min). Interestingly, *C. arabica* exhibited higher concentrations of oxalic acid when higher temperatures were used (230 °C/17.43 min and 275 °C/7.46 min) (Table 4). Coffees with the presence of oxalic acid have been associated with characteristics such as "bland" flavor, caramelized, smooth taste, and some tasters have suggested that oxalic acid enhances the characteristic flavor of coffee (Yeager et al., 2021).

The concentrations of quinic acid in roasted and ground coffee samples varied widely in both *C. canephora* and *C. arabica*, with the lowest concentration found in the 275 °C/7.46 min roasting for *C. canephora*, and no significant differences ($p>0.05$) were observed between the roasting profiles for *C. arabica*. Interestingly, an increase in the concentration of quinic acid was observed in *C. arabica* in roasting profiles with higher temperatures (Table 4). This could be due to the occurrence of chlorogenic acids that degrade into other components, including quinic acid, during the roasting process at higher temperatures. Both compounds are responsible for the characteristic aroma of coffee, as they have a phenolic nature and contribute to roasted

coffee aroma, along with sugars, proteins, and lipids. Quinic acid is sensorially associated with astringency and the characteristic bitterness of coffee (Aree 2019).

Organic acids are the most abundant class of compounds in light and medium roast coffee beans and are responsible for the sour taste of coffee (Wang et al., 2021). They are naturally present in coffee beans as part of the chemical composition of the fruit's husk and berry, and their initial concentration can be a differentiator in quality based on the degradation and formation mechanisms during the roasting process (Yeager et al., 2021). Among the roasting profiles employed, *C. canephora* had higher concentrations of total organic acids ($p<0.05$), except in the 275 °C/7.46 min roasting. The highest relevance in terms of total organic acid concentration was observed in the 210 °C/9.02 min and 210 °C/11.01 min roasting profiles (standard roasting method) in *C. canephora*, while *C. arabica* did not show significant differences between the roasting profiles (Table 4). It should be noted that the greater production of total organic acids in *C. canephora* corresponded to roasting profiles with lower pH values. However, the variation in the concentration of organic acids may be related to the use of different extraction and detection methods, as well as the coffee species and roasting methods used in this study.

3.4. Melanoidins

One of the visual changes observed in foods is the development of a brown color when subjected to thermal treatment, including coffee during the roasting process (Freitas et al., 2023). In the present study, the absorbance at 420 nm (Abs_{420}) was used to measure color compounds, melanoidins (Fig. 3).

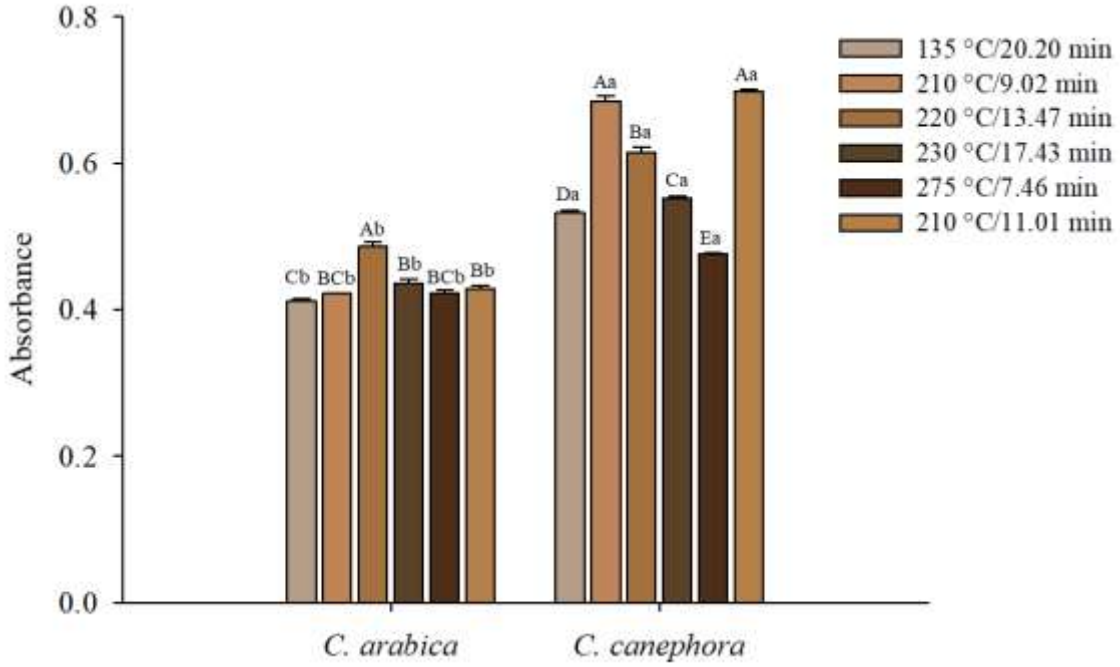


Figure 3. Melanoidins (Abs420 nm) of *canephora* (Robusta) and *arabica* coffee variety Catúai affected by different degrees of roasting.

C. canephora exhibited significantly higher absorbance readings of melanoidins (brown compounds) compared to *C. arabica* in the same roasting profile. The concentrations of this compound were higher in the roasting profiles (210 °C/9.02 min and 210 °C/11.01 min in *C. canephora*) and (220 °C/13.47 min in *C. arabica*) (Fig. 3). Abs_{420} reading is used to indicate the presence of melanoidins in thermally treated foods during their processing and processing. Melanoidin polymers are products resulting from foods heated at high temperatures due to reactions that occur during this process: the Maillard reaction and caramelization (Pastoriza et al., 2014). These reactions occur in products due to the presence of sugars, compounds that are present in our study's raw material in all roasting profiles and analyzed species. The chemical composition of coffee melanoidins consists of 70 % carbohydrates, 12 % proteins, and 13 % phenolics (Feng et al., 2023).

It is worth noting that the variation in melanoidin polymer can also be attributed to differences in genotypes and growing locations, not just variations in roasting profiles (Luiz et al., 2019)

3.5. Multivariate association between the chemical compounds

The Principal Component Analysis (PCA) technique was employed to investigate datasets of chemical nature. The outcomes resulting from the application of PCA, as well as the

distinct separations identified among clusters, were thoroughly examined for their interrelation with the operational variables inherent to the coffee roasting process. Furthermore, this analysis was extended to the datasets corresponding to the coffee species *C. canephora* and *C. arabica* (Fig. 4). The underlying objective was to evaluate how the dissociation observed between the clusters determined by PCA was affected by the intricate processes associated with coffee roasting.

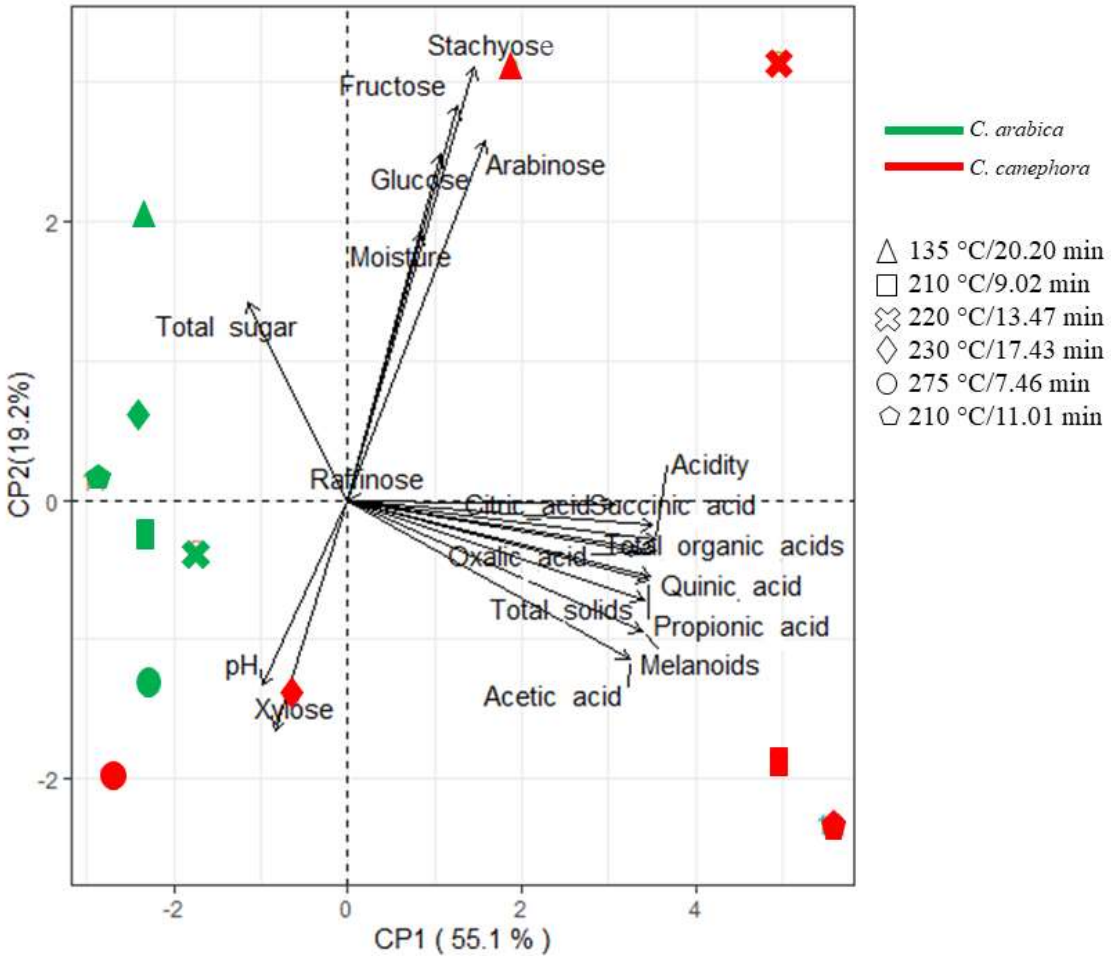


Figure 4. Scatter plot of Principal Component Analysis (PCA) scores of for *canephora* (Robusta) and *arabica* coffee samples after different roasting treatments (PC1 vs. PC2).

The first two principal components (PCs) demonstrated the ability to explain approximately 74.3 % of the variability present in the chemical analysis data. This breakdown of representativeness unfolds as PC1, responsible for explaining 55.1 % of the variation, and PC2, contributing with 19.2 % (Fig. 4). This distinction in the percentage of variation was identified in the resulting score plot of the analysis, indicating a notable contribution of the first two PCs in synthesizing the information contained in the chemical data. From the spatial dispersion of the samples, it is possible to identify four distinct groups, separated by quadrants. In the context of the *C. canephora* species, the roasting profiles were categorized as follows:

135 °C/20.20 min and 220 °C/13.47 min (positive PC1, positive PC2); 230 °C/17.43 min and 275 °C/7.46 min (negative PC1, negative PC2); 210 °C/9.02 min and 210 °C/11.01 min (positive PC1, negative PC2). Regarding the *C. arabica* species, the roasting profiles fit as follows: 135 °C/20.20 min, 230 °C/17.43 min, and 210 °C/11.01 min (negative PC1, positive PC2); 210 °C/9.02 min, 220 °C/13.47 min, and 275 °C/7.46 min (negative PC1, negative PC2). With roasting temperatures at 210 °C/11.01 min and 210 °C/9.02 min, it was observed that they exhibited higher concentrations of these compounds.

However, the application of Principal Component Analysis (PCA) provided a deeper understanding of the complex relationships between coffee species, roasting processes, and resulting chemical characteristics. PCA's ability to highlight related patterns and clusters allowed for a more precise and detailed analysis, thus contributing to knowledge about how roasting processes affect the chemical compositions of different coffee species.

Conclusion

This study investigated the effects of post-harvest roasting temperature and time on the concentrations of sugars and organic acids in coffee species *C. canephora* and *C. arabica*. The results demonstrated that acidity was higher in *C. canephora* coffee, except under specific roasting conditions. The concentration of volatile acids increased with roasting, reaching maximum values around the standard temperature of 210 °C, and decreased with higher temperatures due to the breakdown of chlorogenic acids. pH was influenced by temperature, with lower temperatures resulting in lower values. Moisture was not significantly affected by roasting temperature, except under extreme conditions. Soluble solids concentrations decreased with increasing roasting temperature. Fructose was the most abundant sugar, with higher concentrations at lower temperatures. Concentrations of organic acids varied between species and roasting profiles, with succinic acid predominating. The presence of melanoidins increased in roasting profiles employing higher temperatures. Analyzing the results of Principal Component Analysis (PCA), it was possible to observe the separation of sample groups based on roasting profiles and coffee species. The results indicated that different roasting profiles distinctly affected the concentrations of chemical compounds in the two coffee species.

Overall, this study contributes to the understanding of the effects of roasting on the concentrations of sugars and organic acids in coffee species *C. canephora* and *C. arabica*, providing valuable information for optimizing the roasting process for the final quality of coffee.

References

Ajandouz, E. H., Tchiakpe, L. S., Dalle Ore, F., Benajiba, A., Puigserver, A. (2001). Effects of pH on caramelization and maillard reaction kinetics in fructose-lysine model systems. *Journal of Food Science*, *66*, 926-931. https://doi.org/10.1111/j.1365-2621.2001.tb08213.x

Alyammahi, J., Darwish, A. S., Lemaoui, T., Alnashef, I. M., Hasan, S. W., Taher, H., Banat, F. (2023). Parametric analysis and machine learning for enhanced recovery of high-value sugar from date fruits using supercritical CO2 with co-solvents. *Journal of CO2 Utilization, 72*, article 102511. https://doi.org/10.1016/j.jcou.2023.102511

AOAC - ASSOCIATION OF OFFICIAL ANALYTICAL CHEMISTS. (1990). Official methods of analyses of the Association of Official Analytical Chemists. 15. ed. Washington, 1117.

Aree, T. (2019). Understanding structures and thermodynamics of β-cyclodextrin encapsulation of chlorogenic, caffeic and quinic acids: Implications for enriching antioxidant capacity and masking bitterness in coffee. *Food Chemistry*, *293*, 550-560. https://doi.org/10.1016/j.foodchem.2019.04.084

Avelino, J., Barboza, B., Araya, J. C., Fonseca, C., Davrieux, F., Guyot, B., Cilas, C. (2005). Effects of slope exposure, altitude and yield on coffee quality in two altitude terroirs of Costa Rica, Orosi and Santa Maria de Dota. *Journal of the Science of Food and Agriculture*, *85*(11), 1869-1876. https://doi.org/10.1002/jsfa.2188

Babova, O., Occhipinti, A., Maffei, M. E. (2016). Chemical partitioning and antioxidant capacity of green coffee (*Coffea arabica* and *Coffea canephora*) of different geographical origin. *Phytochemistry*, *123*, 33-39. https://doi.org/10.1016/j.phytochem.2016.01.016

Badmos, S., Lee, S., Kuhnert, N. (2019). Comparison and quantification of chlorogenic acids for differentiation of green Robusta and Arabica coffee beans. *Food Research International*, *126*, 108544. https://doi.org/10.1016/j.foodres.2019.108544

Bae, Y. J., Bak, Y. K., Kim, B., Kim, M. S., Lee, J. H., Sung, M. K. (2011). Coconut-derived D-xylose affects postprandial glucose and insulin responses in healthy individuals. *Nutrition Research and Practice*, *5*(6), 533-539. https://doi.org/10.4162/nrp.2011.5.6.533

Balzer, H. H. (2008). Acids in coffee. In *Coffee: Recent developments*, ed. Ronald Clarke, and O. G. Vitzthum, 18-32. Hoboken, NJ, USA: John Wiley & Sons.

Belitz, H. D., Grosch, W., Schieberle, P. (2009). Coffee, Tea, Cocoa. *Food Chemistry*, 938-970. https://doi.org/10.1007/978-3-540-69934-7

Borém, F. M., Figueiredo, L. P., Ribeiro, F. C., Taveira, J. H. S., Giomo, G. S., Salva, T. J. G. (2016). The relationship between organic acids, sucrose and the quality of specialty coffees. *African Journal of Agricultural Research*, *11*(8), 709-717. https://doi.org/10.5897/AJAR2015.10569

Brands, C. M. J., Van Boekel, M. A. J. S. (2001). Reactions of monosaccharides during heating of sugar-casein systems: Building of a reaction network model. *Journal of Agricultural and Food Chemistry*, *49*, 4667–4675. https://doi.org/10.1021/jf001430b

Bressani, A. P. P., Martinez, S. J., Evangelista, S. R., Dias, D. R., Schwan, R. F. (2018). Characteristics of fermented coffee inoculated with yeast starter cultures using different inoculation methods. *LWT- Food Science and Technology, 92*, 212-219. https://doi.org/10.1016/j.lwt.2018.02.029

Brollo, G., Cappucci, R., Navarini, L. (2008). Acidity in coffee: bridging the gap between chemistry and psychophysics. In *22nd International Conference on Coffee Science, Capinas, SP, Brazil*, 270-280.

Cardoso, W. S., Agnoletti, B. Z., de Freitas, R., Pinheiro, F. A., Pereira, L. L. (2021). Biochemical Aspects of Coffee Fermentation. In: Louzada Pereira, L., Rizzo Moreira, T. (eds) Quality Determinants In Coffee Production. *Food Engineering Series*. Springer, Cham. https://doi.org/10.1007/978-3-030-54437-9_4

Chindapan, N., Soydok, S., Devahastin, S. (2019). Roasting Kinetics and Chemical Composition Changes of Robusta Coffee Beans During Hot Air and Superheated Steam Roasting. *Journal of Food Science*, *84*(2), 292-302. https://doi.org/10.1111/1750-3841.14422

Clifford, M. N. (1979). Chlorogenic acids - Their complex nature and routine determination in coffee beans. *Food Chemistry*, *4*(1), 63-71. https://doi.org/10.1016/0308-8146(79)90031-1

Collazos-Escobar, G. A., Gutiérrez-Guzmán, N., Váquiro-Herrera, H. A., Bom, J., Garcia-perez, J. V. (2022). Thermodynamic analysis and modeling of water vapor adsorption isotherms of roasted specialty coffee (*Coffee arabica* L. cv. Colombia). *LWT- Food Science and Technology 160*, article 113335. https://doi.org/10.1016/j.lwt.2022.113335

Córdoba, N., Moreno, F. M., Osorio, C., Velásquez, S., Ruiz, Y. (2021). Chemical and sensory evaluation of cold brew coffees using different roasting profiles and brewing methods. *Food Research International*, *141*, article 110141. https://doi.org/10.1016/j.foodres.2021.110141

Dong, W., Hu, R., Chu, Z., Zhao, J., Tan, L. (2017). Effect of different drying techniques on bioactive components, fatty acid composition, and volatile profile of robusta coffee beans. *Food Chemistry*, *234*, 121-130. https://doi.org/10.1016/j.foodchem.2017.04.156

Evangelista, S. R., Miguel, M. G. C. P., Silva, C. F., Pinheiro. A. C. M., Schwan, R. F. (2015). Microbiological diversity associated with the spontaneous wet method of coffee fermentation. *International Journal of Food Microbiology*, *210*, 102-112. https://doi.org/10.1016/j.ijfoodmicro.2015.06.008

Evangelista, S. R., Miguel, M. G., Cordeiro, C. S., Silva, C. F., Pinheiro, A. C., Schwan, R. F. (2014). Inoculation of starter cultures in a semi-dry coffee (*Coffea arabica*) fermentation process. *Food Microbiology*, *44*, 87-95. https://doi.org/10.1016/j.fm.2014.05.013

Farah. A. (2012). Coffee constituents. Y. F. Chu (Ed.), Coffee: Emerging health effects and disease prevention, Wiley-Blackwell, Oxford, 21-58.

Feng, J., Berton-carabin, C. C., Guyot, S., Schro, K. (2023). Coffee melanoidins as emulsion stabilizers. *Food Hydrocolloids*, *139*, article 108552. https://doi.org/10.1016/j.foodhyd.2023.108522

Freitas, V. V., Rodrigues, L. L. B., Castro, G. A. D., dos Santos, M. H., Vidigal, M. C. T. R., Fernandes, S. A., Stringheta, P. C. (2023). Impact of different roasting conditions on the chemical composition, antioxidant activities, and color of *Coffea canephora* and *Coffea arabica* L. samples. *Heliyon*, *9*(9), article e19580. https://doi.org/10.1016/j.heliyon.2023.e19580

Gatti, N., Gomez, M. I., Bennett, R. E., Sillett, T. S., Bowe, J. (2022). Eco-labels matter: Coffee consumers value agrochemical-free attributes over biodiversity conservation. *Food Quality and Preference*, *98*, article 104509. https://doi.org/10.1016/j.foodqual.2021.104509

Ginz, M., Balzer, H. H., Bradbury, A. G. W., Maier, H. G. (2000). Formation of aliphatic acids by carbohydrate degradation during roasting of coffee. *European Food Research and Technology, 211*, 404-410. https://doi.org/10.1007/s002170000215

Hazebroek, B. K, & Croijmans, I. (2023). Let's talk over coffee: Exploring the effect of coffee flavour descriptions on consumer imagery and behavior. *Food Quality and Preference*, *105*, article 104757. https://doi.org/10.1016/j.foodqual.2022.104757

Iaccheri, E., Laghi, L., Cevoli, C., Berardinelli, A., Ragni, L., Romani, S., Rocculi, P. (2015). Different analytical approaches for the study of water features in green and roasted coffee beans. *Journal of Food Engineering*, *146*, 28-35. https://doi.org/10.1016/j.jfoodeng.2014.08.016

INMET- Instituto Nacional de Metereologia (2023). Retrieved from: https://clima.inmet.gov.br/

Jayakumar, M., Rajavel, M., Surendran, U., Gopinath, G., Ramamoorthy, K. (2017). Impact of climate variability on coffee yield in India - with a micro-level case study using long-term

coffee yield data of humid tropical Kerala. *Climatic Change*, *145*, 335-349. https://doi.org/10.1007/s10584-017-2101-2

Jeszka-Skowron, M., Sentkowska, A., Pyrzyńska, K., De Pena, M. P. (2016). Chlorogenic acids, caffeine content and antioxidant properties of green coffee extracts: influence of green coffee bean preparation. *European Food Research Technology, 242*, 1403-1409. https://doi.org/10.1007/s00217-016-2643-y

Kalschne, D. L., Viegas, M. C. De Conti, A. J., Corso, M. P., Benassi, M. T. (2018). Steam pressure treatment of defective *Coffea canephora* beans improves the volatile profile and sensory acceptance of roasted coffee blends. *Food Research International*, *105*, 393-402. https://doi.org/10.1016/j.foodres.2017.11.017

Kim, I., Jung, S., Lee, E. K. J., Ha, C. K. J., Jeong, Y. (2021). Physicochemical characteristics of Ethiopian *Coffea arabica* cv. Heirloom coffee extracts with various roasting conditions. *Food Science and Biotechnology*, *30*(2), 235-244. https://doi.org/10.1007/s10068-020-00865-w

Król, K., Gantner, M., Tatarak, A., Hallmann, E. (2020). The content of polyphenols in coffee beans as roasting, origin and storage effect. *European Food Research and Technology*, *246*(1), 33-39. https://doi.org/10.1007/s00217-019-03388-9

Lopez-garcia, E., Guallar-castillon, P., Leon-muñoz, L., Graciani, A., Rodriguez-artalejo, F. (2014). Coffee consumption and health-related quality of life. *Clinical Nutrition*, *33*(1), 143-149. https://doi.org/10.1016/j.clnu.2013.04.004

Ludwig, I. A., Bravo, J., Peña, M. P. De, Cid, C. (2013). Effect of sugar addition (torrefacto) during roasting process on antioxidant capacity and phenolics of coffee. *LWT-Food Science and Technology*, *51*(2), 553-559. https://doi.org/10.1016/j.lwt.2012.12.010

Luiz, A., Mori, B., Viegas, M. C., Fonseca, A. F. (2019). Coffee brews composition from *Coffea canephora* cultivars with different fruit-ripening seasons. *British Food Journal*, *122*(3), 827-840. https://doi.org/10.1108/BFJ-03-2019-0203

Mesías, M., Navarro, M., Martínez-Saez, N., Ullate, M., del Castillo, M. D., Morales, F. J. (2014). Antiglycative and carbonyl trapping properties of the water soluble fraction of coffee silverskin. *Food Research International*, *62*, 1120-1126. https://doi.org/10.1016/j.foodres.2014.05.058

Moon, S., Lee, K., Kyung, M., Jung, S., Park, Y., Yang, C. K. (2012). Study on the proper D-xylose concentration in sugar mixture to reduce glycemic index (GI) value in the human clinical model. *The Korean Journal of Food and Nutrition*, *25*(4), 787-792. https://doi.org/10.9799/ksfan.2012.25.4.787

Moreira, A. S. P., Coimbra, M. A., Nunes, F. M., Rosario, M., Domingues, M. (2013). Roasting-induced changes in arabinotriose, a model of coffee arabinogalactan side chains. *Food Chemistry*, *138*, 2291-2299. https://doi.org/10.1016/j.foodchem.2012.11.130

Mosayebi, M., Kashaninejad, M., Najafian, L. (2018). Optimizing physiochemical and sensory properties of infrared-hot air roasted sunflower kernels using response surface methodology. *Journal of Food Quality, 1*, 1-14. https://doi.org/10.1155/2018/4186050

Murthy, P. S., Basavaraj, K., Kusumoto, K. I. (2019). Modulation of coffee flavor precursors by Aspergillus oryzae serine carboxypeptidases. *LWT - Food Science and Technology, 113*, article 108312. https://doi.org/10.1016/j.lwt.2019.108312

Mussatto, S. I., Machado, E. M. S., Martins, S., Teixeira, J. A. (2011). Production, composition, and application of coffee and its industrial residues. *Food Bioprocess Technology*, *4*, 661-672. https://doi.org/10.1007/s11947-011-0565-z

Park, J. B., Peters, R., Novotny, J. A. (2023). Impact of roasting on javamide-I/-II in Arabica and Robusta coffee beans. *Food Chemistry*, *412*, 135586. https://doi.org/10.1016/j.foodchem.2023.135586

Park, J. B., Wang, T. T., Zhang, D., Vega, F. E., Meinhardt, L. W. (2019). HPLC quantification and MS/NMR confirmation of Javamide-I/-II in Arabica and Robusta coffee beans from different regions for finding better bean sources for Javamide-I/-II. *Austin Chromatography*, *6*(1), 1051. https://doi.org/10.26420/austinchromatogrl.2019.1051.

Pastoriza, S., Rufián-henares, J. A. (2014). Contribution of melanoidins to the antioxidant capacity of the Spanish diet. *Food Chemistry*, *164*, 438-445. https://doi.org/10.1016/j.foodchem.2014.04.118

Poisson, L., Blank, I., Dunkel, A., Hofmann, T. (2017). The chemistry of roasting: Decoding flavor formation. In B. Folmer (Ed.), The craft and science of coffee (273-309). London: Academic Press

Ribeiro, D. E., Borém, F. M., Nunes, Alves, A. P. C., Santos, C. M., Taveira, J. H. S., Dias, L. L. C. (2018). Profile of organic acids and bioactive compounds in the sensory quality discrimination of arabica coffee. *Coffee Science*, *13*(2), 187-197. http://doi:10.25186/cs.v13i2.1415

Ribeiro, L. S., Evangelista, S. R., Miguel, M. G. D. C. P., Van Mullem, J., Silva, C. F., Schwan, R. F. (2018). Microbiological and chemical-sensory characteristics of three coffee varieties processed by wet fermentation. *Annals of Microbiology, 68*(10), 705-716. https://dx.doi.org/10.1007/s13213-018-1377-4

Rune, C. J. B., Giacalone, D., Steen, I., Duelund, L., Münchow, M., Clausen, M. P. (2023). Acids in brewed coffees: Chemical composition and sensory threshold. *Current Research in Food Science*, *6*, article 100485. https://doi.org/10.1016/j.crfs.2023.100485.

Santos, T. B., Budzinski, I. G. F., Marur, C. J., Petkowicz, C. L. O., Pereira, L. F. P., Vieira, L. G. E. (2011). Expression of three galactinol synthase isoforms in *Coffea arabica* L. and accumulation of raffinose and stachyose in response to abiotic stresses. *Plant Physiology and Biochemistry*, *49*(4), 441-448. https://doi.org/10.1016/j.plaphy.2011.01.023

Silva, C. F., Batista, L. R., Abreu, L. M., Dias, E. S., Schwan, R. F. (2008). Succession of bacterial and fungal communities during natural coffee (*Coffea arabica*) fermentation. *Food Microbiology*, *25*(8), 951-957. https://doi.org/10.1016/j.fm.2008.07.003

USDA- United States Department of Agriculture (2021). Coffee: word markets and trade. Disponível em: https://apps.fas.usda.gov/psdonline/circulars/coffee.pdf. Acesso em: 29 set. 2021.

USDA- United States Department of Agriculture (2021). Coffee: word markets and trade. Disponível em: https://apps.fas.usda.gov/psdonline/app/index.html#/app/downloads. Acesso em: 29 set. 2021.

Vitzthum, O. G., Werkhoff, P. (1975). New volatile constituents of black tea aroma. *Journal of Agriculture and Food Chemistry*, *23*(3), 510-516. https://doi.org/10.1021/jf60199a052

Xu, J. L., Kim, T. J., Kim. J., Choi, Y. (2019). Simultaneous roasting and extraction of green coffee beans by pressurized liquid extraction. *Food Chemistry*, *281*, 261-268. https://doi.org/10.1016/j.foodchem.2018.12.061

Wang, Y., Wang, X., Hu, G., Hong, D., Bai, X., Guo, T., Zuo, T., Li. J. Qiu, M. (2021). Chemical ingredients characterization basing on ^{1}HNMR and SHS-GC/MS in twelve cultivars of *Coffea arabica* roasted beans. *Food Research International*, *147*, 110544. https://doi.org/10.1016/j.foodres.2021.110544

Wu, X., Luo, D., Zhang, Y., Jin, L., Crabbe, M. J. C., Qiao, Q., Li, G., Zhang, T. (2023). Integrative analysis of the metabolome and transcriptome reveals the potential mechanism of fruit flavor formation in wild hawthorn (*Crataegus chungtienensis*). *Plant Diversity*. https://doi.org/10.1016/j.pld.2023.02.001

Yeager, S. E., Batali, M. E., Guinard, J. X., Ristenpart, W. D. (2021). Acids in coffee: A review of sensory measurements and meta-analysis of chemical composition. *Critical Reviews in Food Science and Nutrition*, *1*, 1-27. https://doi.org/10.1080/10408398.2021.1957767

Artigo 4*

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Harmonization of sensory characteristics in different roasting profiles of arabica and robusta coffee

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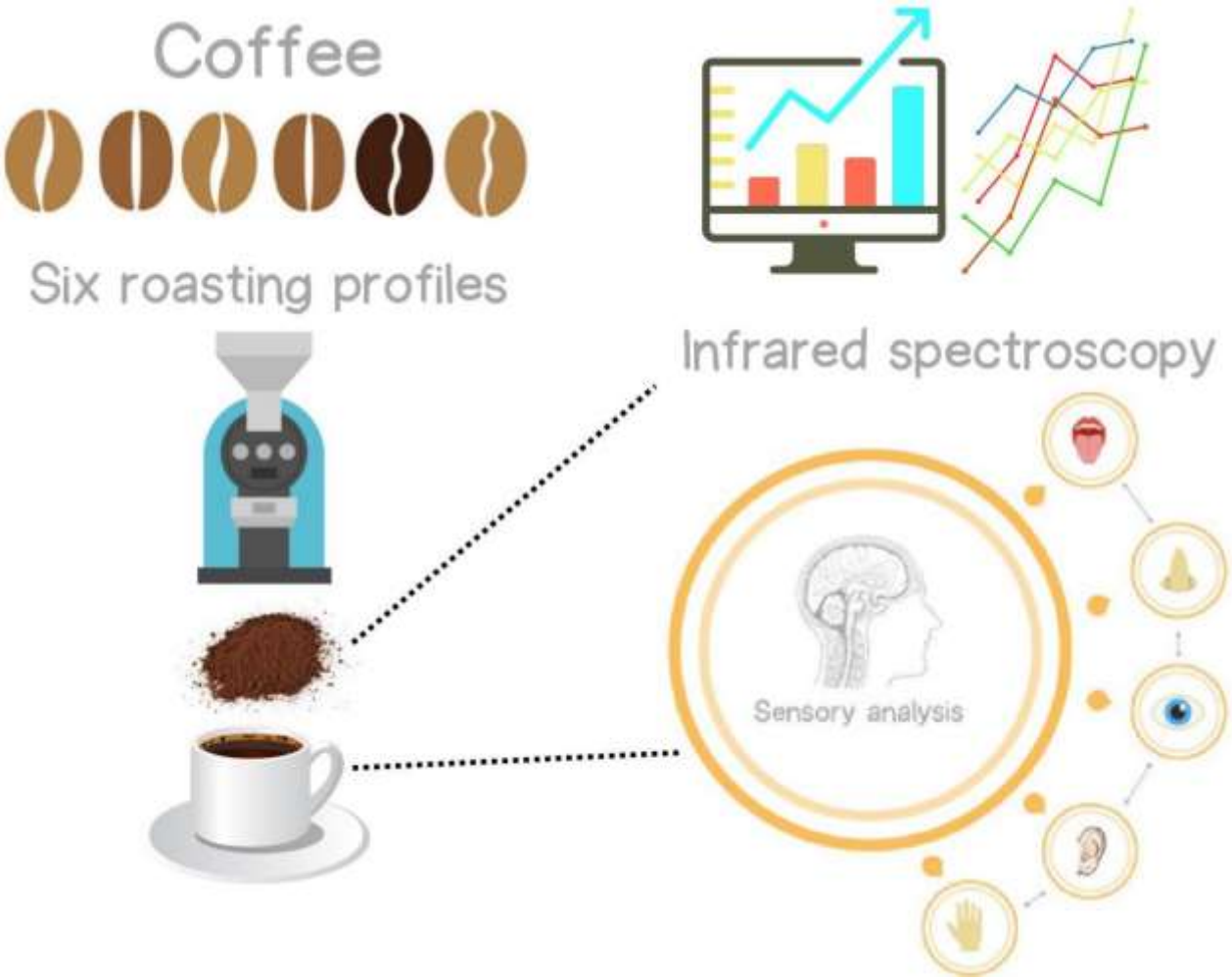
Graphical abstract



Abstract

Coffee plays a significant role in the Brazilian economy, influenced by various factors in its production. This study explored the relationship between sensory analysis and mid-infrared spectroscopy (MIR) in different roasting profiles of arabica and robusta coffee. The objective was to associate sensory characteristics and chemical compositions to identify roasting profiles that resulted in more highly regarded coffees. Principal Component Analysis (PCA) was used to analyze sensory data. The results highlighted spectral ranges associated with chlorogenic acids, lipids, and carbohydrates in coffee. Expert sensory analysis revealed significant differences in attributes, with arabica coffee being evaluated more positively than robusta. Roasting profiles with lower temperatures appear to better preserve the sensory quality of coffee. Consumer sensory evaluation also revealed differences in perceptions of acidity, sweetness, aroma, flavor, and overall impression between varieties and roasting profiles. PCA helped understand the relationship between coffee species, roasting profiles, and sensory attributes, allowing for the visualization of sample groupings and the identification of key influences on data variations. The study demonstrated the effectiveness of MIR spectroscopy in predicting sensory attributes and coffee characteristics, while also highlighting the influence of roasting profiles on consumer perceptions and the final product's quality. Sensory analyses emphasized differences between arabica and robusta coffee, as well as among roasting profiles, underscoring the importance of multiple factors in the quality of the product.

Keywords: Arabica coffee, Robusta coffee, Sensory analysis, Infrared, Tasters.

1. Introduction

The coffee industry holds a significant position in Brazil as one of the most valuable and prolific agricultural commodities. The price of coffee is determined by its potential for final quality, which is a complex attribute influenced by various factors throughout its production, encompassing planting, cultivation, environmental conditions, genetics, harvesting, maturation, processing, roasting, and brewing methods (Borém et al., 2020; Laukaleja & Koppel., 2021; Scholz et al., 2018).

Specifically, key factors influencing coffee quality include fruit ripening, as it necessitates harvesting the beans at an early stage of ripeness. Factors such as altitude and climatic conditions also significantly impact the final product's quality (Scholz et al., 2018). After the harvesting process, coffee beans undergo processing, which can take three different forms: dry processing (the most common and equipment-free method), wet processing, and semi-dry processing (Cassimiro et al., 2020; Ferreira et al., 2023; Frebrianto & Zhu., 2023; Kim et al., 2022; Widodo et al., 2023). Following processing, the beans are subjected to the roasting process, a critical final step with a profound impact on the beverage's quality (Kim et al., 2022).

Coffee roasting is a highly complex process involving mass and energy transfer, including drying, chemical structure modifications, and the enhancement of flavor, aroma, and color (Fadai et al., 2017). Numerous chemical reactions occur during roasting that can significantly affect the sensory attributes of the final product (Freitas et al., 2023). These reactions include dehydration, hydrolysis, fragmentation, cleavage, and enolization (Chang et al., 2020; Pereira et al., 2019). Overall, proper roasting processes lead to the formation of aromatic compounds, enhancing product flavor and ultimately improving food quality for better consumer acceptability (Freitas et al., 2023; Sruthi et al., 2021; Zhang et al., 2021). Roasting is a fundamental and indispensable procedure in coffee production.

Currently, the final beverage's quality is assessed through sensory analysis protocols like the Special Coffee Association (SCA), involving the process of tasting conducted by certified "Q-Graders" (Worch et al., 2010). This sensory analysis is meticulous, complex, and comprehensive, evaluating the beverage qualitatively based on attributes such as acidity, body, sweetness, balance, fragrance, overall impression, aftertaste, flavor, uniformity, and cleanliness of the cup (Ferreira et al., 2023).

In conjunction with the final beverage's quality, the use of near-infrared spectroscopy (MIR) methods has proven effective and cost-efficient. MIR is a rapid technique that does not

require chemicals and provides reliable results (Barrios-Rodríguez et al., 2021; Tugnolo et al., 2021). Recent studies have highlighted that MIR spectroscopy can predict sensory attributes, degree of roasting, product adulterations, and assess coffee composition (Craig et al., 2018a; Craig et al., 2018b). Typically, these analyses are performed in the laboratory after coffee bean roasting.

In light of the above, integrating near-infrared spectroscopy with sensory evaluation by trained "Q-grader" professionals alongside consumer assessments can help predict beverage quality. This approach provides intrinsic data on what constitutes quality coffee, as evaluated by both certified experts and ordinary coffee enthusiasts. To our knowledge, studies that encompass different roasting profiles and involve both trained and non-trained assessors are relatively scarce. Many studies base coffee quality solely on "Q-grader" evaluations, even though a significant portion of the population lacks training to distinguish coffee quality and may have different perceptions of what constitutes quality. Therefore, ensuring the beverage's appeal to all consumers, not just a specific group, is essential. This comprehensive study explores how different roasting profiles can be qualitatively predicted in the final beverage through near-infrared spectra and extensive sensory assessment.

2. Materials and methods

2.1 Materials

This study was conducted on *Coffea arabica* (Arabica) and *Coffea canephora* (Robusta) coffee beans harvested from plantations located in the municipality of São Geraldo, Minas Gerais, Southeastern Brazil. According to the Köppen-Geiger classification, the climate in this region is defined as humid subtropical with a dry winter and a hot summer (Alvares et al., 2013).

The coffee bean roasting process, following dry processing, was carried out using the Probat Leogap TP2 roaster, located in Curitiba, Brazil (Table 1). After this stage, the beans were ground using an electric grinder (Model: Bunn GVH-37, Springfield, Illinois, USA) to achieve a medium particle size and then cooled. The samples were sealed in bags and transported to the Laboratory of Supramolecular Chemistry and Biomimetics in the Department of Chemistry and the Laboratory of Innovation and Natural and Bioactive Dyes (LaCBio) in the Department of Food Technology at the Federal University of Viçosa (UFV).

Table 1. Roasting profile with respective time/temperature binomial.

Roasting profile	Roasting Temperature (°C)	Start time: 1° CRACK (min)	Total roasting time (min)
T1	135	2.16	20.20
T2	210	0.13	9.02
T3	220	4.55	13.47
T4	230	6.20	17.43
T5	275	1.56	7.46
T6	210	2.38	11.01

2.2. Infrared Spectrometry

The infrared spectra (IR) were obtained using a Varian 660 FTIR spectrophotometer equipped with a Gladi ATR (Attenuated Total Reflectance) accessory at the Department of Chemistry - UFV. The spectrophotometer used was a Paragon 1000PC model by Perkin Elmer. A diamond ATR was used as the sampling accessory. The average spectra of the samples were acquired as the mean of 16 consecutive scans in terms of wavenumbers (expressed in cm^{-1}) within the spectral range of 4000 to 400 cm^{-1}. This range corresponds to the mid-infrared region of the spectrum, which is notably rich in exploitable information for the functional assessment of organic compounds. The sample preparation technique employed has proven to be effective for coffee analysis (Ribeiro et al., 2009; Souza et al., 2022). Measurements were conducted in a dry environment at room temperature (20 ± 0.5 °C).

2.3. Sensory analysis with certified Q-grader tasters

The quality of the coffee cup was evaluated through the analysis of its sensory characteristics, following the protocol developed by the Specialty Coffee Association (SCA) (Special Coffee Association, 2018). Three Q-Grader certified tasters conducted the sensory analysis. Initially, coffee samples were roasted according to the roasting profiles indicated in Table 1. The coffee tasting was conducted based on the protocol proposed by the SCA, and the attributes assessed included acidity, aroma/fragrance, body, sweetness, balance, aftertaste, flavor, uniformity, cup cleanliness, and overall cup impression. The rating scale for these attributes ranged from 0 to 10 points. After evaluating all attributes, the tasters assigned an

average score as the final rating, with 10 points being the maximum score a coffee sample can receive. These scores represent the overall quality of the coffee beverage. Therefore, if a coffee sample achieves a final rating of 8 points or higher, it is classified as specialty coffee (SCA, 2018). This study adhered to ethical guidelines and was approved by the Research Ethics Committee for Human Subjects (CEP) under number 69623523.7.0000.5153 at the Federal University of Viçosa (UFV).

2.4. Affective sensory analysis by consumers

The coffee was roasted 24 hours before analysis, and grinding took place 8 hours after roasting. The coffee powder concentration used was 8.25 g for 150 mL of water, following the midpoint of the infusion control chart, considered optimal for achieving the "golden cup standard" (SCA, 2018). The coffee infusion method was conducted with water at temperatures ranging from 92-95 °C.

A total of 110 untrained volunteer tasters (both genders, aged 18 years or older) participated in the study, each evaluating 12 coffee samples. The analysis was conducted in two sessions, with six samples served per session. The inclusion criterion for individuals participating in the research was a habit of consuming coffee, and the exclusion criteria were the claim of not having the habit of consuming coffee and/or experiencing unpleasant symptoms after coffee consumption.

The samples were served individually to consumers in individual booths under white light and evaluated using a hedonic scale ranging from 1 to 9 points, where 1 corresponded to "disliked extremely" and 9 to "liked extremely." Coffee infusions, approximately 20 mL each, were served at 70 °C in plastic cups (50 mL capacity) labeled with three random digits. The presentation order of the samples was randomized for each evaluator. The attributes assessed included acidity, aroma, color, sweetness, flavor, and overall impression (Minim, 2013). This study adhered to ethical guidelines and was approved by the Research Ethics Committee for Human Subjects at the Federal University of Viçosa (UFV).

2.5. Statistical Analysis

The sensory analysis data were analyzed using analysis of variance (ANOVA) followed by means comparison through the Tukey test at a 5 % probability level. The statistical analysis

was performed using the R software (R Core Team, Vienna, Austria). Principal component analysis (PCA) based on the Pearson correlation matrix was conducted to observe differences between the roasting profiles of Arabica and Robusta coffee using R version 4.3.1 (Ry Core Team, Vienna, Austria).

3. Results and Discussion

3.1. Infrared analysis of arabica coffee

Infrared spectroscopy is a technique used to detect subtle changes in the chemical composition of coffee, where the spectral absorption region is examined to differentiate coffee samples with varying chemical compositions. Spectral methods in the near and mid-infrared range have gained significant interest among researchers due to their ability to quickly and non-invasively assess various characteristics of organic materials without the need for extensive sample preparation (Barbin et al., 2014).

Through a detailed analysis of the spectra obtained from Arabica coffee subjected to different roasting profiles (Fig. 1), it was possible to identify that the most significant absorption bands of the samples, those that provide a broader range of information about their characteristics, are found in the spectral regions between 3269 and 2851 cm^{-1}, as well as from 1743 to 1027 cm^{-1}, the latter being within the region known as the "fingerprint region." It is important to emphasize that such prominent absorption bands are universally present in all employed roasting profiles.

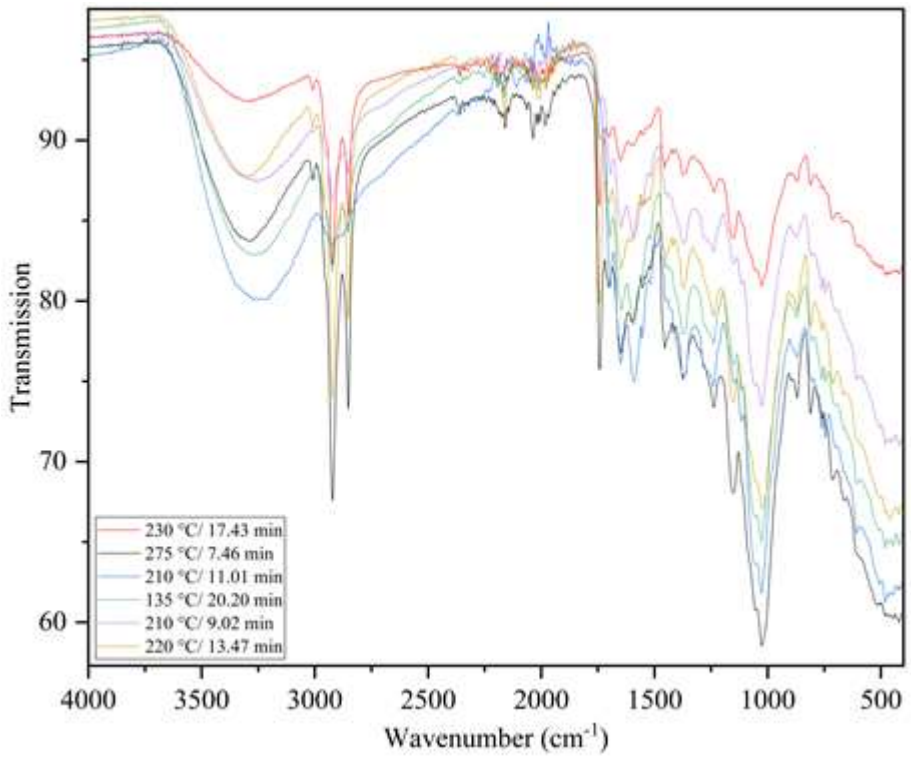


Figure 1. Infrared Spectroscopy in *arabica* coffee variety Catúai affected by different degrees of roasting.

At the specific point of 3269 cm^{-1}, there is a discernible broad amplitude absorption band associated with the vibrational stretching of the O-H bond. This characteristic is observed in a variety of substances present in coffee, including phenols, chlorogenic acids, and carbohydrates (Santos et al., 2016). On the other hand, at the spectral positions of 2922 and 2851 cm^{-1}, two bands of considerable intensity emerge, correlated with the asymmetric and symmetric stretching, respectively, of C-H bonds present in sp^3 carbon atoms. The origin of these stretches is associated with the presence of lipid molecules in roasted coffee, along with other saturated compounds (Barbosa et al., 2013).

Additionally, there is a prominent band at 1743 cm^{-1}, indicating the vibrational stretching of the C=O bond in lipids and aliphatic esters, as exemplified by chlorogenic acid (Barrios-rodríguez et al., 2021; Craig et al., 2018). The stretching of the C=O bond in amides, such as that present in the caffeine structure, is distinctly manifested at 1697 cm^{-1}. A relevant contribution to caffeine characterization is the distinctive band at 1651 cm^{-1}, representing the vibrational stretching of tertiary amides (Craig et al., 2012; Paica et al., 2016).

At the spectral points of 1595 and 1456 cm^{-1}, bands related to the stretching of C=N and CO^{2-} bonds in trigonelline molecules are identified, respectively. Finally, at positions 1151, 1055, and 1027 cm^{-1}, bands indicative of the stretching of ether groups present in carbohydrates,

as well as O-C-O glycosidic bonds present in saccharides like cellulose and sucrose, are observed (Barrios-rodríguez et al., 2021; Paica et al., 2016).

3.2. Infrared analysis of robusta coffee

The analysis of infrared spectra from different roasting profiles of robusta coffee, as illustrated in Figure 2, provides valuable insights into the chemical composition and molecular changes that occur during the roasting process. When examining the spectra, it is notable that certain absorption bands stand out as key points for obtaining essential information about the samples under study. These key bands are concentrated in two specific wavenumber ranges: between 3306 and 2952 cm^{-1} and between 1752 and 1023 cm^{-1}, known as the "fingerprint region" due to the complexity of the information it contains.

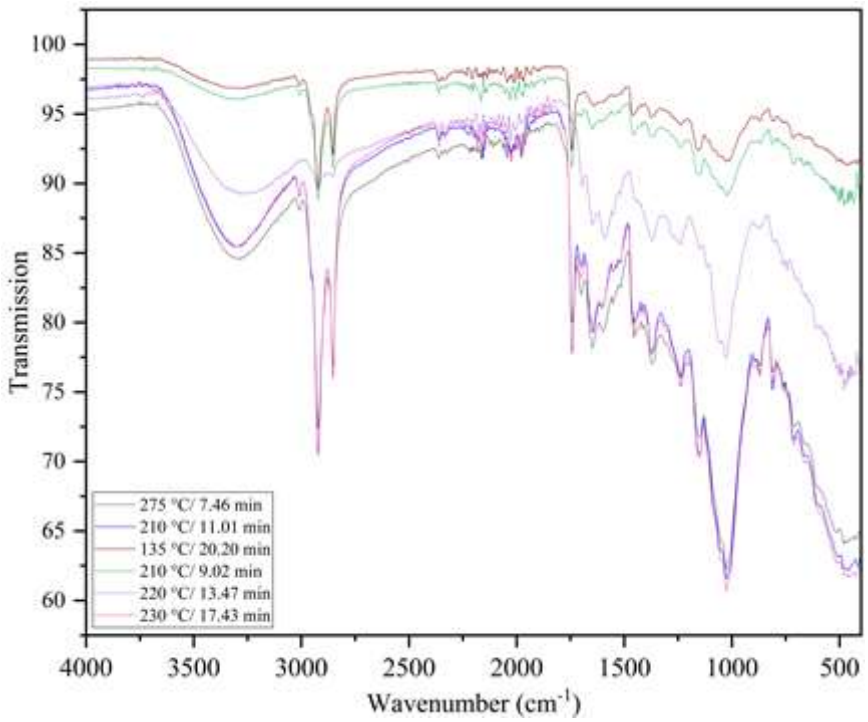


Figure 2. Infrared Spectroscopy in *canephora* (Robusta) coffee affected by different degrees of roasting.

The consistent presence of these important bands in all samples highlights the fundamental nature of the compounds they represent. For example, the broad band observed at 3306 cm^{-1}, related to the stretching of the O-H bond, indicates the presence of essential coffee components such as phenols, chlorogenic acids, and carbohydrates (Santos et al., 2016). These compounds not only contribute to the flavors and aromas of coffee but also play a crucial role in the nutritional and sensory quality of the beverage (Barbosa et al., 2013; Paica et al., 2016).

The intense bands at 2922 and 2852 cm^{-1}, corresponding to the asymmetric and symmetric stretching of C-H bonds in sp^3 carbon atoms, deserve particular attention. These stretches can be attributed to lipid molecules present in roasted coffee, as well as other saturated compounds (Craig et al., 2018). This information suggests the influence of lipid characteristics on the sensory profile and physical properties of coffee, such as crema formation on the surface of an espresso cup.

The analysis of absorption bands at 1742 cm^{-1} reveals the stretching of the C=O bond, which is characteristic of lipids and aliphatic esters, including chlorogenic acid (Craig et al., 2012). The latter is a widely studied compound due to its antioxidant properties and potential impact on human health.

The presence of the band at 1701 cm^{-1}, related to the stretching of the C=O bond in amides such as caffeine, is relevant both for caffeine identification and for assessing coffee quality (Barrios-rodríguez et al., 2021; Craig et al., 2012). This band highlights the presence of nitrogenous compounds like caffeine, which contribute to the flavor and stimulating characteristics of the beverage. Other bands, such as the one observed at 1647 cm^{-1}, specific to the stretching of tertiary amides, are associated with caffeine, providing additional information about this crucial molecule. The presence of bands at 1598 and 1457 cm^{-1} is directly related to trigonelline, a key compound in coffee that plays an essential role in both the flavor and antioxidant properties of the beverage (Barbosa et al., 2013; Craig et al., 2012).

Finally, the bands at 1053 and 1020 cm^{-1} indicate the stretching of ether groups and O-C-O glycosidic bonds in carbohydrates, such as cellulose and sucrose (Barrios-rodríguez et al., 2021). These compounds contribute to the texture, body, and perceived sweetness in coffee.

Taken together, the analysis of absorption bands in infrared spectra provides a detailed and comprehensive insight into the complex chemical composition of arabica and robusta coffee, offering essential information for understanding their quality, taste, aroma, and nutritional impact.

3.3. Sensory analysis by expert panelists

The results of the consensus profile for different coffee roasting profiles are presented in Figure 3 and reveal clear differences between arabica and robusta coffee species. The study considered twelve relevant attributes in coffee evaluation, namely: Acidity, aroma/fragrance, body, sweetness, balance, aftertaste, flavor, uniformity, clean cup, and overall impression. The

minimum and maximum values for individual quality attributes ranged from 6 to 10 on the quality scale, indicating specialty grade.

The "defect" attribute of the product received a score of zero in all used roasting profiles, as expected, to avoid influencing the final coffee score. This is because assigning low scores to this aspect tends to reduce the overall product evaluation. Regarding the "clean cup," "sweetness," and "uniformity" attributes, no significant differences ($p>0.05$) were found between roasting profiles within the same species. However, the "clean cup" attribute showed significant differences ($p<0.05$) between the arabica and robusta species in the 230 °C/17.43 min roasting profile. It is important to emphasize the importance of scores related to "clean cup" since coffees with low ratings in this regard may not result in quality final products as they affect all other attributes. Interestingly, a previous study conducted by Bhumiratana et al. (2011) indicated that coffee prepared at lower temperatures (light roast) is generally sweeter and less bitter than coffees roasted at higher temperatures. However, our results showed a different trend, as different roasting profiles did not exhibit significant differences ($p>0.05$) in the sweetness attribute and achieved significantly high intensity scores, reaching 10 points for both arabica and robusta species in all roasting profiles. These sensory differences likely occur due to changes in volatile substance concentrations, which are determining factors for the final product's quality (Baggenstoss et al., 2008; Buffo & Cardelli-Freire, 2004). These differences were not reported and confirmed in the present study.

Overall, some attributes showed significant differences ($p<0.05$) between the applied roasting profiles, including aftertaste, body, acidity, flavor, fragrance/aroma, balance, overall impression, and final score.

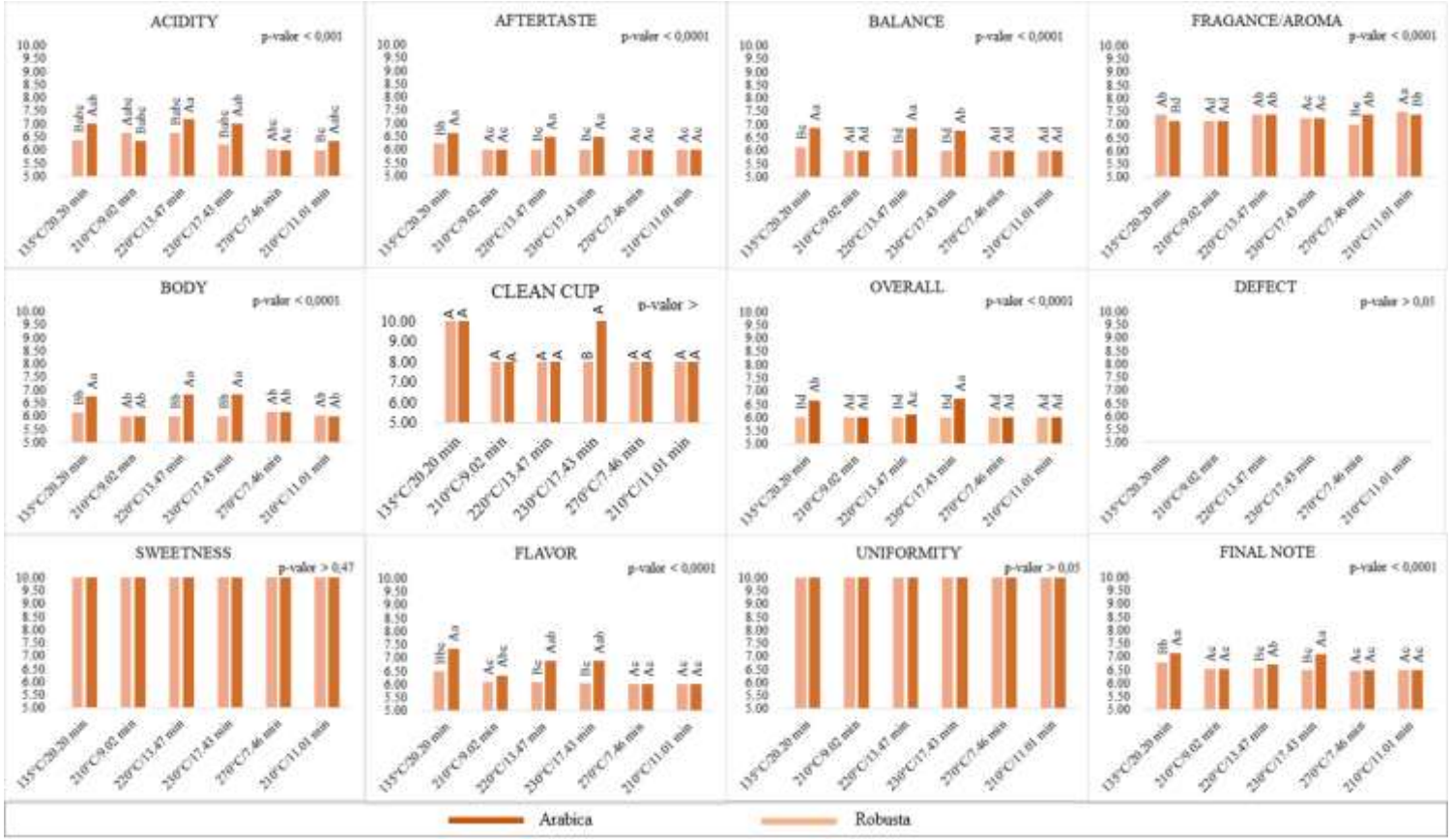


Figure 3. Average values of the attributes and overall qualification by the sensory analysis according to the protocol of the Specialty Coffee Association (SCA) of *canephora* (Robusta) and *arabica* coffee variety Catúai affected by different degrees of roasting. The means followed by the same lowercase letters in all roasting profiles and species, and uppercase letters within the same roasting profile among species, do not differ according to the Tukey test ($p>0.05$).

In arabica coffee, the aftertaste and body attributes received higher scores in the 135 °C/20.20 min, 220 °C/13.47 min, and 230 °C/17.43 min roasting profiles, showing significant differences ($p<0.05$) compared to the other roasting profiles for arabica and robusta coffee. The body attribute, also known as mouthfeel or texture, is an important sensory descriptor for coffee. In instrumental terms, it is often related to total solids and occasionally associated with fat content or fatty acids. Furthermore, to provide a pleasant sensation at the end of coffee consumption, the final coffee flavor must be well-balanced among the aroma, acidity, bitterness, and astringency attributes (Gloess et al., 2013).

The fragrance/aroma attribute received the highest score in arabica coffee in the 210 °C/11.01 min roasting profile (commonly used as the standard profile), with a score of 7.5 points, statistically differing from the other roasting profiles of both arabica and robusta species. Coffee contains various volatile compounds that act as precursors to the beverage's characteristic aroma. During the roasting process, these compounds undergo complex chemical transformations. Several variables, such as coffee variety, cultivation conditions, and processing methods, contribute to the formation of distinct aromas in each type or origin of coffee. Although aroma and flavors are strongly influenced by the locality, it is important to note that the roasting process controls the development of these volatile compounds (Bhumiratana et al., 2011). As a result, differences in aroma complexity arise among coffees subjected to different degrees and roasting conditions. Roasting is, therefore, an essential step to enhance the unique sensory characteristics of each type of coffee, imparting its distinct and pleasing nuances to consumers.

The 135 °C/20.20 min and 220 °C/13.47 min roasting profiles received the highest ratings for the "balance" attribute, both scoring a maximum of 6.88 points. For overall impression, the 230 °C/17.43 min roasting profile received the highest rating, reaching a score of 6.72 points.

The attributes of acidity and flavor exhibited varying scores among the different roasting profiles and analyzed species. For the acidity attribute, scores ranged from 6.0 to 7.17 points for arabica coffee and from 6.0 to 6.67 points for robusta coffee. Flavor scores ranged from 6.0 to 6.88 for arabica coffee and from 6.0 to 6.50 for robusta coffee. Acidity is an essential characteristic of coffee and plays a significant role in consumer perception and response. Along with aroma and bitterness attributes, acidity has long been recognized as a crucial attribute for coffee sensory quality, and it is established that coffee acidity is directly related to the roasting profile to which coffee beans are subjected (Balzer, 2001; Ginz et al., 2000; Rodrigues et al., 2007). Coffee quality is directly influenced by flavor, which results from the chemical

compounds present in coffee beans, also known as precursors. During the roasting process, these compounds undergo transformations and convert into volatile and non-volatile compounds responsible for highlighting the characteristic aromas and flavors of coffee, making this complex chemical reaction occurring during roasting of great importance in the development and highlighting of distinct sensory nuances in the final beverage (Córdoba et al., 2020).

Regarding the final score, the maximum score obtained was 7.12 for the 135 °C/20.20 min roasting profile and 7.08 for the 230 °C/17.43 min roasting profile in arabica coffee. These values showed significant differences ($p<0.05$) both within the arabica coffee context (among the arabica profiles) and in comparison to robusta coffee. It is important to note that the classification of the final product can be influenced by various factors beyond roasting, such as post-harvest processing, crop management, and even the sensory perception of the consumer (Ufer et al., 2019). Therefore, coffee quality is the result of a combination of factors that go beyond the roasting process and involve the entire production chain up to the consumer's experience.

3.4. Consumer sensory analysis

The attributes color, aroma, acidity, sweetness, flavor, and overall impression assessed through the affective test on a 9-point hedonic scale are presented in Table 2.

The "color" attribute was the most highly rated for both coffee species, with Arabica coffee receiving scores ranging from "slight liking" to "liking very much" (6.19 to 7.82 points), with significant differences between roast profiles, and the 135 °C/20.20 min profile being the most highly rated. Robusta coffee received relevant scores in the "color" attribute, ranging from "slight liking" to "moderate liking," with significant variations in statistics ($p<0.05$). When comparing the species and similar roast profiles, only the 135 °C/20.20 min and 220 °C/13.47 min profiles showed significant differences ($p<0.05$). However, the Brazilian consumers in the study exhibited a greater preference for lighter coffee samples, those produced using lower temperatures. The amount of phenolic compounds, sugars, and lipids present in both varieties, along with the degree of roasting, influence the color of the final beverage, with Arabica coffee often exhibiting a lighter color due to these factors (Freitas et al., 2023; Leme et al., 2019; Mehaya & Mohammad 2020; Neves et al., 2023).

The coffee aroma attribute is a distinctive and appealing characteristic resulting from the complex interaction of volatile compounds present in roasted beans. The results related to this attribute are detailed in Table 2. In Arabica coffee, significant differences ($p<0.05$) were observed between roast profiles regarding the aroma attribute. However, Robusta coffee did not show significant differences ($p>0.05$) between roast profiles. When comparing the two species at the same roast profile, only the profiles at 135 °C/20.20 min and 210 °C/11.01 min showed significant differences ($p<0.05$), with Arabica receiving higher scores. These aroma differences between Arabica and Robusta coffees stem from variations in their intrinsic chemical compositions (Haile & Kang 2019; Neves et al., 2023). Arabica coffee tends to contain more sugars and unsaturated fatty acids, while Robusta coffee has higher proportions of saturated fatty acids and elevated total lipids levels (Cheng et al., 2016; Neves et al., 2023; Romano et al., 2014). These differences influence Maillard reactions and chlorogenic acid degradation during roasting, resulting in unique volatile compound profiles contributing to specific aromas in each variety (Kulapichitr et al., 2019; Neves et al., 2023). Additionally, variations in polysaccharide and amino acid compositions also affect the formation of volatile compounds during roasting, contributing to the diversity of aromas detected in Arabica and Robusta coffee beverages (Prakash et al., 2022).

Acidity is a crucial sensory attribute that contributes to the complexity and quality of coffee flavor. The results of the sensory analysis of the acidity attribute are presented in Table 2. In the present study, no significant differences ($p>0.05$) were observed in the acidity attribute among different roast profiles for Arabica coffee. However, in the case of Robusta coffee, significant differences ($p<0.05$) were found between roast profiles, with profiles using milder temperatures (135 °C/20.20 min, 210 °C/9.02 min, and 210 °C/11.01 min) being better evaluated by tasters. This can be explained by the fact that lower temperatures allow for a more gradual and controlled Maillard reaction and caramelization, resulting in greater preservation of compounds that contribute to acidity. At higher temperatures, these reactions occur more intensely, leading to the production of compounds that negatively impact the flavor due to the loss of important acidity-contributing chemical constituents. Among the Arabica and Robusta coffee species, roast profiles at 220 °C/13.47 min, 230 °C/17.43 min, and 275 °C/7.46 min showed significant differences ($p<0.05$). These differences can be attributed to the unique chemical compositions of the two coffee varieties, which react differently to variations in temperature and time during the roasting process. It is important to note that the intrinsic characteristics of Arabica and Robusta coffee, including different levels of compounds such as

sugars, chlorogenic acids, and lipids, directly influence sensory properties (Catão et al., 2022; Mehaya & Mohammad, 2020).

The sweetness of coffee is a complex and desirable sensory aspect influenced by the concentration of natural sugars, roast profile, and brewing method. The average scores assigned to this attribute are presented in Table 2. In Arabica coffee, significant differences ($p<0.05$) were observed between roast profiles, with the 230 °C/17.43 min profile receiving the lowest score (3.79 points). In Robusta coffee, there were no significant differences ($p>0.05$) between roast profiles, with scores ranging from 3.74 to 3.96, indicating moderate to slight dislike. When comparing the two species at the same roast profile, Arabica coffee was generally rated more positively by tasters compared to Robusta, with scores ranging from moderate dislike to slight liking. Sweetness contributes to flavor balance and can vary between species, adding complexity to sensory attributes (Rogers et al., 1999; Neves et al., 2023). The coffee received low ratings for the sweetness attribute due to the fact that Brazilian consumers are accustomed to using sugar in their coffee. However, the samples served in the study were not sweetened, which resulted in lower scores. Coffee culture in Brazil has a long history of appreciating coffee sweetened with sugar, which has become a common preference among consumers. Therefore, when the coffee was evaluated without sugar, many Brazilian consumers could perceive a difference in the sweetness level, leading to lower scores for this attribute. This cultural peculiarity highlights the importance of taking local preferences into account when evaluating food and beverage products in market or sensory studies.

Table 2. Hedonic Scale analysis of *canephora* (Robusta) and *arabica* coffee variety Catúai affected by different degrees of roasting.

Roasting profiles	**Attributes**											
	Acidity		Sweetness		Aroma		Flavor		Color		Overall impression	
	Arabica	Robusta	Arabica	Robusta	Arabica	Robusta	Arabica	Robusta	Arabica	Robusta	Arabica	Robusta
135 °C/20.20 min	5.95 ± 1.67^{Aa}	5.81 ± 2.24^{Aa}	5.10 ± 1.98^{Ba}	3.78 ± 1.57^{Ab}	6.82 ± 2.05^{Aa}	5.60 ± 1.83^{Bb}	6.07 ± 0.98^{Ba}	6.17 ± 1.28^{Aa}	7.82 ± 0.91^{Aa}	6.89 ± 0.84^{ABb}	6.06 ± 1.96^{Aa}	5.43 ± 2.09^{Ab}
210 °C/9.02 min	5.76 ± 1.57^{Aa}	5.30 ± 2.16^{Aa}	5.30 ± 2.03^{ABa}	3.74 ± 1.59^{Ab}	6.00 ± 1.61^{Ba}	5.68 ± 1.75^{Ba}	6.75 ± 0.77^{Aa}	5.89 ± 1.37^{ABb}	7.13 ± 0.96^{Ba}	6.98 ± 0.94^{Aa}	5.59 ± 2.04^{Aa}	5.73 ± 1.93^{Aa}
220 °C/13.47 min	4.53 ± 1.97^{Bb}	5.41 ± 1.72^{Aa}	5.94 ± 1.73^{Aa}	3.87 ± 1.77^{Ab}	5.65 ± 1.83^{Ba}	5.90 ± 1.91^{Ba}	6.84 ± 0.79^{Aa}	5.89 ± 1.55^{ABb}	6.88 ± 0.86^{Ba}	6.55 ± 0.93^{BCb}	5.83 ± 1.99^{Aa}	3.85 ± 1.68^{Bb}
230 °C/17.43 min	3.65 ± 2.12^{Cb}	5.02 ± 1.84^{Aa}	3.79 ± 1.63^{Ca}	3.76 ± 1.58^{Aa}	6.18 ± 1.44^{ABa}	6.00 ± 1.47^{Ba}	6.80 ± 0.75^{Aa}	5.62 ± 1.74^{BCb}	6.50 ± 0.95^{Cb}	6.87 ± 0.87^{ABa}	6.02 ± 2.10^{Aa}	5.89 ± 1.37^{Aa}
275 °C/7.46 min	3.89 ± 1.63^{BCb}	5.40 ± 2.06^{Aa}	4.66 ± 1.83^{Ba}	3.93 ± 1.71^{Ab}	5.54 ± 1.64^{Ba}	5.85 ± 1.93^{Ba}	6.80 ± 0.76^{Aa}	5.41 ± 2.00^{BCb}	6.19 ± 0.98^{Ca}	6.39 ± 1.00^{CDa}	5.62 ± 2.03^{Aa}	3.89 ± 1.55^{Bb}
210 °C/11.01 min	5.37 ± 1.65^{Aa}	5.22 ± 2.01^{Aa}	4.71 ± 1.85^{Ba}	3.75 ± 1.74^{Ab}	5.78 ± 1.76^{Bb}	6.70 ± 1.49^{Aa}	7.24 ± 1.00^{Aa}	5.33 ± 1.56^{Cb}	6.20 ± 0.92^{Ca}	6.11 ± 0.99^{Da}	6.13 ± 1.87^{Aa}	5.28 ± 2.11^{Ab}

Means followed by the same lowercase letters in the row and uppercase letters in the column for each attribute do not differ by Tukey's test (p>0,05).

Coffee flavor plays a fundamental role in the appreciation of the beverage, being influenced by a complex interaction of organic compounds and chemical reactions. The results related to the flavor attribute are presented in Table 2. Significant differences ($p<0.05$) were observed in the flavor attribute between the two coffee species (Arabica and Robusta). Arabica coffee received the lowest score at the 135 °C/20.20 min roast profile among all roast profiles. On the other hand, Robusta coffee showed statistically significant variations ($p<0.05$) among all roast profiles, with scores ranging from 5.33 to 6.17, with the highest score attributed to the 135 °C/20.20 min roast profile. It is relevant to highlight that the highest scores in the flavor attribute were assigned to Arabica coffee ($p<0.05$). The superiority of Arabica coffee flavor compared to Robusta can be attributed to various factors. Arabica coffee is recognized for having higher amounts of sugars, lipids, and aromatic compounds, resulting in a smoother body and greater flavor richness (Cheng et al., 2016; Kulapichitr et al., 2019; Neves et al., 2023; Romano et al., 2014). Additionally, it presents a wider variety of volatile compounds, contributing to complex aromatic notes and sensory nuances. Genetic differences between the two species lead to distinct sensory profiles. Careful cultivation and processing of Arabica under moderate climatic conditions also contribute to its superior flavor (Haile & Kang 2019; Neves et al., 2023).

Finally, the "overall impression" attribute represents the sum of individual impressions and experiences that consumers have when interacting with the product, resulting in an overall positive or negative evaluation. The data related to this attribute are presented in Table 2. Arabica coffee showed no significant differences ($p>0.05$) in this attribute, while Robusta coffee exhibited significant differences ($p<0.05$), with the 220 °C/13.47 min and 275 °C/7.46 min roast profiles being the least well-rated. In terms of species and similar roast profiles, significant differences were observed ($p<0.05$), with Arabica coffee being better rated in all roast profiles.

In summary, consumers evaluated various sensory attributes of Arabica and Robusta coffee, revealing distinct nuances in acidity, sweetness, aroma, flavor, and overall impression. Roast profiles with milder temperatures stood out for Robusta, preserving its acidity and aroma, while Arabica excelled in sweetness and flavor attributes.

3.5. Exploratory analysis of sensory analysis through PCA

Principal Component Analysis (PCA) is an important statistical tool employed to elucidate and analyze differences between samples, as well as the ability to extract more knowledge from variables that primarily affect the spatial distribution of samples. The use of PCA can reduce the dimensionality of the data matrix, capturing a large portion of the original data information, and clarify the relationship between objects and the correlation structure of variables (Alessandrini et al., 2008; Souza et al., 2022). PCA was conducted on the dataset of values to assess the influence of coffee species and roast profiles on sample grouping. The two-dimensional bi-plots of scores and loadings for Arabica and Robusta species in different roast profiles are presented in Figure 4. The Principal Components (PCs) PC1 and PC2 represented 49.5 % and 15.9 % of the total variance, respectively, with the cumulative contribution rate of the first two PCs accounting for 65.4 %.

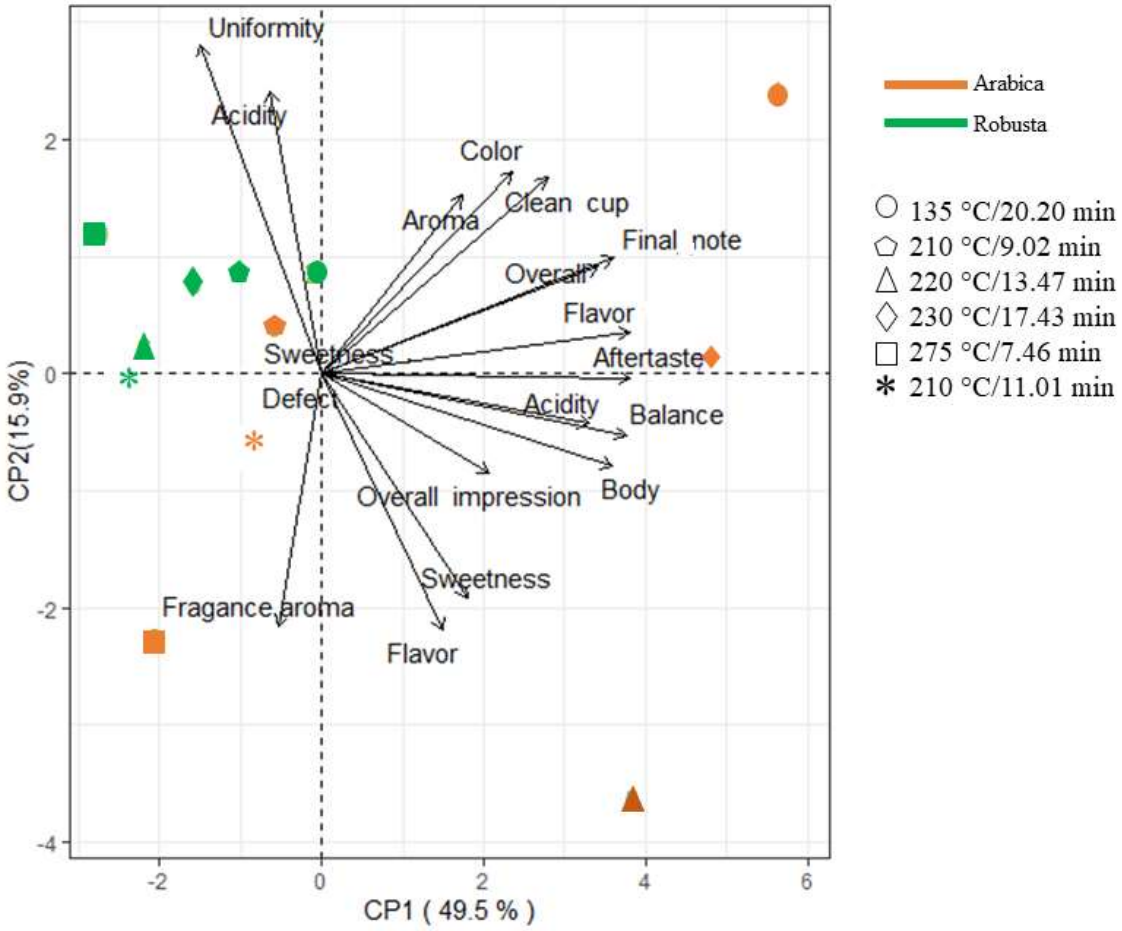


Figure 4. Scatter plot of Principal Component Analysis (PCA) scores from panelist and consumer sensory analysis on samples of canephora (Robusta) and *arabica* coffee after different roasting treatments (PC1 vs. PC2).

In the graphical representation of Principal Component Analysis (PCA), the roast profiles for Arabica coffee at 135 °C/20.20 min and 230 °C/17.43 min were positioned in the positive quadrant of PC1 and PC2. In the case of Robusta coffee, except for the roast profile at 210 °C/11.01 min, which fell into the negative quadrant of both PC1 and PC2, the other roast profiles exhibited a disposition with negative PC1 and positive PC2. Within the context of Arabica coffee, only the roast profile at 210 °C/9.02 min showed a similar disposition, with negative PC1 and positive PC2. The roast profiles at 275 °C/7.46 min and 210 °C/11.01 min, however, positioned themselves in the negative quadrant of PC1 and positive quadrant of PC2. In this negative PC1 and positive PC2 quadrant, the roast profiles were primarily associated with the "fragrance/aroma" attribute. It's worth noting that the only roast profile that exhibited the reverse configuration, with positive PC1 and negative PC2, was Arabica coffee subjected to a temperature of 220 °C/13.47 min, and it was associated with attributes like flavor, acidity, and overall impression by common consumers and attributes like body, balance, and sweetness by trained panelists.

In general, Arabica coffee beans tend to have a higher market value and display more advantageous sensory characteristics compared to Robusta beans (Pinheiro et al., 2021). However, it is worth noting that Robusta coffee boasts significant advantages in terms of its composition. This attribute proves to be a considerable advantage, especially for consumers whose focus extends beyond the sensory aspects of the product, demonstrating a noteworthy concern for the health benefits provided by this variety.

Conclusion

This study investigated the use of different roast profiles for Arabica and Robusta coffee beans, considering compositional aspects (infrared spectroscopy) and sensory evaluation (based on Q-grader certified tasters) as well as consumer preferences (affective evaluation). Infrared analysis and sensory evaluation provided valuable insights into the characteristics of Arabica and Robusta coffees subjected to various roast profiles. Infrared spectra revealed significant absorption bands associated with relevant compounds such as chlorogenic acids, lipids, carbohydrates, and other aromatic compounds. Differences in absorption bands between the coffee species and roast profiles can be explained by variations in the intrinsic chemical composition of coffee varieties and the complex reactions that occur during the roasting process.

The sensory analysis conducted by expert panelists and regular consumers yielded important information about the sensory attributes of the coffees. Attributes like acidity, sweetness, aroma, flavor, and overall impression were evaluated, revealing notable variations among different roast profiles and coffee species. Differences in sensory evaluations can be attributed to the unique chemical compositions of coffee varieties as well as the transformations that occur during roasting.

Principal Component Analysis (PCA) allowed for the visualization of sample distribution based on the assessed sensory attributes. The results showed how different roast profiles influence sample grouping and how specific attributes like fragrance/aroma and flavor are correlated with particular roast profiles.

In summary, the combination of spectral, sensory, and statistical analyses provided a comprehensive understanding of the chemical and sensory characteristics of Arabica and Robusta coffees, enabling the identification of patterns associated with roast profiles and coffee species. These findings may have significant implications for the coffee industry, contributing to the selection of ideal roast profiles that enhance the desired sensory characteristics in each coffee variety.

References

Alessandrini, L., Romani, S., Pinnavaia, G., Dalla Rosa, M. (2008). Near infrared spectroscopy: An analytical tool to predict coffee roasting degree. *Analytica Chimica Acta,* 625(*1*), 95-102. https://doi.org/10.1016/j.aca.2008.07.013

Alvares, C. A., Stape, J. L., Setelhas, P. C., Gonçalves, J. L. M., Sparovek, G. (2013). Köppen's climate classification map for Brazil. *Meteorologische Zeitschrift*, *22*(6), 711-728. https://doi.org/10.1127/0941-2948/2013/0507

Baggenstoss, J., Poisson, L., Kaegi, R., Perren, R., Escher, F. (2008). Coffee roasting and aroma formation: application of different time-temperature conditions. *Journal of Agricultural and Food Chemistry*, *56*(14), 5836-5846.

Barbosa, L. C. A. (2013). Infrared spectroscopy in the characterization of organic compounds. UFV Publisher, 1st edition.

Barbin, D. F., Felicio, A. L. S. M., Sun, Da-Wen., Nixdorf, S. L., Hirooka, E. Y. (2014). Application of infrared spectral techniques on quality and compositional attributes of coffee: An overview. *Food Research International*, *61*, 23-32. https://doi.org/10.1016/j.foodres.2014.01.005

Barrios-Rodríguez, Y. F., Reyes, C. A. J., Campos, J. S. T., Gíron-Hernández, J., Rodríguez-Gamir, J. (2021). Infrared spectroscopy coupled with chemometrics in coffee post-harvest processes as complement to the sensory analysis. *LWT – Food Science and Technology*, *145*, article 111304. https://doi.org/10.1016/j.lwt.2021.111304

Bhumiratana, N., Adhikari, K., Chambers IV, E. (2011). Evolution of sensory aroma attributes from coffee beans to brewed coffee. *LWT-Food Science and Technology*, *44*(10), 2185-2192.

Borém, F. M., Cirillo, M. Â., Alves, A. P. C., Santos, C. M., Liska, G. R., Ramos, M. F., Lima, R. R. (2020). Coffee sensory quality study based on spatial distribution in the Mantiqueira mountain region of Brazil. *Journal of Sensory Studies*, *35(2)*, 1-15. https://doi.org/10.1111/joss.12552

Buffo, R. A., Cardelli-Freire, C. (2004). Coffee flavour: an overview. *Flavour and Fragrance Journal*, *19*(2), 99-104. https://doi.org/10.1002/ffj.1325

Cassimiro, D. M. J., Batista, N. N., Fonseca, H. C., Naves, J. A. O., Coelho, J. M., Bernardes, P. C., Dias, D. R., Schwan, R. F. (2023). Wet fermentation of *Coffea canephora* by lactic acid bacteria and yeasts using the self-induced anaerobic fermentation (SIAF) method enhances the coffee quality. *Food Microbiology*, *110*, article 104161. https://doi.org/10.1016/j.fm.2022.104161

Catão, A. A., Mateus, N. D. S., Garcia, C., Michelle, C., Novaes, F. J. M., Alves, S. Jr, S. (2022). Coffee-roasting variables associated with volatile organic profiles and sensory evaluation using multivariate analysis. *Applied Food Research*, *2*, article 100223. https://doi.org/10.1016/j.afres.2022.100223

Cheng, B., Furtado, A., Smyth, H. E., Henry, R. J. (2016). Influence of genotype and environment on coffee quality. *Trends in Food Science & Technology*, *57*, 20-30. https://doi.org/10.1016/j.tifs.2016.09.003

Córdoba, N., Fernandez-Alduenda, M., Moreno, F. L., Ruiz, Y. (2020). Coffee extraction: A review of parameters and their influence on the physicochemical characteristics and flavour of coffee brews. *Trends in Food Science & Technology*, *96*, 45-60. https://doi.org/10.1016/j.tifs.2019.12.004

Chang, C., Wu, G., Zhang, H., Jin, Q. Wang, X. (2020). Deep-fried flavor: Characteristics, formation mechanisms, and influencing factors. *Critical Reviews in Food Science and Nutrition*, *60*(9), 1496-1514. https://doi.org/10.1080/10408398.2019.1575792

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 Chemistry*, *245*, 1052-1061. https://doi.org/10.1016/j.foodchem.2017.11.066

Craig, A. P., Franca, A. S., Oliveira, L. S. (2012). Discrimination between defective and non-defective roasted coffees by diffuse reflectance infrared Fourier transform spectroscopy. *LWT – Food Science and Technology*, 47(*2*), 505-511.

Craig, A. P., Fraca, A. S., Oliveira, L. S., Irudayaraj, J. (2015). Fourier transform infrared spectroscopy and near infrared spectroscopy for the quantification of defects in roasted coffees. *Talanta*, *134*, 379-386. https://doi.org/10.1016/j.talanta.2014.11.038

Fadai, N. T., Melrose, J., Plese, C. P., Schulman, A., Gorder, R. A. V. (2017). A heat and mass transfer study of coffee bean roasting. *International Journal of Heat and Mass Transfer*, *104*, 787-799. https://doi.org/10.1016/j.ijheatmasstransfer.2016.08.083

Ferreira, L. J. C., Gomes, M. S., Oliveira, L. M., Santos, L. D. (2023). Coffee fermentation process: A review. *Food Research International*, *169*, article 112793. https://doi.org/10.1016/j.foodres.2023.112793

Frebrianto, N. A., Zhu, F. (2023). Coffee bean processing : Emerging methods and their effects on chemical, biological and sensory properties. *Food Chemistry*, *412*, 135489. https://doi.org/10.1016/j.foodchem.2023.135489

Freitas, V. V., Rodrigues, L. L. B., Castro, G. A. D., dos Santos, M. H., Vidigal, M. C. T. R., Fernandes, S. A., Stringheta, P. C. (2023). Impact of different roasting conditions on the chemical composition, antioxidant activities, and color of *Coffea canephora* and *Coffea arabica* L. samples. *Heliyon*, *9*(9), article e19580. https://doi.org/10.1016/j.heliyon.2023.e19580

Ginz, M., Balzer, H. H., Bradbury, A. G., Maier, H. G. (2000). Formation of aliphatic acids by carbohydrate degradation during roasting of coffee. *European Food Research and Technology*, *211*, 404-410.

Gloess, A. N., Schönbächler, B., Klopprogge, B., D`Ambrósio, L., Châtelain, K., Bongartz, A., Strittmatter, A., Rast, M., Yeretzian, C. (2013). Comparison of nine common coffee extraction methods: instrumental and sensory analysis. *European Food Research Technology*, *236*, 607-627. https://doi.org/10.1007/s00217-013-1917-x

Haile, M., & Kang, W. H. (2019). The role of microbes in coffee fermentation and their impact on coffee quality. *Journal of Food Quality*, *2019*, article 4836709. https://doi.org/10.1155/2019/4836709

Kim, C., Park, S. J., Yu, J. S., Lee, D. Y. (2022). Interactive effect of post-harvest processing method, roasting degree, and brewing method on coffee metabolite profiles. *Food Chemistry*, *397*, article 133749. https://doi.org/10.1016/j.foodchem.2022.133749

Kulapichitr, F., Borompichaichartkul, C., Suppavorasatit, I., Cadwallader, K. R. (2019). Impact of drying process on chemical composition and key aroma components of Arabica coffee. *Food Chemistry*, *291*, 49-58. https://doi.org/10.1016/j.foodchem.2019.03.152

Laukaleja, I. & Koppel, K. (2021). Aroma active compound perception in differently roasted and brewed coffees by gas chromatography–olfactometry. *Journal of Sensory Studies*, *36(6)*, 1-15. https://doi.org/10.1111/joss.12708

Leme, D. S., da Silva, S. A., Barbosa, B. H. G., Borém, F. M., Pereira, R. G. F. A. (2019). Recognition of coffee roasting degree using a computer vision system. *Computers and Electronics in Agriculture*, *156*, 312-317. https://doi.org/10.1016/j.compag.2018.11.029

Mehaya, F. M., Mohammad, A. A. (2020). Thermostability of bioactive compounds during roasting process of coffee beans. *Heliyon*, *6*, article e05508. https://doi.org/10.1016/j.heliyon.2020.e05508

Minim, V. P. (2013). Análise sensorial: estudos com consumidores. Editora UFV.

Neves, A. L. S., Martinez, J. R., Maciel, M. I. S., Melo, R. P., Veríssimo, C. M., Arruda, L. L. A. L. (2023). Impact of the physicochemical parameters on the sensory characterization of Brazilian coffee by the CATA method. *Food Chemistry Advances*, *3*, article 100403. https://doi.org/10.1016/j.focha.2023.100403

Paica, D. L., Lampman, G. M., Kriz, G. S., Vyvyan, J. R. (2016). Introduction to spectroscopy. Cengage Learning, 5th edition North American translation.

Pereira, G. V. M., Neto, D. P. C., Júnior, A. I. M., Vásquez, Z. S., Medeiros, A. B. P, Vandenberghe, L. P. S., Soccol, C. R. (2019). Exploring the impacts of postharvest processing on the aroma formation of coffee beans–A review. *Food chemistry*, *272*, 441-452. https://doi.org/10.1016/j.foodchem.2018.08.061

Pinheiro, P.F., Pinheiro, C.A., Osório, V.M., Pereira, L.L. (2021). Chemical Constituents of Coffee. In: Louzada Pereira, L., Rizzo Moreira, T. (eds) Quality Determinants In Coffee Production. *Food Engineering Series. Springer*, Cham. https://doi.org/10.1007/978-3-030-54437-9_5

Prakash, I., Shankar, S. R., Sneha, H. P., Kumar, P., Om, H., Basavaraj, K., Murthy, P. S. (2022). Metabolomics and volatile fingerprint of yeast fermented robusta coffee: A value added coffee. *LWT- Food Science and Technology*, *154*, article 112717. https://doi.org/10.1016/j.lwt.2021.112717

Ribeiro, J. S., Augusto, F., Salva, T. J., Thomaziello, R. A., Ferreira, M. M. C. (2009). Prediction of sensory properties of Brazilian Arabica roasted coffees by headspace solid phase

microextraction-gas chromatography and partial least squares. *Analytica Chimica Acta, 634*(2), 172-179. https://doi.org/10.1016/j.aca.2008.12.028

Rodrigues, C. I., Marta, L., Maia, R., Miranda, M., Ribeirinho, M., Máguas, C. (2007). Application of solid-phase extraction to brewed coffee caffeine and organic acid determination by UV / HPLC. *Journal of Food Composition and Analysis*, *20*, 440-448. https://doi.org/10.1016/j.jfca.2006.08.005

Rogers, W. J., Bastin, M., Bucheli, P. (1999). Changes to the content of sugars , sugar alcohols , myo-inositol , carboxylic acids and inorganic anions in developing grains from different varieties of Robusta (*Coffea canephora*) and Arabica (*C . arabica*) coffees. *Plant Science*, *149*, 115-123. https://doi.org/10.1016/S0168-9452(99)00147-8

Romano, R., Santini, A., Le, L., Manzo, N., Visconti, A., & Ritieni, A. (2014). Identification markers based on fatty acid composition to differentiate between roasted *Arabica* and *Canephora* (Robusta) coffee varieties in mixtures. *Journal of Food Composition and Analysis, 35*(1), 1-9. https://doi.org/10.1016/j.jfca.2014.04.001

Santos, R. S., Lopo, M., Angel, A. O. S. S., Lopes, J. A. (2016). Exploiting near infrared spectroscopy as an analytical tool for on-line monitoring of acidity during coffee roasting. *Food Control*, *60*, 408-415. https://doi.org/10.1016/j.foodcont.2015.08.007

Scholz, M. B. S., Kitzberger, C. S. G., Prudencio, S. H., Silva, R. S. S. F. (2018). The typicity of coffees from different terroirs determined by groups of T physico-chemical and sensory variables and multiple factor analysis. *Food Research International*, *114*, 72-80. https://doi.org/10.1016/j.foodres.2018.07.058

Souza, J. C., Pasquini, C., Hespanhol, M. C. (2022). Feasibility of compact near-infrared spectrophotometers and multivariate data analysis to assess roasted ground coffee traits. *Food Control*, *138*, article 109041. https://doi.org/10.1016/j.foodcont.2022.109041

Specialty Coffee Association (2018). Cupping Protocols. Retrieved from https://sca.coffee/research/protocols-best-practices. Accessed Sep. 16, 2021.

Sruthi, N. U., Premjit, Y., Pandiselvam, R., Kothakota, A., Ramesh, V. (2021). An overview of conventional and emerging techniques of roasting: Effect on food bioactive signatures. *Food Chemistry*, *348*, article 129088. https://doi.org/10.1016/j.foodchem.2021.129088

Tugnolo, A., Giovenzana, V., Malegori, C., Oliveri, P., Casson, A., Curatitoli, M., Guidetti, R., Beghi, R. (2021). A reliable tool based on near-infrared spectroscopy for the monitoring of moisture content in roasted and ground coffee : A comparative study with thermogravimetric analysis. *Food Control*, *130*, article 108312. https://doi.org/10.1016/j.foodcont.2021.108312

Ufer, D., Lin, W., Ortega, D. L. (2019). Personality traits and preferences for specialty coffee: Results from a coffee shop field experiment. *Food Research International*, *125*, article 108504.

Widodo, P. B., Yulianto, M. E., Ariyanto, H. D., Paramita, V. (2023). Materials Today : Proceedings Efficacy of natural and full washed post-harvest processing variations on arabica coffee characteristics. *Materials Today: Proceedings*, *81(1)*, 1-6. https://doi.org/10.1016/j.matpr.2023.02.376

Worch, T., Lê, S., Punter, P. (2010). How reliable are the consumers? Comparison of sensory profiles from consumers and experts. *Food Quality and Preference*, *21*(3), 309-318. https://doi.org/10.1016/j.foodqual.2009.06.001

Zhang, Y., Li, X., Lu, X., Sun, H., Wang, F. (2021). Effect of oilseed roasting on the quality, flavor and safety of oil : A comprehensive review. *Food Research International*, *150*, article 110791. https://doi.org/10.1016/j.foodres.2021.110791

Artigo 5*

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Exploring innovative roasting profiles to enhance the chemical and sensory composition of Arabica coffee

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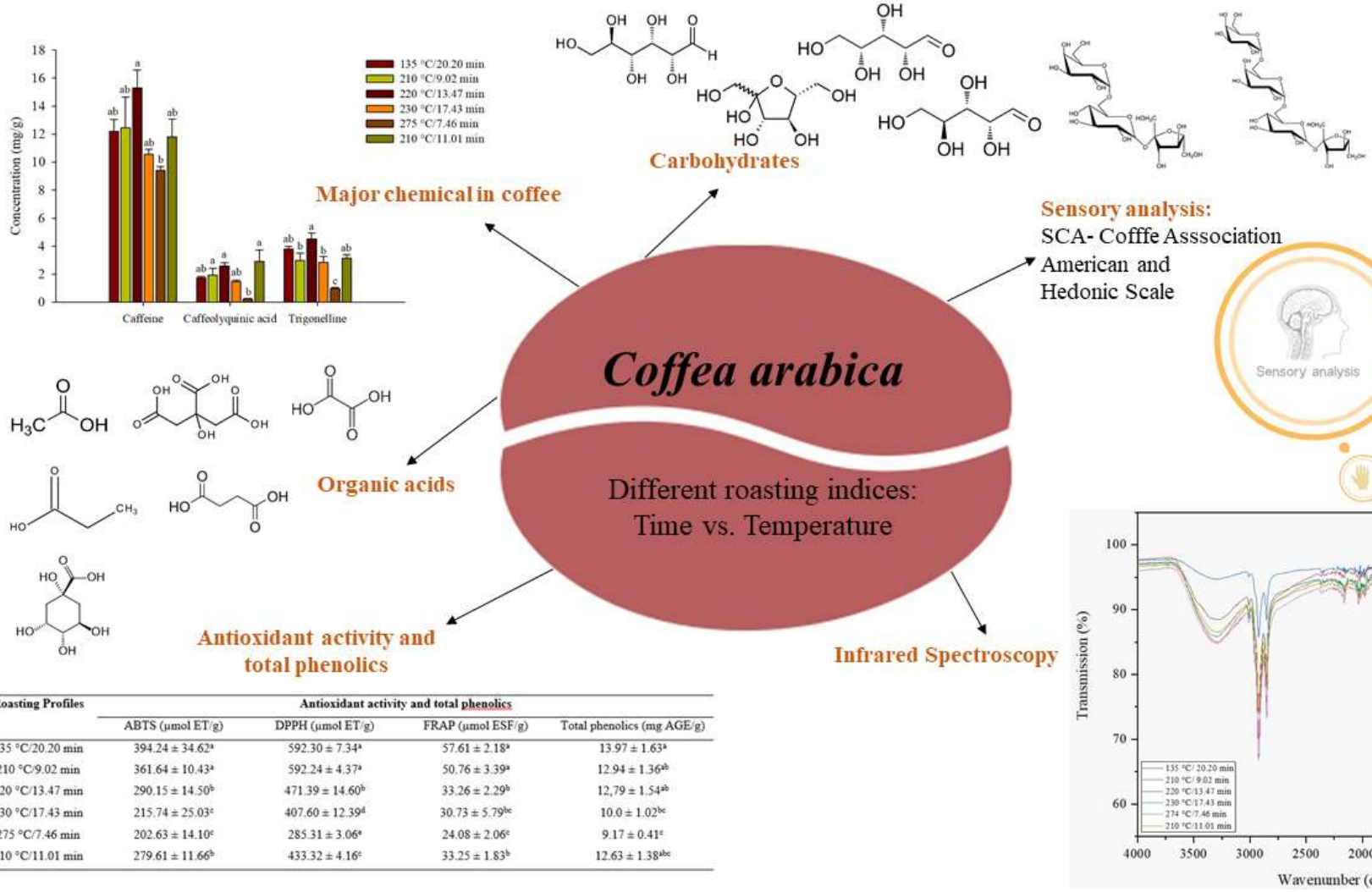
Graphical abstract



Roasting Profiles	Antioxidant activity and total phenolics			
	ABTS (μmol ET/g)	DPPH (μmol ET/g)	FRAP (μmol ESF/g)	Total phenolics (mg AGE/g)
135 °C/20.20 min	394.24 ± 34.62^{a}	592.30 ± 7.34^{a}	57.61 ± 2.18^{a}	13.97 ± 1.63^{a}
210 °C/9.02 min	361.64 ± 10.43^{a}	592.24 ± 4.37^{a}	50.76 ± 3.39^{a}	12.94 ± 1.36^{ab}
220 °C/13.47 min	290.15 ± 14.50^{b}	471.39 ± 14.60^{b}	33.26 ± 2.29^{b}	12,79 ± 1.54^{ab}
230 °C/17.43 min	215.74 ± 25.03^{c}	407.60 ± 12.39^{d}	30.73 ± 5.79^{bc}	10.0 ± 1.02^{bc}
275 °C/7.46 min	202.63 ± 14.10^{c}	285.31 ± 3.06^{e}	24.08 ± 2.06^{c}	9.17 ± 0.41^{c}
210 °C/11.01 min	279.61 ± 11.66^{b}	433.32 ± 4.16^{c}	33.25 ± 1.83^{b}	12.63 ± 1.38^{abc}

Abstract

In this study, different roasting profiles were evaluated to analyze their impact on Arabica coffee in terms of sensory characteristics, chemical composition, and antioxidant activity. The results revealed significant differences in sensory attributes such as flavor, acidity, sweetness, and overall impression among the roasting profiles. Physicochemical characteristics such as phenolic compounds, organic acids, color, and antioxidant activity also varied with the different roasting profiles. It was observed that roasting at lower temperatures resulted in a higher concentration of phenolic compounds and a more attractive color, while roasting at higher temperatures led to a decrease in antioxidant activity. Infrared analysis revealed the presence of various substances such as phenols, chlorogenic acids, carbohydrates, and lipids in coffee. These findings highlight the importance of precise control over roasting parameters to preserve the desirable characteristics of coffee.

Keywords: Organic acids; Carbohydrates; Antioxidant activity; Total phenolics; Infrared; Sensory analysis.

1. Introduction

The coffee roasting process is a fundamental step in the production of the beverage, and its application can positively or negatively affect the final product. In the roasting process, two important factors stand out, namely, temperature and roasting duration (time). The typical temperatures range from 160 °C to 240 °C, with 210 °C being the most common roasting temperature, and the maximum exposure time to heat is 14 minutes (Freitas et al., 2023; Park et al., 2023; Sruthi et al., 2021).

During the roasting process, using temperatures considered high, various chemical reactions occur, including the Maillard reaction and caramelization (Freitas et al., 2023). The Maillard reaction is of great importance in food processing, including coffee. This reaction has the ability to affect the nutritional and sensory aspects of food, as well as produce some desirable and undesirable compounds for human health (Liu et al., 2020; Shakoor et al., 2022; Wei et al., 2015). For this reaction to occur, a free carbonyl group and an amino group are required (Moreira et al., 2017; Jia et al., 2023; Xue et al., 2022). Another reaction that takes place is caramelization, which is a non-enzymatic browning reaction that occurs during the thermal processing of food, leading to the degradation of sugars. As a consequence, it becomes difficult to distinguish the products formed in the Maillard reaction from those formed in caramelization, due to the occurrence of both reactions simultaneously (Sen et al., 2022). These reactions can lead to changes in the taste, aroma, color, and chemical composition of coffee (Freitas et al., 2023; Zuhair et al., 2018). The roasting process can lead to the degradation of proteins, polysaccharides, chlorogenic acids, caffeine, trigonelline, the formation of 5-hydroxymethylfurfural (5-HMF), as well as various other compounds, such as organic acids and melanoidins (Long et al., 2023; Yeager et al., 2021).

Most studies investigating the roasting process focus on light, medium, and dark roast profiles (Acquaticci et al., 2023; Kim et al., 2022). New roasting profiles should be explored because, depending on the temperature and contact time of coffee beans in the roasting process, the concentration of certain compounds can be affected, consequently impacting the quality of the final product. In this context, the present study aimed to obtain results to be used as references for the use of different roasting profiles, seeking information on physical-chemical characteristics, antioxidant activities, total phenolics, color indices (CIE-LAB), melanoidins, sugar and organic acid composition, as well as major compounds, chlorogenic acids (5-CGA),

5-hydroxymethylfurfural (5-HMF), caffeine, and trigonelline, and infrared analysis. The roasting process in this research was conducted at variable temperature and time ranges.

2. Materials and methods

2.1. Materials

The harvest of Coffea arabica variety Red Catuai beans was carried out in the rural area of the city of Coimbra (20°52'12"S, 42°49'22"W), located 868 meters above sea level, in the Southeast Region of Minas Gerais, Brazil. According to the Köppen-Geiger classification, the climate in the region is defined as humid subtropical with a dry winter and hot summer (Alvares et al., 2013).

In the roasting process of the beans after dry processing, a Probat drum roaster (Probat-Werke) was used. After this stage, the samples were packaged and transported to the Laboratory of Natural Dyes and Bioactive Compounds (LacBio) at the Department of Food Technology of the Federal University of Viçosa (UFV) and stored at 5°C for subsequent analyses. Different roasting profiles were created by varying the temperature and time (Table 1). The selection of temperatures was guided by specific criteria. Initially, a review of the existing scientific literature was conducted to identify gaps and inconsistencies in preexisting studies. The approach covered a spectrum ranging from lower temperatures to substantially higher ones, aiming for a comprehensive understanding of the effects on coffee. Additionally, relevant chemical transition thresholds for compounds present in coffee were considered, as well as temperatures that might have practical relevance from an industry perspective.

Table 1. Roasting profile with respective time/temperature binomial.

Roasting profile	Roasting Temperature (°C)	Start time: 1° CRACK (min)	Total roasting time (min)
T1	135	2.16	20.20
T2	210	0.13	9.02
T3	220	4.55	13.47
T4	230	6.20	17.43
T5	275	1.56	7.46
T6	210	2.38	11.01

2.2. Reagents

All the reagents met the required quality standards for analytical-grade reagents. Acetonitrile (HPLC-grade CH_3CN), Folin-Ciocalteu reagent (FCR), acetic acid, caffeic acid, citric acid, chlorogenic acid, phosphoric acid (85% H_3PO_4), gallic acid (>98%), isovaleric acid, 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (Trolox), 2,2-diphenyl-1-picrylhydrazyl (DPPH) acid, lactic acid, malic acid, oxalic acid, propionic acid, quinic acid, succinic acid, tartaric acid, trifenil tetrazolium chloride (TPTZ), caffeine, trigonelline, 5-hydroxymethylfurfural, arabinose, stachyose, fructose, glucose, xylose, and raffinose were acquired from Sigma-Aldrich (St. Louis, MO, USA). Ethyl acetate (≥99.7%), methanol (≥99.9%) were acquired from Chromasolv (Shanghai, China). Ethyl alcohol (≥99.5%), sodium carbonate, ferric chloride, and sodium were acquired from Êxodo Científica (Sumaré, SP, Brazil). Sodium hydroxide (NaOH) was from Synth (Diadema, Brazil).

2.3. Preparation of the extract

The coffee extracts were obtained through solid-liquid extraction using Milli-Q water at 100 °C. To do this, 5 g of each coffee powder sample were mixed with 20 mL of Milli-Q water, and the fluids were centrifuged at 10,000 x g for 10 min (Silva et al., 2008). The extracts were immediately cooled and filtered through a 0.2 μm cellulose acetate filter for subsequent analyses.

2.4. Titratable acidity, pH, moisture, and soluble solids

The acidity was determined by titration with 0.1 N NaOH. The pH was measured using a pH meter DM-20 (Digimed, São Paulo, Brazil). Moisture content was determined using the standard oven method at 105 °C for 24 hours. The soluble solids content was determined using a digital refractometer AR200 (Leica, São Paulo, Brazil) (AOAC, 1990).

2.5. Color attributes and melanoidins

The color of coffee in different roasting profiles was determined using a Colorquest XE Colorimeter (Hunter Lab, Reston, VA), which was previously calibrated. The direct readings of the L* (lightness), a* (redness (+) vs. green (-)) and b* (yellowness (+) vs. blue (-)) values were then taken. The hue (h*) and chroma (c*) parameters were calculated from the values of a* and b* according to equations 1 and 2, respectively.

$$h^* = \arctan\left(\frac{b^*}{a^*}\right) \qquad (1)$$

$$c^* = \sqrt{a^{*2} + b^{*2}} \qquad (2)$$

For the determination of melanoidins, 200 µL of coffee extracts were diluted in 4 mL of distilled water. Melanoidins were quantified by measuring the absorbance at 420 nm using a spectrophotometer (UV-M51, Bel Photonics, Monza, Italy) (Ludwig et al., 2013).

2.6. Total phenolic content and determination of antioxidant activity

The quantification of total phenolic compounds was performed according to the method described by Singleton & Rossi (1965). The results were expressed as gallic acid equivalents per gram of coffee. The DPPH radical scavenging activity was determined according to the method described by Kim et al. (2002). The Ferric Reducing Antioxidant Power (FRAP) assay followed the method of Boroski et al. (2015). The ABTS (2,2′-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid)) assay was conducted using the method proposed by Re et al. (1999).

2.7. Analysis of caffeine, chlorogenic acid (5-CQA), trigonelline, caffeic acid, and HMF (Hydroxymethylfurfural) composition

Caffeic acid, chlorogenic acid, caffeine, trigonelline, and hydroxymethylfurfural were determined in roasted coffee samples following the methodology adapted by Vignoli et al. (2014). The analyses were performed by high-performance liquid chromatography (HPLC) using a Thermo Scientific Accela LC system (diode array detector (DAD), autoinjector, and pump Accela) (Thermo Fisher Scientific, TX, USA). The column used for separation was the Lichrospher 100 RP-18 reverse-phase column (250 x 4.6 mm, 5 µm particle size, and 10 nm pore size) (Merck, Germany). The mobile phase consisted of water (A) and methanol (B), with elution in an isocratic mode from 0 - 6 minutes (90 % A and 10 % B), a gradient mode from 6

- 7 minutes (90 - 80 % A and 10 – 20 % B), an isocratic mode from 7 - 23 minutes (80 % A and 20 % B), a gradient from 23 - 24 minutes (80 – 0 % A and 20 – 100 % B), 24 - 25 minutes (0 – 90 % A and 100 – 10 % B), and finishing with an isocratic mode from 25 - 26 minutes (90 % A and 10 % B). The flow rate was 1 mL min-1, and the injection volume was 1 µL (partial loop), with a temperature of 25 °C for the injector and 40 °C for the column. Peaks were detected at a wavelength of 272 nm. Caffeine, chlorogenic acid (5-CQA), trigonelline, caffeic acid, and HMF were identified by injecting standards and calibration curves. The calibration curves obtained for trigonelline, HMF, chlorogenic acid, caffeic acid, and caffeine showed linearity ranges between concentrations of 2.5 mg/L^{-1} and 600 mg/L^{-1}, 1.7 mg/L^{-1} and 200 mg/L^{-1}, 2.5 mg/L^{-1} and 600 mg/L^{-1}, 1.7 mg/L^{-1} and 400 mg/L^{-1}, and 5.0 mg/L^{-1} and 1200 mg/L^{-1}, respectively. The equations of the lines obtained were as follows: trigonelline: y = 7953.6x + 23878, with R^2 = 0.9976; HMF: y = 46062x + 296356, with R^2 = 0.9972; chlorogenic acid: y = 8394.6x + 94087, with R^2 = 0.9974; caffeic acid: y = 17096x + 42049, with R^2 = 0.9997; and caffeine: y = 24942x + 431009, with R^2 = 0.9982.

2.8. Organic acids composition analysis

The analyses were performed using High-Performance Liquid Chromatography (HPLC) on a Thermo Scientific Accela LC system (Diode Array Detector (DAD), autoinjector, and pump Accela) (Thermo Fisher Scientific, TX, USA). The column used for separation was the reverse-phase Lichrospher 100 RP-18 column (250 x 4.6 mm, with a particle size of 5 µm and a pore size of 10 nm) (Merck, Germany). The mobile phase consisted of water acidified with 0.1 % phosphoric acid. The flow rate was 600 µL min^{-1}, and the injection volume was 2 µL (partial loop), with a temperature of 25 °C for the injector and 50 °C for the column. Peaks were detected at a wavelength of 210 nm. Peak identification was performed by comparing the retention time in the chromatogram and the UV spectra with those of separately injected standards. The concentration of oxalic acid, quinic acid, acetic acid, citric acid, succinic acid, and propionic acid was calculated based on the area of each peak at 210 nm using the calibration curve. The calibration curves obtained for oxalic acid, quinic acid, acetic acid, citric acid, succinic acid, and propionic acid showed a linear range between concentrations of 100 mg/L^{-1} and 8000 mg/L^{-1}. The equations for the calibration curves were as follows: oxalic acid: y = 3203.5x + 435068, with R^2 = 0.9905; quinic acid: y = 178.69x - 26232, with R^2 = 0.9923; acetic acid: y = 212.19x + 15254, with R^2 = 0.9990; citric acid: y = 438.65x + 46680, with R^2 =

0.9990; succinic acid: y = 92.684x + 11416, with R^2 = 0.9980; and propionic acid: y = 201.56x + 14884, with R^2 = 0.9988.

2.9. Sugar composition analysis

Sugars were quantified using high-performance liquid chromatography (HPLC). This process was carried out on the Shimadzu CBM-20A/20Alite chromatograph model, equipped with a refractive index detector RID-20A (Shimadzu).

Quantification of monomeric sugars was performed using the BioRad Aminex7 HPX87H column. The flow rate used was 0.6 mL/min, and the oven temperature was set at 45 °C. Elution was carried out isocratically using a 0.005 mol/L sulfuric acid solution, following the protocol established by Alyammahi et al., (2023), which is known to enable the separation and detection of sugars by refractive index.

To construct the analytical curve, standards of arabinose, stachyose, fructose, glucose, xylose, and raffinose were used at concentrations of 0.1, 0.5, 1.0, 2.0, 5.0, and 10.0 g/L. These standards served as references for the quantification of sugars present in the sample under study. The equations of the lines were obtained as follows: Arabinose: y = 111245x + 1495.2, with R2 = 0.9999; Stachyose: y = 126912x + 103425, with R2 = 0.9848; Fructose: y = 120753x + 11839, with R2 = 0.9973; Glucose: y = 138289x + 814.48, with R2 = 0.9979; Xylose: y = 112158x + 5632.1, with R2 = 0.9997; Raffinose: y = 114705x + 202955, with R2 = 0.9333.

2.10. Infrared spectroscopy

The infrared spectra (IR) were obtained using a Varian 660 FTIR spectrophotometer equipped with a Gladi ATR (Attenuated Total Reflectance) accessory (Department of Chemistry - UFV, Brazil), Paragon 1000PC model (Perkin Elmer), equipped with a diamond ATR accessory. The spectra of the samples were obtained as the average of 16 consecutive scans within the range of 4000 to 400 cm^{-1}. This range corresponds to the mid-infrared spectrum region and can be used for a functional assessment of organic compounds. The approach used for sample preparation has proven to be effective in coffee analysis (Ribeiro et al., 2009; Souza et al., 2022). The measurements were conducted in a dry environment at room temperature (20 ± 0.5 °C).

2.11. Sensory analysis with trained panelists

The sensory evaluation of coffee flavor, obtained from different roasting methods, was conducted following the SCA (Specialty Coffee Association) protocol from 2018. The study involved the participation of three trained Q-Grader panelists who specialize in coffee assessment.

Participants used a scale ranging from 6 to 10 to evaluate 10 sensory attributes: fragrance/aroma, flavor, finish, acidity, body, balance, uniformity, cup cleanliness, sweetness, and defects. This scale allowed for a detailed assessment of the sensory quality of each coffee sample. It is important to mention that, according to the SCA protocol, defects were scored negatively, indicating undesirable characteristics that reduce the final score of the coffee.

After evaluating each attribute, participants assigned an overall score to each coffee sample, representing the overall quality of the prepared coffee. The team's average score was calculated for each sample, providing a representative measure of the overall quality.

This study adhered to ethical guidelines and was approved by the Human Research Ethics Committee (CEP), under protocol number 69623523.7.0000.5153, at the Federal University of Viçosa (UFV).

2.12. Consumer sensory analysis

A panel of 110 untrained coffee evaluators was randomly recruited from regular coffee consumers, with a minimum age of 18 years, at the Federal University of Viçosa (UFV), Brazil. The panel consisted of 47 male individuals and 63 female individuals, with ages ranging from 18 to 75 years (26.25 ± 7.23 years for males and 26.10 ± 6.10 years for females). None of the participants were informed about the coffee preparation methods. The Ethics Committee for Human Research at the Federal University of Viçosa approved the study.

A 9-point hedonic scale was employed in the study to assess the attributes of acidity, aroma, color, sweetness, flavor, and overall impression. When using the hedonic scale, participants assigned a score from 1 to 9 for each attribute, indicating their level of satisfaction or pleasure (Minim, 2013).

2.13. Statistical Analysis

The data were analyzed using analysis of variance (ANOVA), and the means of three repetitions were subjected to the Tukey test at a 5% probability level. Statistical analysis was performed using the R program (R Core Team, Vienna, Austria). Principal component analysis (PCA) based on the Pearson correlation matrix was conducted to observe the differences among the various roasting profiles in Arabica coffee using R version 4.3.1 (R Core Team, Vienna, Austria).

3. Results and discussion

3.1. Acidity, pH, moisture, and soluble solids

The values of acidity, pH, moisture, and soluble solids found in the roasted and ground coffee samples from different roasting profiles are presented in Table 2. These results are important as they can provide a comparison of the current data on the physicochemical characteristics of coffee subjected to the roasting process with previously published data. Furthermore, they describe valuable compositional data that can serve as an indication of the potential final quality of coffee infusions.

There was no significant difference ($p>0.05$) in acidity and soluble solids parameters for Arabica coffee in all the roasting profiles employed. The roasting profile at 275°C/7.46 min showed the highest pH value (6.66), and the highest moisture content was observed in the roasting profile at 135°C/20.20 min (10.13%). The differences observed in the physicochemical characteristics of Arabica coffee can be attributed to the inherent properties of coffee beans (microbiota, grain maturity, climate, seasonality, and processing) (Livramento et al., 2017; Sunarharum et al., 2014).

Table 2. Physicalchemical characteristics of *arabica* coffee variety Catúai Red affected by different degrees of roasting.

Roasting profiles	*Coffea arabica*			
	Moisture (%)	pH	Acidity	Soluble solids
135 °C/20.20 min	10.13 ± 0.97^{a}	5.41 ± 0.02^{e}	11.88 ± 0^{a}	5.20 ± 0^{a}
210 °C/9.02 min	2.01 ± 0.03^{b}	5.80 ± 0.04^{d}	12.36 ± 0^{a}	5.43 ± 0^{a}
220 °C/13.47 min	1.05 ± 0.04^{bc}	6.44 ± 0.01^{b}	12.03 ± 0^{a}	5.23 ± 0^{a}
230 °C/17.43 min	0.31 ± 0.06^{c}	6.39 ± 0.07^{bc}	12.36 ± 0^{a}	5.43 ± 0^{a}
275 °C/7.46 min	0.04 ± 0.03^{c}	6.66 ± 0.05^{a}	11.83 ± 0.64^{a}	4.26 ± 0^{b}
210 °C/11.01 min	2.15 ± 0.48^{b}	6.27 ± 0.04^{c}	11.13 ± 1.53^{a}	5.23 ± 0^{a}

Means followed by the same lowercase letters in the column do not differ by Tukey's test ($p>0.05$).

3.2. Color analysis and melanoidin analysis

Color indices are considered one of the main physical properties of food and food products due to their influence on consumer acceptability. An important factor to be controlled and monitored in coffee is its coloration because this characteristic is directly related to the final quality of the product after the roasting process. Modifications in color parameters can either enhance or diminish consumer perception and determine their preference and choice of the product (Anette & Stafford 2023; Dong et al., 2017). The colorimetric coordinates and quantification of melanoidins in the Arabica coffee roasting profiles are presented in Table 3.

In all the roasting profiles employed in this study, the values of the L, a*, and b* coordinates did not show significant differences ($p>0.05$). Generally, as the roasting temperature increases, coffee becomes darker in color, and the yellowish variation decreases, and consequently, the b* parameter decreases, tending toward a bluish hue. However, the exposure time of coffee beans to heat is also a factor that can affect the color of roasted coffee beans, making the samples darker. The values of the a* parameter being higher than the b* parameter indicate that the green/yellow variation changes to blue/red due to the application of heat, thus indicating the occurrence of Maillard and caramelization reactions during this process (Dong et al., 2017; Santos et al., 2016).

The coffees roasted at 135 °C/20.20 min, 220 °C/13.47 min, and 275 °C/7.46 min showed higher hue (h) values (Tab. 3). For the c parameter (chroma), no significant differences ($p>0.05$) were observed among the roasting profiles employed. Color is considered an intrinsic factor of products of great importance, and several studies have reported that changes in color saturation can impact consumer choices and preferences (Carvalho & Spence 2019; Sousa et al., 2020).

Table 3. Average attributes color and melanoidins of *arabica* coffee variety Catúai Red affected by different degrees of roasting.

Roasting profiles	*Coffee arabica*					
	L	a*	b*	h (hue)	C (chroma)	Abs_{420}
135 °C/20.20 min	30.26 ± 0.98^{a}	19.77 ± 1.69^{a}	11.52 ± 1.95^{a}	59.90 ± 2.03^{a}	22.90 ± 2.42^{a}	0.396 ± 0.00^{d}
210 °C/9.02 min	34.21 ± 2.98^{a}	19.87 ± 3.97^{a}	17.55 ± 5.15^{a}	48.98 ± 4.83^{bc}	26.57 ± 6.16^{a}	0.426 ± 0.00^{bc}
220 °C/13.47 min	31.53 ± 1.69^{a}	20.37 ± 1.06^{a}	12.71 ± 1.93^{a}	58.16 ± 2.57^{a}	24.03 ± 1.92^{a}	0.461 ± 0.00^{a}
230 °C/17.43 min	34.38 ± 1.95^{a}	20.06 ± 3.31^{a}	17.27 ± 2.69^{a}	49.22 ± 4.15^{bc}	26.51 ± 3.84^{a}	0.425 ± 0.00^{c}
275 °C/7.46 min	31.74 ± 0.89^{a}	21.83 ± 0.58^{a}	13.76 ± 1.06^{a}	57.78 ± 2.18^{ab}	25.82 ± 0.70^{a}	0.417 ± 0.00^{cd}
210 °C/11.01 min	34.19 ± 2.37^{a}	20.23 ± 3.27^{a}	17.78 ± 4.17^{a}	48.92 ± 2.44^{c}	26.95 ± 5.17^{a}	0.450 ± 0.00^{ab}

Means followed by the same lowercase letters in the column do not differ by Tukey's test ($p>0.05$).

The roasting process of coffee beans triggers the formation of the characteristic aroma of coffee and brown-colored compounds (Bekedam et al., 2008). In the present study, regarding melanoidins, Arabica coffee showed significant differences ($p < 0.05$) among the roasting profiles. The highest absorbance of melanoidins (brown compounds) was found in the roasting profiles at 220 °C/13.47 min and 210 °C/11.01 min, and the lowest absorption was observed in the roasting profiles at 135 °C/20.20 min and 275 °C/7.46 min (Tab. 3). Probably in the roasting profile at 135 °C/20.20 min, the Maillard reaction was not as intense, resulting in lower levels of melanoidins, and at 275 °C/7.46 min, due to the high temperature, the compounds were degraded, a process that may have occurred in melanoidins. Specifically, melanoidins are interesting not only for their contribution to the color of coffee but also for enhancing taste properties, presenting antioxidant activity, metal-chelating properties, as well as their reactivity in coffee infusion (aiding in the aging process of the beverage) (Bekedam et al., 2008).

3.3. Antioxidant activity and total phenolics

The roasting profiles of Arabica coffee at 135 °C/20.20 min and 210 °C/9.02 min showed higher antioxidant activity ($p<0.05$) than the other roasting profiles in the ABTS method. The antioxidant activity of Arabica coffee significantly decreased with increasing roasting temperature. The decreasing trend was observed starting from the roasting at 210 °C/11.01 min, as antioxidant activity values gradually decreased after this roasting, demonstrating that roasting time also interferes with the antioxidant activity of Arabica coffee (Tab. 4).

The antioxidant activity values by the DPPH and FRAP methods showed the same decreasing trend in antioxidant activity with increasing roasting temperature (Tab. 4). Some studies have found that antioxidant activity increases up to a certain roasting time and then decreases (Freitas et al., 2023; Sacchetti et al., 2009; Vignoli et al., 2014). One of the main causes of variations in antioxidant activity in the different roasting profiles used in coffee processing is related to reactions occurring during this process, such as the Maillard reaction and the degradation of chlorogenic acids. During the roasting process, non-covalent interactions occur between phenolics and melanoidins (products of the Maillard reaction and caramelization). The antioxidant activity of melanoidins is likely due to the incorporation of chlorogenic acids into their structure during the roasting process (Kwon et al., 2022).

Table 4. Antioxidant activities by ABTS, DPPH, FRAP and total phenolic methods of roasted *Coffea arabica* variety Catuái Vermelho according to the roasting profile used.

Roasting Profiles	**Antioxidant activity and total phenolics**			
	ABTS (µmol ET/g)	DPPH (µmol ET/g)	FRAP (µmol ESF/g)	Total phenolics (mg AGE/g)
135 °C/20.20 min	394.24 ± 34.62^{a}	592.30 ± 7.34^{a}	57.61 ± 2.18^{a}	13.97 ± 1.63^{a}
210 °C/9.02 min	361.64 ± 10.43^{a}	592.24 ± 4.37^{a}	50.76 ± 3.39^{a}	12.94 ± 1.36^{ab}
220 °C/13.47 min	290.15 ± 14.50^{b}	471.39 ± 14.60^{b}	33.26 ± 2.29^{b}	12.79 ± 1.54^{ab}
230 °C/17.43 min	215.74 ± 25.03^{c}	407.60 ± 12.39^{d}	30.73 ± 5.79^{bc}	10.0 ± 1.02^{bc}
275 °C/7.46 min	202.63 ± 14.10^{c}	285.31 ± 3.06^{e}	24.08 ± 2.06^{c}	9.17 ± 0.41^{c}
210 °C/11.01 min	279.61 ± 11.66^{b}	433.32 ± 4.16^{c}	33.25 ± 1.83^{b}	12.63 ± 1.38^{abc}

Means followed by the same lowercase letters in the column do not differ by Tukey's test ($p>0.05$).

Phenolic compounds are important secondary metabolites found in plants and are abundant in roasted coffee, considered healthy for human consumption. These compounds have significant antioxidant potential (Agunbiade et al., 2022; Liao et al., 2022). The total phenolic content is presented in Table 4.

In general, roasting profiles with lower temperatures had higher total phenolic content (TPC), and an increase in temperature gradually decreased their content, indicating a decrease of 65.64 % (Tab. 4). This decrease in total phenolic concentration may result from the degradation of some compounds that, when exposed to very high temperatures, such as chlorogenic acid, are degraded into other compounds, giving rise to new acids and phenolics, such as quinic acid (Mehaya & Mohammad, 2020).

3.4. Caffeine, chlorogenic acid (5-CQA), trigonelline, caffeic acid, and HMF (Hydroxymethylfurfural)

The effect of roasting on the concentrations of caffeine, chlorogenic acid (5-CQA), trigonelline, caffeic acid, and HMF was investigated in Arabica coffee. Caffeic acid and HMF were not detected in the samples from the different roasting profiles analyzed (Fig. 1).

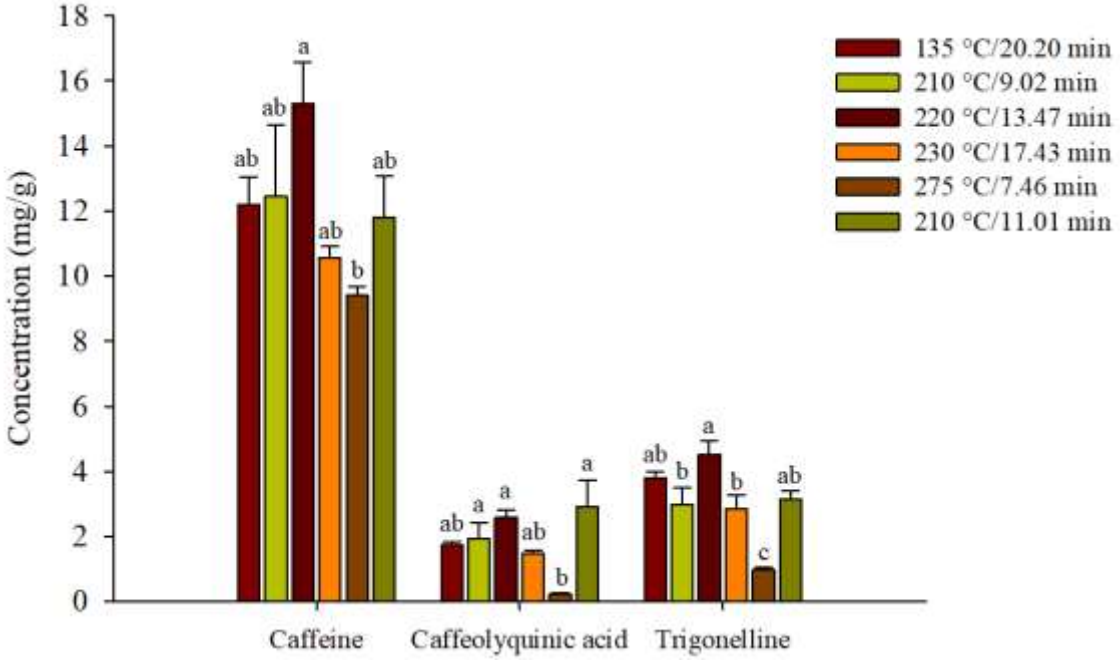


Figure 1. Caffeine, caffeoylquinic acid (5-CQA), trigonelline, caffeic acid and hydroxymethylfurfural (HMF) (mg/g) content in arabica coffee variety Red Catúai affected by different degrees of roasting.

In the six roasting profiles, caffeine was detected in concentrations ranging from 9.40 mg/g to 15.3 mg/g (Fig. 1). Caffeine is a methylxanthine, being one of the most abundant compounds in coffee, known for its high thermal stability and possessing antioxidant and anti-inflammatory properties (Rodrigues et al., 2023).

In addition to caffeine, coffee is rich in trigonelline, which is a bioactive alkaloid with significant biological activity. This compound is the second most abundant alkaloid in coffee berries, derived from enzymatic methylation of nicotinic acid, and trigonelline concentrations were detected in the range of 0.98 mg/g to 4.51 mg/g. The highest concentration of trigonelline was found in roasting profiles at 135 °C/20.20 min, 210 °C/11.01 min, and 220 °C/13.47 min. The lowest concentration of trigonelline (0.98 mg/g) was observed with the high temperature profile at 275 °C/7.46 min, indicating a decrease when high temperatures are used in the coffee roasting process (Fig. 1). Trigonelline has potential anticancer activity, neuroprotective effects, and can lower blood sugar, cholesterol, and lipid levels (Hu et al., 2019; Jeszka-skowron et al., 2020; Wu et al., 2022).

Chlorogenic acids are an important class of phenolics in coffee and are water-soluble esters between quinic acid and hydroxycinnamic acids, showing temperature sensitivity, indicating their susceptibility to deterioration (Vilas-boas et al. 2020). 5-CQA was detected in the present study at concentrations ranging from 0.22 mg/g to 2.57 mg/g in the analyzed roasting profiles (Fig. 1). It has been reported that the roasting process reduces the concentrations of 5-CQA in coffee (Bastian et al., 2021), and the intake of this acid by active coffee consumers varies between 0.5 g and 1.0 g per day (Olthof et al., 2001). High concentrations of chlorogenic acids have the ability to reduce the sensory quality of the beverage, especially in terms of taste attribute, due to relatively high concentrations of oxidized products generated before roasting (Farah, 2012; Zanir et al., 2016). It is evident that geographical location, cultivation conditions and practices, as well as processing through roasting, can be linked to the losses of 5-CQA in the chemical composition of coffee (Illy & Viani, 2005; Perrone et al., 2010; Zanir et al., 2016).

The importance of these phenolics in coffee lies in the formation of the characteristic and unique flavor and bitterness of coffee, as well as their potential benefits to human health due to their antioxidant activity, anti-inflammatory characteristics, and antimicrobial properties (Farah & dePaula Lima, 2019). As observed, coffee beans contain various bioactive components, especially caffeine, which is considered a natural stimulant, phytoestrogen trigonelline, and chlorogenic acids (5-CQAs) with antioxidant properties.

3.5. Composition of organic acids and sugars

The compositions of organic acids (acetic, citric, isovaleric, lactic, malic, oxalic, propionic, quinic, succinic, and tartaric) were verified using HPLC. Lactic, malic, tartaric, and isovaleric acids were not detected (Tab. 5).

The levels of acetic, citric, propionic, quinic, and succinic acids did not show significant differences ($p>0.05$) among the analyzed roasting profiles. Propionic and succinic acids had the highest fractions of organic acids in mg/g. Oxalic acid showed significant differences among the analyzed roasting profiles ($p<0.05$).

Acidity is considered a sensorially important attribute in coffee, as a correlation has been demonstrated between roasting profiles and the perceived acidity in coffee (Yeager et al., 2021). This attribute is closely related to the composition and levels of organic acids present in roasted coffee (Rune et al., 2023; Wang et al., 2023). Acids are considered natural contributors to the final quality of coffee and are responsible for the authentic experience of the beverage. They are valued by coffee enthusiasts who savor this acidity and seek roasting adjustments to achieve the highest sensitivity to this attribute. Acidity is a pleasant sensation that enhances the sweetness of coffee (Rune et al., 2023; Thomas et al., 2017).

Quantitative analyses of carbohydrates were conducted for glucose, fructose, xylose, stachyose, arabinose, and raffinose in coffee samples subjected to different roasting profiles (Tab. 6). It was noted that raffinose was not detected in any of the investigated roasting profiles. In terms of sugar concentrations, stachyose exhibited the highest amounts, ranging from 4.88 to 6.42 mg/mL, showing no significant differences ($p>0.05$) between the different roasting profiles tested in this study. Fructose followed, with concentrations ranging from 4.20 to 4.94 mg/mL. The highest concentration of fructose was observed in the roasting profile at 210 °C/11.01 min, while the lowest concentration occurred in the roasting profile at 275 °C/7.46 min ($p<0.05$).

Table 5. Organic acid content of *arabica* coffee variety Catúai Red affected by different degrees of roasting.

Roasting profiles	**Organic acid content**					
	Acetic acid	Citric acid	Oxalic acid	Propionic acid	Quinic acid	Succinic Acid
135 °C/20.20 min	3.47 ± 1.75^{a}	7.48 ± 1.14^{a}	2.60 ± 0.43^{bc}	50.60 ± 11.04^{a}	27.70 ± 5.02^{a}	48.33 ± 10.33^{a}
210 °C/9.02 min	6.30 ± 0.23^{a}	5.74 ± 0.03^{a}	2.37 ± 0.01^{bc}	41.22 ± 0.66^{a}	12.36 ± 0.52^{a}	39.82 ± 4.03^{a}
220 °C/13.47 min	9.48 ± 1.47^{a}	7.97 ± 1.05^{a}	3.53 ± 0.32^{ab}	33.02 ± 4.39^{a}	17.64 ± 5.11^{a}	44.25 ± 5.07^{a}
230 °C/17.43 min	8.43 ± 2.12^{a}	7.23 ± 0.23^{a}	3.14 ± 0.14^{b}	25.55 ± 2.88^{a}	14.17 ± 2.07^{a}	51.57 ± 0.77^{a}
275 °C/7.46 min	5.83 ± 1.46^{a}	5.65 ± 1.22^{a}	1.66 ± 0,29^{c}	20.57 ± 4.85^{a}	9.19 ± 2.09^{a}	30.84 ± 6.50^{a}
210 °C/11.01 min	8.41 ± 0.53^{a}	6.27± 0.60^{a}	4.85 ± 0.02^{a}	40.58 ± 0.95^{a}	12.06 ± 0.54^{a}	37.59 ± 0.91^{a}

Means followed by the same lowercase letters in the column do not differ by Tukey's test ($p>0.05$).

The concentrations of glucose, xylose, and arabinose, on the other hand, did not show significant differences between the different roasting profiles, with values ranging from 0.29 to 0.37 mg/mL, 0.79 to 1.01 mg/mL, and 1.73 to 2.06 mg/mL, respectively. These concentrations did not exhibit notable disparities among the various roasting profiles analyzed. During the roasting process, there is a reduction in the concentrations of raffinose and stachyose, attributed to the occurrence of thermal hydrolysis of these oligosaccharides. Simultaneously, the concentrations of glucose and fructose increase, resulting from both the hydrolysis of sucrose into various products and thermal degradation through the caramelization process (Chindapam et al., 2019; Ginz et al., 2000; Poisson et al., 2017). The presence of sugars in coffee beans is crucial for the quality of the final beverage as they influence the taste, aroma, acidity, sweetness, body, and texture of the product.

3.6. Infrared

The infrared spectra of the six coffee samples obtained from different roasting conditions are presented in Fig. 2. When observing the spectra, it is noted that the most important absorption bands of the samples, those that provide the most information about the samples, are in the regions from 3306 to 2097 cm^{-1} and from 1745 to 1024 cm^{-1} (part of the fingerprint region). It is worth noting that these important bands are present in all samples.

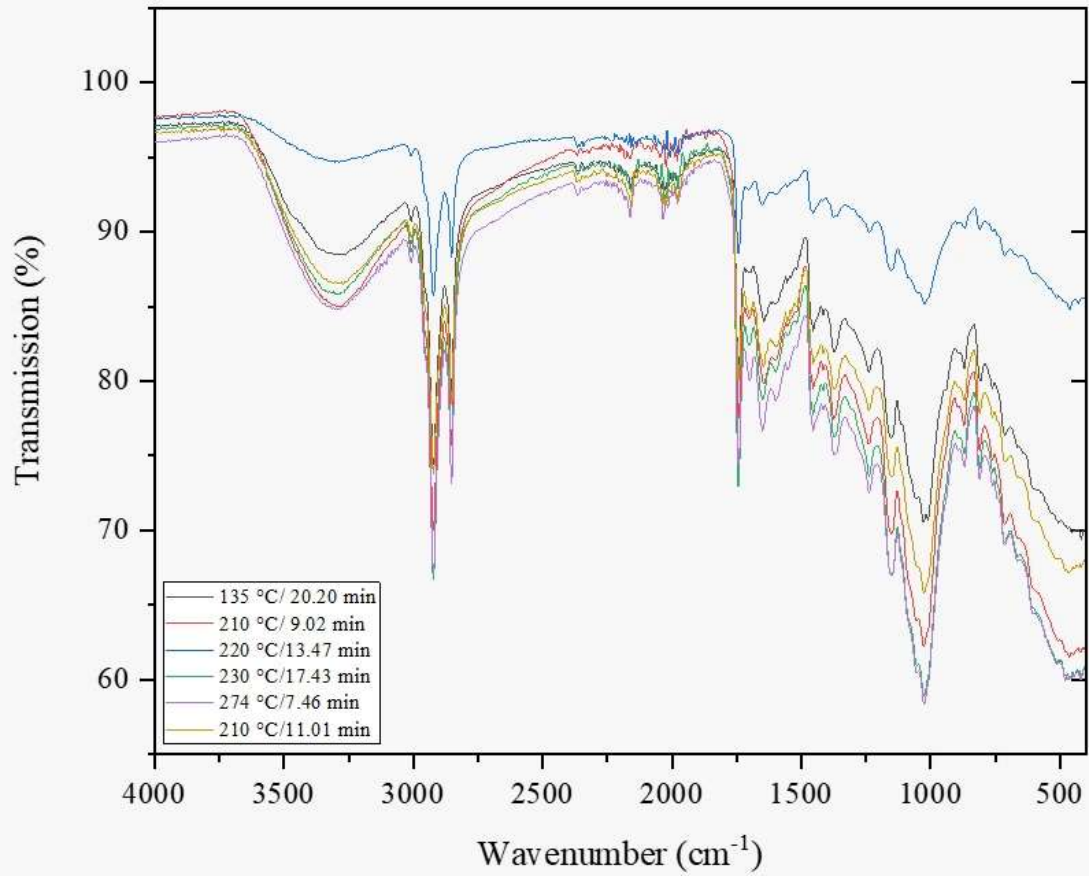


Figure 2. Infrared Spectroscopy in arabica coffee variety Red Catúai affected by different degrees of roasting.

At 3306 cm^{-1}, a broad band is observed, which corresponds to the stretching of the O-H bond, present in numerous coffee substances such as phenols, chlorogenic acids, and carbohydrates. At 2922 and 2847 cm^{-1}, two intense bands are observed, corresponding to the asymmetric and symmetric stretching of C-H bonds of sp^3 carbon. These stretches can come from lipid molecules present in roasted coffee, as well as some other saturated compounds. In addition to these, there is also a high-intensity band at 1745 cm^{-1}, which is characteristic of the stretching of the C=O bond in lipids and aliphatic esters (such as chlorogenic acid). The stretching band of the C=O bond in amides, such as caffeine, is observed at 1701 cm^{-1}. Another band related to the caffeine molecule is at 1648 cm^{-1}, which is specific to the tertiary amide stretching. Bands at 1596 and 1455 cm^{-1} are present in the spectrum and can be related to the stretching of the C=N and CO_2 bonds, respectively, in trigonelline. Finally, at 1154, 1057, and 1024 cm^{-1}, there are bands inherent to the stretching of ether groups present in carbohydrates and the O-C-O glycosidic bonds of saccharides like cellulose and sucrose (Barbosa, 2013; Barrios-Rodríguez et al., 2021; Paiva et al., 2016).

3.7. Sensory analysis with Q-graders panel

According to the methodological protocol of the Special Coffee Association (SCA-2018), we observed that the scores assigned to different roast profiles had similar final scores and did not show significant differences ($p>0.05$) in the final score (Fig. 3). All analyzed coffees received a final score ranging from 6.58 to 7.17 points (Fig. 3). In another study, it was observed that the variation in temperature/time gradient was not significant in distinguishing the roast profiles used in their sensory analysis (Anastácio et al., 2023). However, the results revealed that the roast profile at 135 °C/20.20 min showed significantly higher scores ($p<0.05$) in the final score, indicating that the use of lower temperatures with longer heat contact time favored the overall perception of the beverage. Furthermore, the "balance" attribute also showed significant differences ($p<0.05$) among the analyzed roast profiles, receiving lower scores for roasts conducted at 210 °C/9.02 min, 230 °C/17.43 min, and 270 °C/7.46 min. The body and flavor of the beverage also received lower scores for the roast profiles at 230 °C/17.43 min and 270 °C/7.46 min. The acidity of the product showed significant differences among the different roast profiles, with the temperature of 275 °C/7.46 min resulting in the lowest acidity (Fig. 3). This can be attributed to the use of high temperatures, which ended up impacting the degradation of various chemical compounds present in the coffee.

The obtained results can be attributed to the use of prolonged roast times and moderate temperatures, which may result in less physical wear and subtler chemical changes in the coffee beans. The lack of proper adjustment of time and temperature conditions during the coffee roasting process can lead to the formation of compounds that negatively affect the sensory characteristics of the final coffee beverage (Yang et al., 2016). It is worth noting that carefully considering roasting parameters is essential to achieve the desired sensory attributes in the final product, such as aroma, body, and flavor of the coffee beverage.

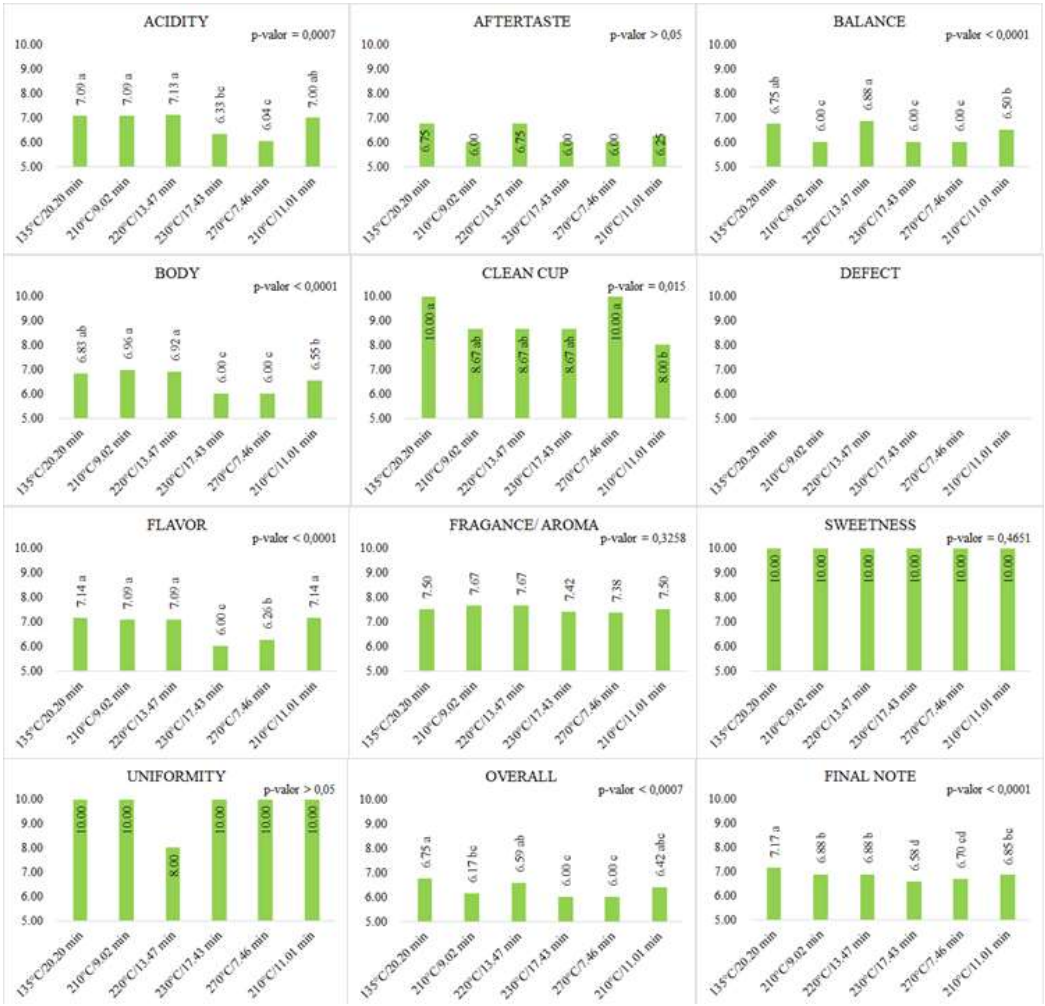


Figure 3. Average values of the attributes and overall qualification by the sensory analysis according to the protocol of the Specialty Coffee Association (SCA) of coffee obtained by different roasting profiles.

3.8. Consumer sensory analysis

The sensory attributes of the coffees were analyzed, and the consistency of the sensory analysis method through the affective acceptance test was related to the scores assigned to the different roast profiles used in this study. The mean values (and standard deviations) for each sensory attribute analyzed, according to the 110 coffee tasters (consumers who claimed to appreciate the beverage), and the overall impression are presented in Table 7.

The acidity attribute was perceived with lower sensitivity by the tasters in the roast profiles at 230 °C/17.43 min and 275 °C/7.46 min, showing statistically significant differences ($p<0.05$) compared to the other roast profiles. Intrinsic observations revealed a correlation between the scores assigned to this attribute and the acidity measured by titration (Table 2), indicating that there were no statistically significant differences ($p<0.05$) in roasts at 135 °C/20.20 min, 210 °C/9.02 min, 220 °C/13.47 min, and 210 °C/11.01 min. Acidity, along with aroma and bitterness, is widely recognized as a crucial factor for the sensory quality of coffee in the final cup (Rune et al., 2023; Thomas et al., 2017). Especially in the *C. arabica* species subjected to lighter and medium roasts, acidity plays a central role in the flavor of the beverage. On the other hand, when coffees are roasted at higher temperatures, acidity is typically reduced, allowing bitterness to become the dominant flavor (Chindapan et al., 2019). It is worth noting that in observations, some tasters referred to acidity as "fruity."

Statistically significant differences ($p<0.05$) were observed in flavor scores for the different roast profiles. The most appreciated roast profiles were as follows: 135 °C/20.20 min, 210 °C/9.02 min, and 210 °C/11.01 min. On the hedonic scale, these roasts received average ratings ranging from "liked slightly" to "liked moderately." Considering the common practice of consuming coffee with added sugar in Brazil, these roasts received favorable ratings in terms of flavor. It is important to highlight that the characteristic flavor of coffee is influenced by the presence and concentrations of various chemical compounds, such as phenolic compounds, organic acids, sugars, and proteins (Febrianto & Zhu, 2023; Pimenta et al., 2021; Wang et al., 2023). In this study, the roast at 135 °C/20.20 min exhibited a high concentration of total phenolic compounds, while organic acids were predominant in this same roast. Some tasters noted the presence of citrus fruit flavors in this specific roast profile.

Table 7. Sensory attributes by *arabica* coffee variety Catúai Red affected by different degrees of roasting by acceptance test.

Roasting profiles	*Coffea arabica*					
	Sensory Attributes					
	Acidity	Aroma	Color	Sweetness	Flavor	Overall impression
135 °C/20.20 min	7.2 ± 1.1^{a}	7.1 ± 0.8^{b}	6.1 ± 0.8^{b}	3.1 ± 0.2^{ab}	6.9 ± 1.3^{a}	6.7 ± 1.3^{a}
210 °C/9.02 min	7.1 ± 2.1^{a}	8.4 ± 1.2^{a}	7.8 ± 1.2^{a}	2.9 ± 0.2^{ab}	6.7 ± 0.6^{a}	6.3 ± 2.0^{b}
220 °C/13.47 min	6.9 ± 0.9^{a}	8.1 ± 1.3^{a}	6.7 ± 0.3^{b}	2.7 ± 0.4^{ab}	6.1 ± 2.2^{b}	5.8 ± 1.1^{c}
230 °C/17.43 min	6.0 ± 0.9^{a}	7.2 ± 2.1^{b}	5.8 ± 2.0^{b}	2.4 ± 1.0^{b}	6.2 ± 1.4^{b}	5.6 ± 0.8^{c}
275 °C/7.46 min	5.9 ± 1.5^{b}	6.2 ± 1.7^{c}	5.6 ± 1.8^{bc}	2.3 ± 0.6^{b}	6.0 ± 0.9^{b}	5.5 ± 0.7^{c}
210 °C/11.01 min	6.9 ± 2.2^{b}	8.1 ± 0.7^{a}	7.7 ± 0.8^{a}	3.0 ± 1.0^{ab}	6.7 ± 1.3^{a}	6.8 ± 0.4^{a}

Means followed by the same lowercase letters in the column do not differ by Tukey's test ($p>0.05$).

The scores assigned to the sweetness attribute varied negatively, ranging from "disliked extremely" to "disliked slightly." These evaluations can be justified by the prevalent habit of consuming coffee with added sugar in the coffee context (Eulalia et al., 2022). Therefore, in this study, regardless of the roast profile used, the analyzed coffees did not provide a pleasant sensory experience to the tasters' palates. Sweetness is a crucial sensory attribute for coffee flavor appreciation and can be influenced by various factors, including the chemical compounds present in the beverage, and it is important to note that sweetness perception is mediated by the interaction between compounds such as carbohydrates, organic acids, and phenolic compounds (Chindapan et al., 2019; Lopes et al., 2021; Yeager et al., 2021). However, the results obtained in this study indicate that even with variations in roast profiles, the coffee samples evaluated failed to provide a positive sensory experience regarding sweetness. These findings reinforce the importance of considering local consumption habits when assessing coffee sensory quality. The habit of adding sugar to coffee can affect taste perceptions and influence individual consumer preferences (Eulalia et al., 2022). Therefore, when developing new products or adjusting roasting processes, it is essential to take into account the preferences of the target audience and seek to enhance the sensory experience, including sweetness, to meet consumer expectations and demands.

In this study, the roast at 275 °C/7.46 min resulted in a lower appreciation of aroma by the tasters, suggesting that the temperature used in this roast profile may have been excessively severe. This more rigorous roasting condition may have led to more pronounced degradation reactions, resulting in the loss or alteration of important aromatic compounds. These findings highlight the importance of precise control of roasting parameters to preserve desirable sensory characteristics of coffee. Proper selection of the roast profile, including temperature and exposure time, can directly influence the formation and preservation of aromatic compounds (Caporaso et al., 2018; Kim et al., 2022; Pimenta et al., 2021). Understanding the relationships between roasting parameters and the sensory properties of coffee is essential for improving the quality of the final product and meeting consumer preferences (Bemfeito et al., 2021).

The color attribute showed significant differences ($p<0.05$) among the roast profiles. The roast profiles at 210 °C/9.02 min and 210 °C/11.01 min received the highest scores. This suggests that roasting parameters, such as temperature and time, influence the coloration of the beverage. Color is an important sensory attribute and can affect the perception of coffee quality by consumers (Anette & Stafford 2023; Bemfeito et al., 2021; Carvalho & Spence 2019; Dong et al., 2017; Sousa et al., 2020). Therefore, it is essential to optimize roasting parameters to

achieve an attractive and pleasant color to satisfy consumers' visual expectations and provide a positive sensory experience.

The overall impression of the coffee showed significant differences ($p<0.05$) among the roast profiles. The lowest scores were attributed to coffees roasted at 220 °C/13.47 min, 230 °C/17.43 min, and 275 °C/7.46 min. These results suggest that exposing the beans to higher temperatures may lead to the degradation of important compounds in the final beverage quality, negatively affecting the overall impression of the coffee.

Overall, untrained consumers had a similar taste perception to certified tasters (Q-graders). Their evaluations are not significantly inferior to those of experts. These results emphasize the importance of considering consumers' perceptions in the development and evaluation of coffee beverages, respecting their preferences. Therefore, it is crucial to improve sensory evaluation methods to encompass the diversity of coffee sensory perspectives.

3.9. Principal component analysis

Principal Component Analysis (PCA) is a widely used statistical technique for reducing the dimensionality of complex datasets. Through this approach, it is possible to transform a large number of correlated variables into a smaller set of uncorrelated principal components. In the specific context of a dataset containing information about roasting profiles, PCA was employed to investigate the relationship between these variables and the formation of sample groups (Fig. 4).

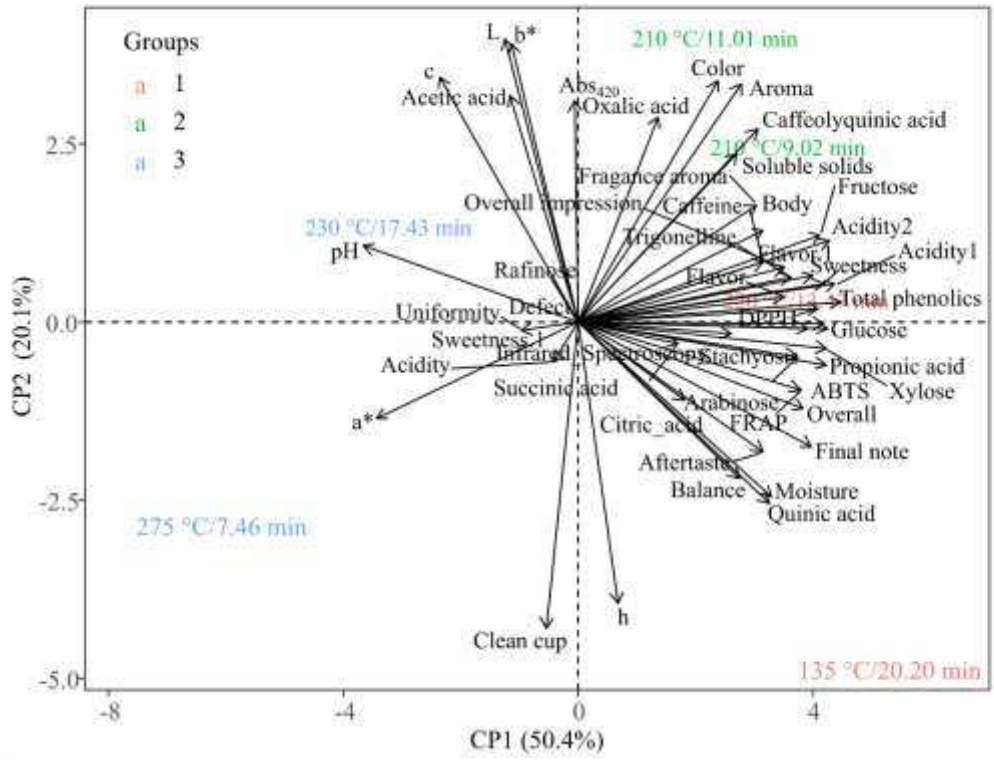


Figure 4. Data from the principal component analysis of chemical compounds and sensory attributes of Arabica coffee variety Red Catúai subjected to different roasting profiles.

The similarity and divergence between samples of roasting profiles can be represented through a Principal Component Analysis (PCA) with two principal components (PCs), displaying the distribution of samples on a new coordinate graph according to their scores. Additionally, the loading plot shows the relationship between variables and a specific principal component. According to the PCA data, as demonstrated in Fig. 4, the explained variance was 70.5 %. The first principal component (PC1) contributed 50.4 % to the total variance of the data, while the second principal component (PC2) explained 20.1 % of the variance (Fig. 4). The PCA analysis indicated a clear segregation of roasting profiles, corresponding to temperatures from milder to more intense, which is in agreement with the results reported by Alcantara et al. (2021). In an exploratory study, Alcantara and colleagues identified a clear distinction between traditional and specialty coffees using PCA analysis. From the spatial representation of the samples, four distinct groups were identified and separated into the following quadrants: 210 °C/9.02 min, 210 °C/11.01 min, and 220 °C/13.47 min (positive PC1, positive PC2); 230 °C/17.43 min (negative PC1, positive PC2); 275 °C/7.46 min (negative PC1, negative PC2); 135 °C/20.20 min (positive PC1, negative PC2) (Fig. 4).

In conclusion, Principal Component Analysis (PCA) revealed a relationship of similarity among different coffee samples, distinguishing roasting profiles based on the use of

temperatures ranging from low to high, arranged in four quadrants that correlate with the compounds of each principal component (PC). Thus, it became evident that the relationship between the chemical and sensory components of coffee, as well as its quality, could be easily observed through the application of PCA.

Conclusion

The results of this study have demonstrated that different roasting profiles significantly impact the physicochemical, sensory, and antioxidant characteristics of Arabica coffee. Variations in roasting temperatures and times influenced the composition of organic acids, total phenolics, caffeine, sugars, melanoidins, and aromatic compounds, as well as the acidity, color, and antioxidant activity of the beverage.

These findings underscore the importance of precise control over roasting parameters to achieve desirable sensory characteristics in coffee, such as aroma, flavor, acidity, and color. Furthermore, the results highlight the need to consider consumer preferences when developing new products or adjusting roasting processes in order to meet their expectations and demands.

In this way, the study contributes to the understanding of the relationships between roasting parameters and the chemical and sensory properties of Arabica coffee, providing valuable information for the coffee industry in its pursuit of high-quality products that align with consumer preferences. Future research can further explore the effects of different roasting temperatures and times on other coffee varieties and under different cultivation conditions, aiming to further enhance the quality and diversity of flavors in coffee offered to enthusiasts of this globally consumed beverage.

References

Acquaticci, L., Angeloni, S., Cela, N., Galgano, F., Vittori, S., Caprioli, G., Condelli, N. (2023). Impact of coffee species, post-harvesting treatments and roasting conditions on coffee quality and safety related compounds. *Food Control*, *149*, 109714. https://doi.org/10.1016/j.foodcont.2023.109714

Agunbiade, H. O., Fagbemi, T. N., Aderinola, T. A. (2022). Antioxidant properties of beverages from graded mixture of green/roasted coffee and hibiscus sabdariffa calyx flours. *Applied Food Research*, *2*(2), 100163. https://doi.org/10.1016/j.afres.2022.100163

Alcantara, G. M. R. N., Dresch, D., Melchert, W. R. (2021). Use of non-volatile compounds for the classification of specialty and traditional Brazilian coffees using principal component analysis. *Food Chemistry*, *360*, article 130088. https://doi.org/10.1016/j.foodchem.2021.130088

Alvares, C. A., Stape, J. L., Setelhas, P. C., Gonçalves, J. L. M., Sparovek, G. (2013). Köppen's climate classification map for Brazil. *Meteorologische Zeitschrift*, *22*(6), 711-728. https://doi.org/10.1127/0941-2948/2013/0507

Alyammahi, J., Darwish, A. S., Lemaoui, T., Alnashef, I. M., Hasan, S. W., Taher, H., Banat, F. (2023). Parametric analysis and machine learning for enhanced recovery of high-value sugar from date fruits using supercritical CO2 with co-solvents. *Journal of CO2 Utilization, 72*, article 102511. https://doi.org/10.1016/j.jcou.2023.102511

Anastácio, L. M., DaSilva, M. A. D. C. S., Debona, D. G., Veloso, T. G. R., Estringer, T. L., Bullergahn, V. B., DaLuz, J. M. R., Moreli, A. P., Megumi, M. C., Pereira, L. L. (2023). Relationship between physical changes in the coffee bean due to roasting profiles and the sensory attributes of the coffee beverage. *European Food Research and Technology*, *249*(2), 327-339. https://doi.org/10.1007/s00217-022-04118-4

Annette, M., & Stafford, L. D. (2023). How colour influences taste perception in adult picky eaters. *Food Quality and Preference*, *105*, article 104763. https://doi.org/10.1016/j.foodqual.2022.104763

AOAC - ASSOCIATION OF OFFICIAL ANALYTICAL CHEMISTS. (1990). Official methods of analyses of the Association of Official Analytical Chemists. 15. ed. Washington, 1117.

Barbosa, L. C. de A. (2013). Luiz Cláudio de Almeida Barbosa. Espectroscopia no infravermelho na caracterização de compostos orgânicos. Editora UFV, 1ª edição.

Bastian, F., Hutabarat, O. S., Dirpan, A., Nainu, F., Harapan, H., Emran, T. Bin, Simal-gandara, J. (2021). From Plantation to Cup: Changes in Bioactive Compounds during Coffee Processing. *Foods*, *10*, 1-27. https://doi.org/10.3390/foods10112827

Barrios-Rodríguez, Y. F., Reyes, C. A. J., Campos, J. S. T., Giron-Hernandez, J., Rodríguez-Gamir, J. (2021). Infrared spectroscopy coupled with chemometrics in coffee post-harvest processes as complement to the sensory analysis. *LWT - Food Science and Technology, 145*, 111304. https://doi.org/10.1016/j.lwt.2021.111304

Bekedam, E. K., Loots, M. J., Schols, H. A., Van Boekel, M. A. J. S., Smit, J. (2008). Roasting Effects on Formation Mechanisms of Coffee Brew Melanoidins. *Journal of Agricultural and Food Chemistry, 56*(16), 7138-7145. https://doi.org/10.1021/jf800999a

Bemfeito, C. M., Guimarães, A. S., Oliveira, A. L. De, Andrade, B. F., Paula, M. L. A. F., Pimenta, C. J. (2021). Do consumers perceive sensory differences by knowing information about coffee quality?. *LWT- Food Science and Technology*, *138*, article 110778. https://doi.org/10.1016/j.lwt.2020.110778

Boroski, M., Visentainer, J., Cottica, S., Morais, D. (2015). *Antioxidantes: Princípios e Métodos Analíticos* (1st ed.). Appris.

Caporaso, N., Whitworth, M. B., Cui, C., Fisk, I. D. (2018). Variability of single bean coffee volatile compounds of Arabica and robusta roasted coffees analysed by SPME-GC-MS. *Food Research International*, *108*, 628-640. https://doi.org/10.1016/j.foodres.2018.03.077

Carvalho, F. M., & Spence, C. (2019). Cup colour influences consumers' expectations and experience on tasting specialty coffee. *Food Quality and Preference*, *75*, 157-169. https://doi.org/10.1016/j.foodqual.2019.03.001

Chindapan, N., Soydok, S., Devahastin, S. (2019). Roasting Kinetics and Chemical Composition Changes of Robusta Coffee Beans During Hot Air and Superheated Steam Roasting. *Journal of Food Science*, *84*(2), 292–302. https://doi.org/10.1111/1750-3841.14422

Dong, W., Hu, R., Chu, Z., Zhao, J., Tan, L. (2017). Effect of different drying techniques on bioactive components, fatty acid composition, and volatile profile of robusta coffee beans. *Food Chemistry*, *234*, 121-130. https://doi.org/10.1016/j.foodchem.2017.04.156

Eulalia, C., Luciano, N., Gasparini, P., & Robino, A. (2022). Are taste variations associated with the liking of sweetened and unsweetened coffee? *Physiology & Behavior*, *244*, artcle 113655. https://doi.org/10.1016/j.physbeh.2021.113655

Farah, A. (2012). Coffee constituents. Y. F. Chu (Ed.), Coffee: Emerging health effects and disease prevention, *59*, 22-57. https://doi.org/10.1002/9781119949893.ch2

Farah, A., Lima, J. D. P. (2019). Consumption of Chlorogenic Acids through Coffee and Health Implications. *Beverages*, *5*(1), 1-29. https://doi.org/10.3390/beverages5010011

Febrianto, N. A., & Zhu, F. (2023). Coffee bean processing : Emerging methods and their effects on chemical, biological and sensory properties. *Food Chemistry*, *412*, article 135489. https://doi.org/10.1016/j.foodchem.2023.135489

Freitas, V. V., Rodrigues, L. L. B., Castro, G. A. D., dos Santos, M. H., Vidigal, M. C. T. R., Fernandes, S. A., Stringheta, P. C. (2023). Impact of different roasting conditions on the chemical composition, antioxidant activities, and color of *Coffea canephora* and *Coffea arabica* L. samples. *Heliyon*, *9*(9), article e19580. https://doi.org/10.1016/j.heliyon.2023.e19580

Ginz, M., Balzer, H., Bradbury, A. G. W., Maier, H. G. (2000). Formation of aliphatic acids by carbohydrate degradation during roasting of coffee. *European Food Research and Technology*, *211*, 404-410. https://doi.org/10.1007/s002170000215

Hu, G. L., Wang, X., Zhang, L., Qiu, M. H. (2019). The sources and mechanisms of bioactive ingredients in coffee. *Food Function*, *10*(6), 3113-3126. https://doi.org/10.1039/c9fo00288j

Jeszka-skowron, M., Frankowski, R., Zgo, A. (2020). Comparison of methylxantines , trigonelline , nicotinic acid and nicotinamide contents in brews of green and processed Arabica and Robusta coffee beans – Influence of steaming , decaffeination and roasting processes on coffee beans. *LWT - Food Science and Technology*, *125*, article 109334. https://doi.org/10.1016/j.lwt.2020.109344

Jia, W., Guo, A., Zhang, R., Shi, L. (2023). Mechanism of natural antioxidants regulating advanced glycosylation end products of Maillard reaction. *Food Chemistry*, *404*, article 134541. https://doi.org/10.1016/j.foodchem.2022.134541

Kim, C., Jin, S., Seok, J., Yup, D. (2022). Interactive effect of post-harvest processing method, roasting degree, and brewing method on coffee metabolite profiles. *Food Chemistry*, *397*, article 133749. https://doi.org/10.1016/j.foodchem.2022.133749

Kim, I., Jung, S., Lee, E. K. J., Ha, C. K. J., Jeong, Y. (2021). Physicochemical characteristics of Ethiopian *Coffea arabica* cv. Heirloom coffee extracts with various roasting conditions. *Food Science and Biotechnology*, *30*(2), 235-244. https://doi.org/10.1007/s10068-020-00865-w

Kwon, S., Young, H. Y., Poung, N. T, Lee, G. Y, Jang, K., Joe, E., Lee, Y., Jeon, J. (2022). Humic-like crop stimulatory activities of coffee waste induced by incorporation of phytotoxic phenols in melanoidins during coffee roasting : Linking the Maillard reaction to humification. *Food Research International*, *162*, article 112013. https://doi.org/10.1016/j.foodres.2022.112013

Liao, Y., Kim, T., Silva, J. L., Hu, W., Chen, B. (2022). Effects of roasting degrees on phenolic compounds and antioxidant activity in coffee beans from different geographic origins. *LWT - Food Science and Technology*, *168*, article 113965. https://doi.org/10.1016/j.lwt.2022.113965

Liu, X., Xia, B., Hu, L., Ni, Z., Thakur, K., Wei, Z. (2020). Maillard conjugates and their potential in food and nutritional industries: A review. *Food Frontiers*, *1(4)*, 382-397. https://doi.org/10.1002/fft2.43

Livramento, K. G., Borém, F. M., José, A. C., Santos, A. V., Livramento, D. E., Alves, J. D., Paiva, L. V. (2017). Proteomic analysis of coffee grains exposed to different drying process. *Food Chemistry*, *221*, 1874-1882. https://doi.org/10.1016/j.foodchem.2016.10.069

Lopes, G. R., Passos, P., Petronilho, S., Rodrigues, C., Teixeira, J., Coimbra, M. A. (2021). Carbohydrates as targeting compounds to produce infusions resembling espresso coffee brews using quality by design approach. *Food Chemistry*, *344*, article 128613. https://doi.org/10.1016/j.foodchem.2020.128613

Long, L., Zhu, M., Ma, Y., Huang, Y., Gan, B., Yu, Q., Xie, J., Chen, Y. (2023). Variation of bioactive compounds and 5-hydroxymethyl furfural in coffee beans during the roasting process using kinetics approach. *Food Chemistry Advances*, *2*, article 100242. https://doi.org/10.1016/j.focha.2023.100242

Ludwig, I. A., Bravo, J., Peña, M. P. De. Cid, C. (2013). Effect of sugar addition (torrefacto) during roasting process on antioxidant capacity and phenolics of coffee. *LWT-Food Science and Technology*, *51*(2), 553-559. https://doi.org/10.1016/j.lwt.2012.12.010

Illy, A., & Viani, R. (Eds.). (2005). *Espresso coffee: the science of quality*. Academic Press.

Mehaya, F. M., Mohammad, A. A. (2020). Thermostability of bioactive compounds during roasting process of coffee beans. *Heliyon*, *6*, article e05508. https://doi.org/10.1016/j.heliyon.2020.e05508

Mehari, B., Redi-Abshiro, M., Chandravanshi, B. S., Atlabachew, M., Combrinck, S., McCrindle, R. (2016). Simultaneous determination of alkaloids in green coffee beans from Ethiopia: Chemometric evaluation of geographical origin. *Food analytical methods*, *9*, 1627-1637. https://doi.org/10.1007/s12161-015-0340-2

Minim, V. P. (2013). Análise sensorial: estudos com consumidores. Editora UFV.

Moreira, A. S. P., Nunes, F. M., Simões, C., Maciel, E., Domingues, P., Domingues, M. R. M., Coimbra, M. A. (2017). Transglycosylation reactions, a main mechanism of phenolics incorporation in coffee melanoidins: Inhibition by Maillard reaction. *Food Chemistry*, *227*, 422-431. https://doi.org/10.1016/j.foodchem.2017.01.107

Olthof, M. R., Hollman, P. C. H., Katan, M. B. (2001). Human Nutrition and Metabolism Chlorogenic Acid and Caffeic Acid Are Absorbed in Humans. *Journal of Nutrition*, *131*(1), 66-71. https://doi.org/10.1093/jn/131.1.66

Paiva, D. L., Lampman, G. M., Kriz, G. S., Vyvyan, J. R. (2016). Introdução à espectroscopia. Cengage Learning, tradução da 5ª edição norte-americana.

Park, J. B., Peters, R., Novotny, J. A. (2023). Impact of roasting on javamide-I/-II in Arabica and Robusta coffee beans. *Food Chemistry*, *412*, 135586. https://doi.org/10.1016/j.foodchem.2023.135586

Perrone, D., Donangelo, R., Donangelo, C. M., Farah, A. (2010). Modeling weight loss and chlorogenic acids content in coffee during roasting. *Journal of Agricultural and Food Chemistry*, *58*(23), 12238-12243. https://doi.org/10.1021/jf102110u

Poisson, L., Blank, I., Dunkel, A., & Hofmann, T. (2017). The chemistry of roasting: Decoding flavor formation. In B. Folmer (Ed.),. The craft and science of coffee (273–309). London: Academic Press.

Re, R., Pellegrini, N., Proteggente, A., Pannala, A., Yang, M., Rice-Evans, C. (1999). Antioxidant activity applying an improved abts radical cation decolorization assay. *Free Radical Biology & Medicine*, *26*, 1231-1237. https://doi.org/10.1016/S0891-5849(98)00315-3

Ribeiro, J. S., Augusto, F., Salva, T. J., Thomaziello, R. A., Ferreira, M. M. C. (2009). Prediction of sensory properties of Brazilian Arabica roasted coffees by headspace solid phase microextraction-gas chromatography and partial least squares. *Analytica Chimica Acta, 634*(2), 172-179. https://doi.org/10.1016/j.aca.2008.12.028

Rodrigues R, Oliveira MBPP, Alves RC. Chlorogenic Acids and Caffeine from Coffee By-Products: A Review on Skincare Applications. *Cosmetics*, *10*(1), 1-12. https://doi.org/10.3390/cosmetics10010012

Rune, C. J. B., Giacalone, D., Steen, I., Duelund, L., Münchow, M., Clausen, M. P. (2023). Acids in brewed coffees: Chemical composition and sensory threshold. *Current Research in Food Science*, *6*, article 100485. https://doi.org/10.1016/j.crfs.2023.100485.

Sacchetti, G., Mattia, C. Di, Pittia, P., Mastrocola, D. (2009). Effect of roasting degree, equivalent thermal effect and coffee type on the radical scavenging activity of coffee brews and their phenolic fraction. *Journal of Food Engineering*, *90*, 74-80. https://doi.org/10.1016/j.jfoodeng.2008.06.005

Santos, J. R., Viegas, O., Páscoa, R. N. M. J., Ferreira, I. M. P. L. V. O., Rangel, A. O. S. S., Lopes, J. A. (2016). In-line monitoring of the coffee roasting process with near infrared spectroscopy: Measurement of sucrose and colour. *Food* Chemistry, *208*, 103-110. https://doi.org/10.1016/j.foodchem.2016.03.114

Sen, D., & Gokmen, V. (2022). Kinetic modeling of Maillard and caramelization reactions in sucrose-rich and low moisture foods applied for roasted nuts and seeds. *Food Chemistry, 395,* article 133583. https://doi.org/10.1016/j.foodchem.2022.133583

Shakoor, A., Zhang, C., Xie, J., Yang, X. (2022). Maillard reaction chemistry in formation of critical intermediates and flavour compounds and their antioxidant properties. *Food Chemistry*, *393*, article 133416. https://doi.org/10.1016/j.foodchem.2022.133416

Specialty Coffee Association (2018). Cupping Protocols. Retrieved from https://sca.coffee/research/protocols-best-practices. Accessed Sep. 16, 2021.

Silva, C. F., Batista, L. R., Abreu, L. M., Dias, E. S., Schwan, R. F. (2008). Succession of bacterial and fungal communities during natural coffee (*Coffea arabica*) fermentation. *Food Microbiology*, *25*(8), 951-957. https://doi.org/10.1016/j.fm.2008.07.003

Singleton, V. L., & Rossi, J. A. J. (1965). Colorimetry of Total Phenolics with Phosphomolybdic-Phosphotungstic Acid Reagents. *American Journal of Enology and Viticulture*, *16*, 144-158.

Sousa, M. M. M. De, Carvalho, F. M., Pereira, R. G. F. A. (2020). Colour and shape of design elements of the packaging labels influence consumer expectations and hedonic judgments of specialty coffee. *Food Quality and Preference*, *83*, article 103902. https://doi.org/10.1016/j.foodqual.2020.103902

Souza, J. C., Pasquini, C., Hespanhol, M. C. (2022). Feasibility of compact near-infrared spectrophotometers and multivariate data analysis to assess roasted ground coffee traits. *Food Control*, *138*, article 109041. https://doi.org/10.1016/j.foodcont.2022.109041

Sruthi, N. U., Premjit, Y., Pandiselvam, R., Kothakota, A., Ramesh, V. (2021). An overview of conventional and emerging techniques of roasting: Effect on food bioactive signatures. *Food Chemistry*, *348*, article 129088. https://doi.org/10.1016/j.foodchem.2021.129088

Sunarharum, W. B., Williams, D. J., Smyth, H. E. (2014). Complexity of coffee flavor: A compositional and sensory perspective. *Food Research International*, *62*(1), 315-325. https://doi.org/10.1016/j.foodres.2014.02.030

Thomas, E., Puget, S., Valentin, D., Songer, P. (2017). Sensory evaluation-profiling and preferences. The Craft and Science of Coffee, *Elsevier Inc*. https://doi.org/10.1016/B978-0-12-803520-7.00018-9

Viencz, T., Acre, L. B., Rocha, R. B., Alves, E. A., Ramalho, A. R., Benassi, M. D. T. (2023). Caffeine, trigonelline, chlorogenic acids, melanoidins, and diterpenes contents of *Coffea canephora* coffees produced in the Amazon. *Journal of Food Composition and Analysis*, *117*, article 105140. https://doi.org/10.1016/j.jfca.2023.105140

Vignoli, J. A., Marcelo, C. V., Denisley, G. B., Marta, T. N. (2014). Roasting process affects differently the bioactive compounds and the antioxidant activity of arabica and robusta coffees. *Food Research International*, *61*, 279-285. http://dx.doi.org/10.1016/j.foodres.2013.06.006

Vilas-boas, A. A., Oliveira, A., Jesus, D., Rodrigues, C., Figueira, C., Gomes, A. (2020). Chlorogenic acids composition and the impact of in vitro gastrointestinal digestion on espresso

coffee from single-dose capsule. *Food Research International*, *134*, article 109223. https://doi.org/10.1016/j.foodres.2020.109223

Wang, Y., Wang, X., Hu, G., Zhang, Z., Al-romaima, A., Bai, X. Li, J., Zhou, L., Li, Z., Qiu, M. (2023). Comparative studies of fermented coffee fruits post-treatments on chemical and sensory properties of roasted beans in Yunnan, China. *Food Chemistry*, *423*, article 136332. https://doi.org/10.1016/j.foodchem.2023.136332

Wei, F., & Tanokura, M. (2015).Chemical changes in the components of coffee beans during roasting. Coffee in health and disease prevention. *Elsevier*, 83-91. https://doi.org/10.1016/B978-0-12-409517-5.00010-3

Wu, H., Gu, J., Bk, A., Nawaz, M. A., Barrow, C. J., Dunshea, F. R., Suleria, H. A. R. (2022). Effect of processing on bioaccessibility and bioavailability of bioactive compounds in coffee beans. *Food Bioscience*, *46*, article 101373. https://doi.org/10.1016/j.fbio.2021.101373

Xue, C., Quan, W., Li, Y., He, Z., Qin, F., Wang, Z., Chen, J., Zeng, M. (2022). Mitigative capacity of Kaempferia galanga L. and kaempferol on heterocyclic amines and advanced glycation end products in roasted beef patties and related mechanistic analysis by density functional theory. *Food Chemistry*, *385*, article 132660. https://doi.org/10.1016/j.foodchem.2022.132660

Yang, N., Liu, C., Liu, X., Degn, T. K., Munchow, M., Fisk, I. (2016). Determination of volatile marker compounds of common coffee roast defects. *Food Chemistry*, *211*, 206-214. https://doi.org/10.1016/j.foodchem.2016.04.124

Yeager, S. E., Batali, M. E., Guinard, J. X., Ristenpart, W. D. (2021). Acids in coffee: A review of sensory measurements and meta-analysis of chemical composition. *Critical Reviews in Food Science and Nutrition*, *1*, 1-27. https://doi.org/10.1080/10408398.2021.1957767

Zanin, R. C., Corso, M. P., Kitzberger, C. S. G., Scholz, M. B. S., Benassi, M. T. (2016). Good cup quality roasted coffees show wide variation in chlorogenic acids content. *LWT - Food Science and Technology*, *74*, 480-483. https://doi.org/10.1016/j.lwt.2016.08.012

Zuhair, M., Zain, M., Salihin, A., Bakr, A. (2018). Effect of polyphenols enriched from green coffee bean on antioxidant activity and sensory evaluation of bread. *Journal of King Saud University - Science*, *30*(2), 278-282. https://doi.org/10.1016/j.jksus.2017.12.003

2. CONCLUSION

This comprehensive study on coffee highlights the importance of the roasting process as a critical factor that influences both the chemistry and the coffee experience, a widely consumed beverage worldwide. The five chapters of this work take us on a journey of discovery, exploring everything from the origin and market of coffee to roasting profiles, chemical composition, properties, and innovations in the process.

In the first chapter, we are introduced to the general context of coffee, its global relevance, and the importance of quality in the roasting process. In the second chapter, we examine how different roasting profiles affect the chemical composition, antioxidant activity, and color of different coffee varieties, *Coffea canephora* and *Coffea arabica*.

The third chapter explores post-harvest roasting conditions, focusing on the composition of carbohydrates, organic acids, and melanoidins, revealing how these elements contribute to the unique flavor and aroma of coffee. The fourth chapter investigates the harmonization of sensory characteristics in different roasting profiles, using advanced techniques such as infrared spectroscopy analysis to deepen our understanding of the complex chemical interactions involved.

Finally, in the fifth and last chapter, we are introduced to innovative roasting profiles that have the potential to enhance both the chemical composition and the experience of arabica coffee. The study covers a comprehensive analysis of the total chemical composition of this coffee, demonstrating the potential for roasting advancements to further elevate the quality of this beloved beverage.

In summary, this work underscores the deep relationship between chemistry, the roasting process, and the appreciation of coffee, offering valuable insights that can benefit both the industry and enthusiasts of this globally cherished beverage.

3. REFERENCES

Acquaticci, L., Angeloni, S., Cela, N., Galgano, F., Vittori, S., Caprioli, G., Condelli, N. (2023). Impact of coffee species, post-harvesting treatments and roasting conditions on coffee quality and safety related compounds. *Food Control*, *149*, article 109714. https://doi.org/10.1016/j.foodcont.2023.109714

Aguiar, J., Estevinho, B. N., Santos, L. (2016). Microencapsulation of natural antioxidants for food application - The specific case of coffee antioxidants - A review. *Trends in Food Science & Technology*, *58*, 21-39. https://doi.org/10.1016/j.tifs.2016.10.012

Akash, M. S. H., Rehman, K., Chen, S. (2014). Effects of coffee on type 2 diabetes mellitus. *Nutrition*, *30*(8), 755-763. https://doi.org/10.1016/j.nut.2013.11.020

Alongi, M., & Anese, M. (2018). Effect of coffee roasting on in vitro α-glucosidase activity: Inhibition and mechanism of action. *Food Research International*, *111*, 480-487. https://doi.org/10.1016/j.foodres.2018.05.061

Alongi, M., Calligaris, S., Anese, M. (2019). Fat concentration and high-pressure homogenization affect chlorogenic acid bioaccessibility and α-glucosidase inhibitory capacity of milk-based coffee beverages. *Journal of Functional Foods*, 58, 130-137. https://doi.org/10.1016/j.jff.2019.04.057

Alongi, M., Frías Celayeta, J. M., Vriz, R., Kinsella, G. K., Rulikowska, A., Anese, M. (2021). In vitro digestion nullified the differences triggered by roasting in phenolic composition and α-glucosidase inhibitory capacity of coffee. *Food Chemistry*, 342, article 128289. https://doi.org/10.1016/j.foodchem.2020.128289

Anese, M., Alongi, M., Cervantes-Flores, M., Simental-Mendía, L. E., Martínez-Aguilar, G., Valenzuela-Ramírez, A. A., Rojas-Contreras, J. A., Guerrero-Romero, F., Gamboa-Gómez, C. I. (2023). Influence of coffee roasting degree on inflammatory and oxidative stress markers in high-fructose and saturated fat-fed rats. *Food Research International*, *165*, article 112530. https://doi.org/10.1016/j.foodres.2023.112530

Baggenstoss, J., Poisson, L., Kaegi, R., Perren, R., Escher, F. (2008). Coffee roasting and aroma formation: application of different time-temperature conditions. *Journal of Agricultural and Food Chemistry*, *56*(14), 5836-5846. https://doi.org/10.1021/jf800327j

Chaichi, M., Ghasemzadeh-Mohammadi, V., Hashemi, M., Mohammadi, A. (2015). Furanic compounds and furfural in different coffee products by headspace liquid-phase micro-extraction followed by gas chromatography–mass spectrometry: Survey and effect of brewing

procedures. *Food Additives & Contaminants*, *8*(1), 73-80. https://doi.org/10.1080/19393210.2014.981601

Chindapan, N., Soydok, S., Devahastin, S. (2019). Roasting Kinetics and Chemical Composition Changes of Robusta Coffee Beans During Hot Air and Superheated Steam Roasting. *Journal of Food Science*, *0*, 1-11. https://doi.org/10.1111/1750-3841.14422

Cortés-Macías, E. T., López, C. F., Gentile, P., Girón-Hernández, J., López, A. F. (2023). Impact of post-harvest treatments on physicochemical and sensory characteristics of coffee beans in Huila, Colombia. *Postharvest Biology and Technology*, *187*, article 111852. https://doi.org/10.1016/j.postharvbio.2022.111852

Hall, R. D., Trevisan, F., de Vos, R. C. (2022). Coffee berry and green bean chemistry–Opportunities for improving cup quality and crop circularity. *Food Research International*, *151*, article 110825. https://doi.org/10.1016/j.foodres.2021.110825

Klaidaeng, C., Chudjuarjeen, S., Pomsen, C., Charoenwiangnuea, P. (2023). Prediction of roasted coffee bean level from a coffee house-ware using fuzzy logic. *Materials Today: Proceedings*. https://doi.org/10.1016/j.matpr.2023.04.524

Li, X., Yang, L., Hao, M., Song, T., He, Y., Yang, M., Zhang, J. (2023). Chlorogenic acid as an indispensible partner of caffeic acid in coffee via selective regulation of prooxidative actions of caffeic acid. *Food Research International*, article 113482. https://doi.org/10.1016/j.foodres.2023.113482

Lopes, G. R., Passos, C. P., Rodrigues, C., Teixeira, J. A., Coimbra, M. A. (2020). Impact of microwave-assisted extraction on roasted coffee carbohydrates, caffeine, chlorogenic acids and coloured compounds. *Food Research International*, *129*, article 108864. https://doi.org/10.1016/j.foodres.2019.108864

Mehaya, F. M., Mohammad, A. A. (2020). Thermostability of bioactive compounds during roasting process of coffee beans. *Heliyon*, *6*, article e05508. https://doi.org/10.1016/j.heliyon.2020.e05508

Park, J. B., Peters, R., Novotny, J. A. (2023). Impact of roasting on javamide-I/-II in Arabica and Robusta coffee beans. *Food Chemistry*, *412*, article 135586. https://doi.org/10.1016/j.foodchem.2023.135586

Pereira, L. L., Júnior, D. B., de Sousa, L. H. B. P., dos Santos, W. G., Cardoso, W. S., Guarçoni, R. C., ten Caten, C. S. (2021). Relationship Between Coffee Processing and Fermentation. Quality Determinants In Coffee Production, 255-301. https://doi.org/10.1007/978-3-030-54437-9

Pimpley, V., Patil, S., Srinivasan, K., Desai, N., Murthy, P. S. (2020). The chemistry of chlorogenic acid from green coffee and its role in attenuation of obesity and diabetes. Preparative *Biochemistry & Biotechnology*, *50*(10), 969-978. https://doi.org/10.1080/10826068.2020.1786699

Poisson, L., Blank, I., Dunkel, A., & Hofmann, T. (2017). The chemistry of roasting: Decoding flavor formation. In B. Folmer (Ed.), the craft and science of coffee (pp. 273–309). London: Academic Press.

Poltronieri, P., Rossi, F. (2016). Challenges in Specialty Coffee Processing and Quality Assurance. *Challenges*, 7, 19. https://doi.org/10.3390/challe7020019

Shahinfar, H., Jayedi, A., Khan, T. A., Shab-Bidar, S. (2021). Coffee consumption and cardiovascular diseases and mortality in patients with type 2 diabetes: A systematic review and dose–response meta-analysis of cohort studies. *Nutrition, Metabolism and Cardiovascular Diseases*, *31*(9), 2526–2538. https://doi.org/10.1016/j.numecd.2021.05.014

Silva, C. W., Zanardi, K. R., Grancieri, M., Costa, N. M. B., Trivillin, L. O., Viana, M. L., Silva, P. I., & Costa, A. G. V. (2022). Green coffee extract (Coffea canephora) improved the intestinal barrier and slowed colorectal cancer progression and its associated inflammation in rats. PharmaNutrition, 22, 100314. https://doi.org/10.1016/j.phanu.2022.100314

Sruthi, N. U., Premjit, Y., Pandiselvam, R., Kothakota, A., Ramesh, S. V. (2021). An overview of conventional and emerging techniques of roasting: Effect on food bioactive signatures. *Food Chemistry*, *348*, article 129088. https://doi.org/10.1016/j.foodchem.2021.129088

Van der Werf, R., Marcic, C., Khalil, A., Sigrist, S., Marchioni, E. (2014). ABTS radical scavenging capacity in green and roasted coffee extracts. *LWT - Food Science and Technology*, *58*(1), 77-85. https://doi.org/10.1016/j.lwt.2014.02.053

Worku, M., Astatkie, T., Boeckx, P. (2023). Quality and biochemical composition of Ethiopian coffee varied with growing region and locality. *Journal of Food Composition and Analysis*, *115*, article 105015. https://doi.org/10.1016/j.jfca.2022.105015

Wu, H., Gu, J., BK, A., Nawaz, M. A., Barrow, C. J., Dunshea, F. R., Suleria, H. A. R. (2022). Effect of processing on bioaccessibility and bioavailability of bioactive compounds in coffee beans. *Food Bioscience*, *46*, article 101373. https://doi.org/10.1016/j.fbio.2021.101373