Chemical and Sensory discrimination of coffee: Impacts of the planting altitude and fermentation

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Research Article

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Abstract

Edaphoclimatic conditions, planting altitudes, soil, the microbiome of plants and fruits, genotypes, and postharvest processing are variables that contribute to the chemical and sensory quality of the coffee. Thus, the objective of this study was to evaluate the impacts of planting altitude and fermentation of fruits on the chemical and sensory quality of the coffee using nuclear magnetic resonance (NMR) and linear discriminant analysis (LDA). Cherry coffees were harvested in 8 points of altitudes between 826 and 1078.08 meters. A completely randomized design with 8 planting altitudes, 5 fermentation processes, and 5 repetitions was performed. Lipids, trigonelline, citrate, and malate were the compounds that most contribute to the chemical discrimination of coffee in the altitudes below 969 m. While, in the high altitudes (> 1000 m), this discrimination was due to the HMF, quinic acid, caffeine, and formic acid and the global notes of coffee drink were higher than 80 points. In fermented coffee, the LDA of the chemical data indicates the formation of five clusters, showing how the compounds can suffer changes depending on the form of processing used in coffee. The best score was observed in samples of 1078.08 m and dry fermentation and only in 969 m was observed significant difference between spontaneous fermentation and induced fermentation. Thus, coffee sensory scores were dependent on planting and fermentation methods and NMR and LDA techniques proved to be important in chemical and sensory discrimination of coffees.

Introduction

Many variables contribute to the coffee quality, especially when considering the relationship between the chemical compounds and sensory attributes of the roasted coffee. Aroma precursors, such as trigonelline, manifest after roasting coffee, being responsible for flavor formation, such as pyridine, alkyl-pyridines, and furans (Duarte et al. 2010). The caffeine is odorless and has a bitter taste that is important to the taste and aroma of coffee (Pereira et al. 2020).

Conversely, the components negatively related to coffee sweetness, such as citrate and malate, have a very strong sour taste. The relationship between sweetness and sourness is variably affected at low intensities/concentrations but symmetrically suppressive at medium and high intensities/concentrations. Similar to bitterness, coffee astringency had a positive relationship with lipids, quinic acids, mannose, and quinine and negative relation with chlorogenic acids, citrate, malate, trigonelline, arabinose, and galactose (Wei et al. 2014).

In recent years, studies have indicated that edaphoclimatic conditions, planting altitudes, soil, the microbiome of plants and fruits, genotypes, and postharvest processing are also factoring determinants of the chemical and sensory quality of the coffee (Brioschi Junior et al., 2021, Chindapan, et al., 2019, De Bruyn, et al., 2017, Pereira et al., 2021, Martinez et al., 2021, Veloso et al., 2021).

The microbial metabolites affect the chemical and sensory composition of fermented coffee (Evangelista et al. 2014; Lee et al. 2016; Lee et al. 2017; Pereira et al. 2017). However, there are two distinct scientific
trends regarding the impact of fermentation on the chemical, nutritional, and sensorial quality of coffee. To the first trend, this quality is due to the spontaneous fermentation that occurred in coffee fruits (Alvarado and Linnemann 2010; Bertrand et al. 2006; De Bruyn et al. 2017; Pereira et al., 2018a; Pereira et al., 2020). This fermentation is affected by the processing of coffee cherries (Pereira et al. 2020), the genetic variety of the plant (Bertrand et al. 2006), and natural coffee microbiota (De Bruyn et al. 2017). Another trend argues that coffee quality can be optimized with the application of microorganism's starters that modify the taste and texture (Bressani et al. 2021; Evangelista et al. 2015; Martinez et al. 2021; Pereira et al. 2017; Pereira et al. 2021; Tang et al. 2021). Moreover, the production of specialty coffees has suffered a profound revision in the form of processing, through the understanding and introduction of fermentation techniques, focusing on the observation of how chemical compounds interact with sensory profiles of the coffee drink (Avelino et al. 2015; Brioschi Junior et al. 2021; Pereira et al., 2018a).

In this range of interactions between chemical compounds and microbial agents, processing techniques need to be better understood to determine the best strategies for the production of specialty coffees. Thus, the objective of this study was to evaluate the impacts of planting altitude and fermentation of fruits on the chemical and sensory quality of the coffee. For this, we used the Nuclear magnetic resonance (NMR) technique to determine the chemical compounds with the highest contribution to the sensory attributes of coffee samples and linear discriminant analysis to evaluate the grouping relationship of chemical and sensory classes according to the production zones (altitude) and how the variables are related about the final quality of the coffee.

**Materials And Methods**

In this study, we evaluated the impact of planting altitude and fermentation of coffee cherries on the chemical and sensory quality of the coffee.

The samples of cherry coffee were harvested in the maturation period in 8 different points of the state of Espírito Santo, Brazil (Supplementary material S1). Only coffee in the full maturity stage (90 %) was collected.

After harvesting, the coffees were taken to the processing unit to be washed in 1000-liter plastic boxes to separate the floating fruits. After washing, the fruits were peeled with the DPMM-04 equipment (coffee peeler).

The freshwater used in the processing of the coffees is by CONAMA guideline n. 357/2005, which deals with the classification of water bodies such as the recommendation of Pereira et al. (2020).

**Analysis of chemical and sensory quality Cherry coffee of different altitude**

The 8 points of sampling had between 826 and 1078.08 meters of altitude (Supplementary material S1). The samples were used to determines the chemical compounds by NMR and sensory attributes.
Supplementary material S1: Location of the farmers and points of samples of the Cherry coffee (1 to 8) at different altitudes.

**Fermentation of the Cherry coffee**

A completely randomized design with 8 planting altitudes, 5 fermentation processes (Table 1), and 5 repetitions was carried out to evaluate the impacts of the spontaneous and induced fermentation on the chemical and sensory quality of the coffee. These fermentations were performed following the recommendations of Pereira et al. (2020).

Table 1: Fermentations of Cherry coffee produced an altitude of 826 to 1078.08 m.

| Fermentation                        | Description                                                                                                                                                                                                 |
|-------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Semi-dry                            | 25 kg of Cherry coffee with mucilage were peeled and placed on drying in a suspended terrace (African Bed System), for drying with the mucilage on the parchment. There is no microbial inoculation and spontaneous fermentation took place at 21 °C for 36 hours. |
| Washed                              | 25 kg of Cherry coffee with mucilage were immersed in 12.5 liters of water. There is no microbial inoculation and spontaneous fermentation took place at 21 °C for 36 hours.                                              |
| Yeast fermentation (Washed with microbial inoculation) | 25 kg of cherry coffee with mucilage were immersed in 12.5 liters of water. The inoculation was performed with *Saccharomyces cerevisiae* (10⁶ UFC) at 1% (w/v). Induced fermentation by starter culture took place at 21 °C for 36 hours. |
| Fully washed                        | 25 kg of Cherry coffee with mucilage were placed dry (without additional water) to carry out the fermentation. There is no microbial inoculation and spontaneous fermentation took place at 21 °C for 36 hours. The coffee samples were washed after the fermentation processing finished. |
| Dry fermentation (Fully washed with microbial inoculation) | 25 kg of Cherry coffee with mucilage were placed dry (without additional water) to carry out the fermentation. The inoculation was performed with *Saccharomyces cerevisiae* (10⁶ UFC) at 1% (w/v). Induced fermentation by starter culture took place at 21 °C for 36 hours. The coffee samples were washed after the fermentation processing finished. |
The coffees were removed from the fermentation tanks and immediately taken to drying in a suspended bed with a plastic cover until reduced to 11 % (b.u) for safe storage.

**Roasting procedures and grinding**

The roasting procedures of coffee were carried out in a Probation roaster (Probat), with roasting curves of 140 °C to 190 °C. The roasted coffees were placed in packages (*aluminum*), respecting 8 hours after roasting.

The coffees were also ground in a disk mill (Bunn Coffee Mill, model G3A HD), with granulometry between 70 and 75 % of the particles passing through a 20-mesh sieve (standard US Standards).

**NMR data analysis**

The $^1$H NMR spectra of ground coffee were obtained at Laboratory of Research and Development of Methodologies for Analysis of Oils (LabPetro) Chemistry Department, Federal University of Espirito Santo, Campus Goiabeiras, Vitoria – ES, in a Varian spectrometer of 400 MHz, using a probe of 5 mm 1H/X/D Broadband at 25 °C and a 90° pulse. First, the T1 values were optimized, using 3 different coffee samples, which had very different sensory characteristics, so that the waiting time at the time of analysis was determined. In addition, the coffee extraction temperature was tested by the solvent, 95 °C and room temperature (around 20 °C), showing that there were no significant differences between the spectra.

After optimization, the samples were prepared by dissolving 0.07g of ground coffee in D2O, totaling a volume of 700 µL. Wait 4 minutes and the supernatant was collected for analysis. The instrumental conditions were a spectral window, 4401.4 Hz; acquisition time, 7,445 s; standby time, 27 seconds; pulse, 90; number of transients, 64. Chemical shifts were obtained using maleic acid (6.40 ppm) as a reference signal, using an insertion tube, and the phase and baseline were manually adjusted.

**Sensory analysis procedures**

Coffee brewing was performed following the recommendations of the Specialty Coffee Association (SCA).

The cupping protocol used contains 10 attributes, namely: fragrance/aroma, flavor, aftertaste, acidity, body, balance, uniformity, clean cup, sweetness, and overall. The grades in each attribute range from 6 to 10 (SCAA 2013). The coffees were evaluated by six professional judges (Q-graders), following the guidance of Pereira et al. (2018b).

**Data Analysis**

Statistical analysis was performed using the Linear Discriminant Analysis (LDA) supervised classification method using Matlab® Software. LDA is a multivariate classification method that uses the Mahalanobis
metric to calculate the discrepancies of each sample at the center of each identified class. The probability that a sample belongs to a class is all the greater the shorter the distance from that class.

Four LDA models were made using the chemical compounds and sensory attributes of Cherry Coffee. The chemical and sensory discrimination of these coffees about planting altitude is observed in the first and second models, while the impacts of fermentation can be observed in the third and fourth models.

Sensory scores data were also submitted to analysis of variance and Scott-Knott test at 5 % probability (p < 0.05).

Results

The $^1$H-NMR spectra were integrated into the areas described in figure 1 and water signals (H$_2$O; bins 4.50–5.50 ppm) were removed. For multivariate analysis, these data were referenced with maleic acid, phased, baseline corrected, aligned, and normalized by MestRe Nova Software, and then the data between -1.00 and 10.00 ppm were reduced for spectral ranges (Figure 1).

3.1 Analysis of chemical and sensory quality Cherry coffee of different altitude

The lipids (3) and trigonelline (13 and 14) in 826 m and the lipids (1), citrate and malate (6), and trigonelline (11) in 907.08 m were the compounds that most contribute to the chemical discrimination of coffee about altitude (Figures 1 and 2). In the intermediate zone, 969 to 1021 meters was observed a general contribution of all compounds (Figures 1 and 2). In the high altitudes of 1033 to 1078.08 m, the HMF (15), quinic acid (4), caffeine (10), and formic acid (12) were the compounds that most contribute to group discrimination (Figures 1 and 2). These results show variations in chemical composition in the function of the planting altitude.

For the sensory data, the uniformity in 826 m and the overall in 1005 and 1078.08 m were the sensory attributes that most contributed to the discrimination of the groups (Figure 3). At other altitudes, there was no significant difference between attributes in sensory discrimination of Cherry coffee.

3.2 Analysis of chemical and sensory quality Cherry coffee of different altitudes after fermentations

The results of the LDA analysis with the chemical data indicate the formation of five clusters, showing how the compounds can suffer changes depending on the form of processing used in coffee (Figures 1 and 4). The washed processing has the lipids (3), formic acid (12), and HMF (15), as an antagonist (Figure 3, Table 2). In the fully washed method, the trigonelline (11 and 14) and lipids (1) were compounds that most contribute by clusters formation. The yeast fermentation, the compounds most contribute to discrimination in the LDA method were caffeine (10) and trigonelline (13). These compounds were antagonistic in the dry fermentation (Figures 1 and 4). Furthermore, washed and fully washed methods were in opposite positions in the scores on canonical variable 1, while yeast
fermentation and semidry were in the opposite position to dry fermentation in the scores on canonical variable 2 (Figure 4A).

Nothing cluster was observed in the LDA of the fermentations and sensory attributes (Figure 5). However, the fermented coffee has sensory scores greater than 78 points, and regardless of the planting altitude; these scores were higher than 80 points in the Washed fermentation (Table 2). Furthermore, the best score was observed in samples of 1078.08 m and dry fermentation, and only in 969 m was observed significant difference (p< 0.05) between spontaneous fermentation and induced fermentation (Table 2). Thus, sensory scores of coffees depend on the planting system and fermentation methods.

Table 2. Global note of Cherry coffee of planting different altitude after 5 types of fermentation (see table 1).

| Planting altitude (m) | Fermentations       |
|-----------------------|----------------------|
|                       | Semi-dry  | Washed   | Yeast fermentation | Fully washed | Dry fermentation |
| 826.00                | 79.87 aA  | 80.46 aA | 78.69 bA           | 78.15 bB     | 79.48 bB         |
| 907.08                | 80.98 aB  | 81.48 aA | 79.48 bC           | 79.29 bC     | 81.44 aA         |
| 969.00                | 79.54 bC  | 80.03 bB | 81.52 aA           | 78.36 bC     | 82.08 aA         |
| 1005.00               | 87.09 aA  | 87.63 aA | 85.11 bB           | **84.48 bB** | 85.73 bB         |
| 1021.00               | 81.63 bC  | 80.78 bC | 83.36 aB           | 83.75 aA     | 84.34 aA         |
| 1033.00               | 82.68 bB  | 85.39 aA | 82.70 bB           | 83.17 bB     | 83.81 bB         |
| 1052.00               | 80.64 cC  | 82.03 cB | 82.97 bB           | 80.74 cC     | 84.41 aA         |
| 1078.08               | 84.75 bB  | 83.98 bC | 84.14 bB           | 84.09 bB     | 86.99 aA         |

Means with the same lowercase letter in the vertically and uppercase in the horizontally do not differ by Scott-Knott test at 5 % probability.

**Discussion**

The reduction of spectral ranges (Fig. 1) is according to Arana et al. (2015), Tavares and Ferreira (2006), and Wei et al. (2014). In these spectra, we identified 12 chemicals in the Coffee samples produced in different planting altitudes (Fig. 1). While, about 20 compounds (e.g. formic acid, fumaric acid, quinic acid, caffeine, sugar, trigonelline, and lipids) were observed in the $^1$H NMR spectra of coffees beans produced in Portugal, Timer-Leste, Kenyan, Colombia, and Brazil in the coffees (Wang et al. 2021). According to these authors, the planting region influences the chemical composition of the coffee cherry and in the principal component analysis, the 12 coffee cultivars were grouped into four groups in the function of the chemical compounds. These results showed the potential of NMR for Chemical discrimination of cultivars coffee.
The altitude range of 826 to 907.08 m was opposite the ranges of high altitudes by canonical variable 1 in the LDA model (Fig. 2). These results show a variation in the chemical composition of the coffee in the function of the planting altitude. Other studies have also shown significant differences in the chemical composition of the coffees produced at different planting altitudes (Avelino et al. 2005 and 2015; Martinez et al. 2021; Pereira et al. 2021). The concentration of acetic acid was greater in coffees produced at an altitude of 1,200 m than in the samples from the lowest altitudes (Martinez et al. 2021). Furthermore, according to Pereira et al. (2021), coffees produced in altitudes of 300 to 600 m have about 30 volatile compounds. Therefore, these coffees can be grouped in the function of the composition of volatile compounds.

The clusters of the relationships between planting altitude and the chemical compounds can be due to the plant variety, the microbiota of the fruits and soil, and edaphoclimatic conditions (Fig. 2). The genetic factor was the main responsible for the presence of lipids and trigonelline in roasted coffee (del Campo et al. 2009; Duarte et al. 2010). Environmental factors (e.g., altitude, solar radiation, soil temperature, and chemical content of the soil) influence the microbiota of the fruits and soil that produce the main sensory compounds of the coffee beverage (Veloso et al. 2020). According to these authors, coffee trees at higher altitudes tended to have more bacteria shared between the soil and fruits, and fungi-fungi and fungi-bacteria connections are inversely proportional to ground altitudes. Furthermore, these indigenous coffee microorganisms promote spontaneous fermentations (Pereira et al. 2020). Because of these interactions, the terroir effects can be understanding from these perspectives.

In high planting altitude (> 1000 m), the global notes were higher than 80 points (Table 2) indicating that edaphoclimatic conditions of this environment favor the formation of organoleptic compounds, for example, sugar, quinic acids, acetic acid, formic acid, citrate, malate, HMF, and caffeine (Figs. 1 to 3). Quinic acid, malic acid, and gluconic acid were the compounds most abundant in the mucilage of green coffee beans produced in 1.329 m of altitude (De Bruyn et al. 2017).

Acetic acid and formic acid are contributors to the overall sensory perceived acidity of coffee (Chindapan et al. 2019). Few studies relate the composition of formic acid to the sensory quality of coffee (del Campo et al. 2010; Pereira et al., 2020).

Citrate and malate have a very strong sour taste and a negative correlation between these compounds content and coffee sweetness has been observed (Wei et al. 2014). Furthermore, in the altitude range with the occurrence of these compounds, the sensory results were also above 80 points, however, the processing with microbial inoculation indicated a score below SCA quality standards (Figs. 1, 2, and 4, Table 2).

HMF formed in foods during heating is considered a marker of the extent of Maillard and sugar dehydration reactions. However, the HMF content of different types of beers is relatively low, indicating its potential for degradation during fermentation (Akillioglu et al. 2011). According to Pereira et al. (2020), the observation regarding the increase of the level of HMF with the altitude for process semi-dry reinforces the indication that the residual sugars of the parchment can be incorporated into the coffee,
due to the sensory observations of the Q-Graders, with the semi-dry providing softer and sweeter coffees.

Although caffeine content was not found to have a direct effect on beverage quality, levels of this alkaloid are higher in samples of high-quality coffee than other samples of coffees (Franca et al. 2005). Furthermore, a significant linear regression was found between caffeine content and planting altitude in Arabica coffees (Bertrand et al. 2006).

The overall, body, and uniformity were the sensory attributes that most influenced the discrimination of coffee by planting altitude (Fig. 3). However, these attributes are sensory characteristics that normally the Q-Graders are free to highlight the notes. Q-Graders can raise or lower their grades according to their criteria. The body is a sensory perception of the weight of the drink on the tongue. Thus, the altitude/body ratio can vary according to the nature of the taster-Grader. Furthermore, a high body score can also be perceived as a defect in some cases, mainly for low-altitude coffees (Avelino et al. 2005).

Lipids, trigonelline, formic acid, and HMF were important variables in the chemical discrimination of the fermented coffee (Figs. 1 and 4). The lipids extracted from coffee beans contain about 75% of triacylglycerols with a high percentage of unsaponifiable compounds, including diterpene alcohols and sterols, and low tocopherols contents (Calligaris et al. 2009). Furthermore, there is the migration of lipids from the endosperm to the surface of the coffee bean (Williamson and Hatzakis 2019) that can contribute to fermentation.

Microbial degradation of this biomolecule can produce sensory compounds, such as fatty acids and citrate. The degradation of lipids by microbial enzymes has been observed in the growth of different microorganisms, for example, S. cerevisiae (Bustamante-Torres et al. 2021; Darvishi 2012). Furthermore, lipids oxidation also causes off-flavors (Alvarenga 2017). Thus, the lipids degradation shows the importance of the fermentation in the chemical and sensory quality of the coffee beverage.

Formic acid has been reported as the natural presence in plants and fruits, and it can be an additional mechanism for defense against diseases or alterations produced by bacteria and fungi (Berregi et al. 2007). The concentration of this acid in green coffee is very low, but it represents about 10% of the organic acids in the dried coffee beans (Dong et al. 2017). Furthermore, formic acid has been reported as well as strong contributors to total sensory perceived acidity of the coffee drink (Chindapan et al. 2019).

For washed fermentation, the formic acid can also be formed by the action of the Enterobacteriaceae and Pantoea bacteria through carbohydrates degradation (Ndayambaje et al. 2019).

The production of sugar reduction and microbial proteins by fermentation can have influenced the HMF contents of coffee. This compound is formed during the roasting of coffee by reactions of Maillard and sugar dehydration (Akillioglu et al. 2011). Furthermore, 5-HMF is recognized as an indicator of quality deterioration in a wide range of foods (del Campo et al. 2010).
The HMF formation is greater in the semi-dry method than in other fermentation processes due to sugar dehydration (Pereira et al. 2020). However, the degradation of these compounds was observed in the yeast fermentation and occurred faster when there is sugar in the must (Akillioglu et al. 2011; Feldman et al. 2015).

In the fully washed, the coffee grains are left to rest for a spontaneous fermentation to occur, without adding water (Pereira et al. 2020). The major loss of biomass in this process must be due to the consumption of organic matter by microbial respiration and/or fermentation (Bytof et al. 2007).

The degradation and formation of chemical compounds by processing (Figs. 1 and 4) and roasting of the grains produce the coffee flavor (Sunarharum et al. 2014). The trigonelline and lipids degradation had been observed washed fermentation (De Bruyn et al. 2017; Leloup et al. 2005). The impact of the roasting on flavor is due to the Maillard reactions, breakdown of amino acids, and degradation of trigonelline, quinic acid, pigments, and lipids (Sunarharum et al. 2014).

In yeast fermentation, the chemical discrimination of coffee was due to caffeine and trigonelline (Fig. 4). These two compounds are responsible for the bitterness and astringency of coffee beverages (De Bruyn et al. 2017).

The quinic acid had no significant contribution to the chemical discrimination of coffee after the fermentation, which may be due to its degradation by microorganisms of the must (Figs. 1 and 5). The degradation of this acid during fermentation of the green coffee beans may be linked to fungal metabolism (Lee et al. 2016). However, the decrease level of this compound was also observed during the immersion of the coffee grains in water for fermentation (De Bruyn et al., 2017; Lee et al., 2016). Furthermore, De Bruyn et al. (2017) also observed that the concentrations of citric acids, quinic acid, caffeine, and trigonelline were greater before than after the soaking step. Thus, upstream, and downstream fermentation influenced the chemical composition of the coffee.

During coffee fermentation, potentially lactic bacteria can decompose phenolic compounds to obtain carbon and energy sources. The metabolism of hydroxycinnamic acids through the activities of the enzymes acid phenol decarboxylases and reductases was confirmed after 24 hours of fermentation by heterofermentative lactic acid bacteria (Filannino et al. 2014).

In the wet processing of coffee grains, the acidification of must was due to the accumulation of lactic acid and acetic acid produced by lactic acid bacteria belonging to the taxa *Lactococcus sp.*, *Leuconostoc sp.*, and *Weissella sp.* of the mucilage (De Bruyn et al. 2017). Thus, more controlled studies need to be applied for a broader understanding of microbial, biochemical, chemical, and sensory processes regarding this method.

The sensory data show that the processing of Cherry coffee was no a determining factor for the chemical and sensory composition of coffee drinks (Table 2). The planting altitude had a higher contribution in the composition of organic acids and volatile compounds of the *C. canephora* than processing by dry
method (Pereira et al. 2021). However, the microbiota of the planting region and physical and chemical conditions of the processing had important contributions in these data that corroborate with the hypothesis established by De Bruyn et al. (2017). According to Veloso et al. (2020), studies on the microbiota of coffee have addressed its role during the fermentation process, however, the knowledge of indigenous microorganisms harbored in fruits and soil of coffee trees growing in fields are essential, as they can contribute to fermentation. Furthermore, the research of the coffee ecosystem contributes to a better understanding of a state-of-the-art framework for the further analysis and subsequent control of this complex biotechnological process. Microorganisms from the fruit, seed, handlers, water and processing machinery can all seed the fermentation and have the potential to affect the sensory and chemical quality of the coffee.

The washed and semi-dry process and sensory attributes overall and uniformity were the variables that most contributed to the discrimination for sensory of coffee after fermentation (Fig. 5). Sensorial results addressed by Pereira et al. (2020) indicate that in high altitude areas, the semi-dry method is capable of producing coffees with different sensory profiles in the same way as the washed method. The overall can be directly influenced by the preference of Q-graders, while, the uniformity indicates a good consistency of the coffee drink. The application of the semi-dry method has been described by the high standard of sweetness and harmony between the sensory attributes (Poisson et al. 2009). Furthermore, sucrose content in coffee seeds processed by the semi-dry method was significantly higher than in those processed by the wet method (Duarte et al. 2010).

From the perspective of the production of specialty coffees, it is important to understand in depth the maximum variables that are inherent in the definition of a good coffee aiming at a relationship between applied technologies, processing, fermentations, and edaphoclimatic conditions aiming at a broader understanding of the interactions that are possible in the course of producing specialty coffees. Furthermore, the interactions between soil, fruit, altitude, and slope exposures concerning the sun are important to understand the microbiome in coffee (Veloso et al. 2020).

The results of this study indicate that the chemical discrimination of the coffee is dependent on the planting altitude and the two distinct scientific trends regarding the impact of fermentation on the chemical, nutritional, and sensory quality of the coffee are true. Both spontaneous and induced fermentations to contribute the chemical and sensory quality do the coffee drink. Furthermore, coffee sensory scores are dependent on planting and fermentation methods and NMR and LDA techniques proved to be important in chemical and sensory discrimination of coffees.

Therefore, future studies need to demonstrate the interactions between anabolism and catabolism during fermentation processes, in association with chemical and sensory interaction, aiming at a real understanding of the quality expressed in the coffee cup.

Declarations

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Declarations

The authors declare no conflict of interest. This article does not contain any studies with human participants or animals performed by any of the authors.

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**Figures**

| Assignment            | Chemical shifts region (ppm) |
|-----------------------|-----------------------------|
| 1 Lipids              | 1.01 - 0.76                 |
| 2 Lactates            | 1.43 - 1.27                 |
| 3 Lipids              | 1.65 - 1.54                 |
| 4 Quinic and chlorogenic acids | 2.13 - 1.95          |
| 5 γ-butyrolactone     | 2.28 - 2.13                 |
| 6 Citrate and malate  | 2.97 - 2.60                 |
| 7 Caffeine             | 3.48 - 3.26                 |
| 8 Sugars (caffeine in 3,87) | 4.50 - 3.52           |
| - Maleic acid pattern | 6.70 - 6.16                 |
| 9 chlorogenic acids   | 7.70 - 6.70                 |
| 10 Caffeine            | 7.90 - 7.78                 |
| 11 Trigonelline       | 8.14 - 7.90                 |
| 12 Formic acids       | 8.51 - 8.35                 |
| 13 Trigonelline       | 8.91 - 8.73                 |
| 14 Trigonelline       | 9.20 - 9.02                 |
| 15 5-hydroxymethylfurfural (HMF) | 9.50 - 9.39          |

**Figure 1**

Spectrum and integration regions of the Nuclear magnetic resonance. The chemical compounds identified in the coffee samples are numbered from 1 to 15.
Figure 2

Linear Discriminant Analysis of the chemical composition of Cherry coffee of different altitudes (826 to 1078.08 m). The clusters (A) are based on 8 planting altitudes and 15 chemical compounds (B) of the Nuclear magnetic resonance spectrum (Figure 1).

Figure 3

Linear Discriminant Analysis of the chemical composition of Cherry coffee of different altitudes (826 to 1078.08 m). The clusters (A) are based on 8 planting altitudes and 8 sensory attributes (B).
Figure 4

Linear Discriminant Analysis of the chemical composition of Cherry coffee of different altitudes (826 to 1078.08 m) after fermentation. The clusters (A) are based on 5 fermentations and 15 chemical compounds (B) of the Nuclear magnetic resonance spectrum (Figure 1).

Figure 5

Linear Discriminant Analysis of the chemical composition of Cherry coffee of different altitudes (826 to 1078.08 m) after fermentation. The clusters (A) are based on 5 fermentations and 8 sensory attributes (B) of the Nuclear magnetic resonance spectrum (Figure 1).

Supplementary Files

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