Evaluation of differences in the antioxidant capacity and phenolic compounds of green and roasted coffee and their relationship with sensory properties.

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Abstract

This study aimed to identify the main compounds and sensory attributes found in green and roasted coffee brews. To this end, sensory analysis techniques and a sensory discrimination test were conducted, and antioxidant capacity and individual phenolic compounds were analyzed. Multivariate statistical analysis was then conducted to identify characteristic compounds and sensory attributes. Antioxidant capacity assays did not show any significant differences between green and roasted coffee brews. However, both the individual phenolic and sensory profiles of green and roasted coffee brews were significantly different. Finally, we were able to identify through multivariate analysis, the sensory attributes and phenols that characterize each type of coffee. In this sense, green coffee brews are characterized by floral, and thin aqueous flavors, whereas, roasted coffee brews are characterized by flavors of chocolate and caramel, and creamy and intense flavors.

Keywords: Sensory analysis; Green coffee; Roasted coffee; Phenolic compounds; Multivariate analysis

1 Introduction

Coffee is one of the most consumed beverages worldwide and is ranked as the second most traded commodity after petroleum (Getachew & Chun, 2016; Şemen, Mercan, Yayla, & Açıkkol, 2017). Since the early ages,

coffee has been related to health and it remains a frequently studied item in recent times in research projects related to chronic diseases (Galluzzi Bizzo et al., 2015). The protective role of coffee on health is thought to be mostly related to its high antioxidant capacity and is also linked to its high consumption (Saura-Calixto & Goñi, 2006). Coffee brews have a wide range of antioxidant compounds such as different types of phenolics (hydroxycinnamic acids such as caffeic, ferulic, coumaric and chlorogenic acids), aromatic compounds and Maillard reaction products such as melanoidins (Pastoriza & Rufián-Henares, 2014). Phenolic compounds, for instance, have been reported to exert a protective role against several diseases such as cardiovascular or neurodegenerative diseases and cancer thanks to their ability to protect cells against oxidation (Galluzzi et a., 2015).

On the other hand, *Coffea arabica* is not only beneficial as a result of its potential health effects, but also due to its sensory properties (Philippe, Benoít, & Hervé, 2009, pp. 525–543). This makes sensory analysis one of the most important techniques for assessing coffee quality. However, the flavor of coffee and its other distinctive sensory qualities can be very different from one place to another depending on coffee genetic strain, geographical location, exposure to a unique climate, agricultural practices and coffee variations resulting from processing after harvest (Sunarharum, Williams, & Smyth, 2014). Accordingly, coffee sensory evaluation should be carried out by especially trained tasters (Bhumiratana et al., 2011; Ribeiro et al., 2017). Further, in order to properly achieve a standardized evaluation, in 1982, the Specialty Coffee Association of America (SCAA) came up with standards for evaluating the quality of coffee beverages (Association of America, 2003).

Currently, coffee is mostly consumed roasted in the form of a drink. Roasting involves high temperature treatments which prompts non-enzymatic browning reactions, polymer breakdown (proteins, fats, carbohydrates), polyphenol breakdown and other chemical changes (Wei & Tanokura, 2015, pp. 83–91). In the case of phenolic compounds, this process causes a significant degradation of chlorogenic acids with the simultaneous formation of new antioxidants such as those produced during the Maillard reaction (Budryn, Nebesny, & Oracz, 2015). Thus, it is a process that changes the color, flavor and odor of green coffee beans, and could even modify their biological activity (Zain, Baba, & Shori, 2018). Nevertheless, nowadays, green coffee is receiving considerable attention because of its potential health benefits, which are currently under discussion (Onakpoya, Terry, & Ernst, 2011; Şemen et al., 2017). It is, therefore, convenient to characterize the sensory attributes, antioxidant capacity and phenolic profile of green and roasted coffee brews.

Accordingly, the aim of the present research was to identify the main compounds or sensory attributes characterizing green and roasted coffee. For this, a descriptive analysis of the sensory profiles of coffee drinks was carried out by professional testers, and antioxidant capacity and individual polyphenols were measured and analyzed using multivariate statistical analysis.

2 Materials and methods

2.1 Reagents, standards and solvents

Trolox ((±)-6-Hydroxy-2,5,7,8-tetramethylchromane-2-carboxylic acid), 2,2′-Azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) diammonium salt, 2,4,6-Tri(2-pyridyl)-*s*-triazine (TPTZ), potassium persulphate, caffeic acid, dimethyl caffeic, chlorogenic acid, ferulic acid, coumaric acid, gallic acid, tyrosol, p-hydroxybenzoic acid, m-hydroxyphenylacetic acid, Folin-Ciocalteu reagent, sodium acetate, and ethanol were purchased from Sigma-Aldrich (Darmstadt, Germany).

2.2 Coffee samples

Two types of coffee samples were analyzed, green coffee (*Coffee arabica*) from Colombia (n = 12) and roasted coffee (*Coffee arabica*) from Colombia (n = 12). Coffee samples were purchased from Cafés Cumbal S.L. (Granada, Spain) and kept in storage in their respective sealed containers whilst awaiting analysis. This avoided the loss of volatile compounds.

Samples were prepared according to standards of the International Organization for Standardization for the preparation of samples for the sensory analysis of green coffee (ISO, 2008: 2008). Different established norms and protocols were also used (Association of America, 2003; ISO, 2003; ISO, 2004; ISO, 2005a, b; ISO, 2012a, b).

Coffee milling was performed for 15–30 min before brewing. This was performed for green coffee brew roasted coffee brew separately, and for a combination of the two. Coffee brews were prepared as follows: 6 g of ground coffee were mixed with 100 mL of low mineralization water (100–200 mg/L) filling only 2/3 of the cup. These samples were stored until further analysis. In order to avoid fatigue in the panelists, a maximum of 5 samples per session were evaluated.

2.3 Antioxidant capacity

The antioxidant capacity of green and roasted coffee samples was estimated using two different methods: The ABTS assay was conducted as described by Re and colleagues (Re et al., 1999) with slight modifications. The FRAP assay was measured following methods proposed by (Benzie & Strain, 1997).

Total phenolic compound content was measured following the procedure of Folin-Ciocalteu, with some modifications (Moreno-Montoro, Olalla-Herrera, Gimenez-Martinez, Navarro-Alarcon, & Rufián-Henares, 2015).

All experiments were carried out in triplicate. Antioxidant capacity was expressed as mmol Trolox equivalents/L of coffee in line with FRAP and ABTS methods, and in mg Gallic acid equivalents/L in line with the Folin-Ciocalteu method.

2.4 Individual phenolic compounds

A slightly modified version of the UPLC-Q-TOF-MS method (Rivera-Dominguez, Yahia, Wlodarchak, & Kushad, 2010; Rueda, Cantarero, Seiquer, Cabrera-Vique, & Olalla, 2017) was used to quantify phenolic compound content (Muñoz et al., 2018). ESI-MS2 experiments were performed with a hybrid mass spectrometer (SYNAPT G2 HDMS Q-TOF) with UPLC liquid chromatography system. UPLC separation and mass spectrometer conditions were the same as those previously used by (Muñoz et al., 2018).

Phenolic compounds were quantified with 0.5–50 ppm concentration standards and masses were compared with those reported by previous authors. MassLynx V4 software (Waters Laboratory ISO, 2008) was used for instrument control, data acquisition and data analysis. A calibration curve was made for each phenolic compound with a linearity of $R2 \geq 0.99$. All experiments were carried out in triplicate.

2.5 Sensory evaluation

The materials used for tasting were as follows: temperature resistant conical ceramic cups with a minimum capacity of 150 mL and a maximum of 250 mL, a stainless-steel spoon, odor-free paper, and a cleaned and odor-free water heater that was suitable for boiling water. All materials were washed with neutral soap.

Tastings took place in a well ventilated and illuminated room, without surrounding smells or noise in order to facilitate tasters' concentration. Each respondent was given mineral water (this was also used to prepare coffee brews) in a glass (at room temperature) to rinse their mouth before and after testing. Sensory analysis was performed by trained panelists.

2.6 Sensory profiles

A descriptive analysis was carried out to evaluate and characterize the sensory attributes of green coffee and roasted coffee. A well-trained sensory panel responded to numerical scales, allowing the statistical treatment of results. ISO (2003) methodology was followed. This enables description and evaluation of the olfactory-gustatory properties of a product in a way that can be reproduced. According to this method, the attributes that contribute to the overall impression of the product are identified separately and the intensity of each one is evaluated in order to establish a description of these properties. The ISO (2012a) standard was applied with regards to qualification level, selection and skills. All tasters (a minimum number of 5–8) held a similar qualification level and were chosen after receiving training from a group of experts in this type of tests. For the selection of descriptors, the "independent" method was followed (it is not necessary to reach a consensus). For this method, tasters discuss the olfactory-gustatory properties of the product within the group and then independently record their perceptions. Samples were evaluated by 12 panelists (7 men and 5 women). First, cups containing ground coffee were placed on the panelists' table so that the aroma could be evaluated before the water was poured. The water was heated below boiling point (85–94 °C) and cups were then filled, allowing the infusion stand for 3–5 min. Next, the surface crust was broken with the tasting spoon and was gently stirred to allow sedimentation. Following this, the aroma was re-evaluated.

Following 10 min of infusion, the coffee was tasted with the help of the spoon, perceiving the different flavors and taste sensations. The evaluation ended when the temperature reached approximately 20 °C.

Sensory attributes were evaluated in order of perception: olfactory perception (intensity, harmony, persistence, floral, fruity, caramel, chocolate, nuts and spices) and gustative perception (sweet, salty, sour, bitter, astringent, intensity, harmony, persistence, watery/thin, rough, creamy, thick/meaty and heavy). Finally, a global assessment was made.

For the evaluation of these parameters, a graphic structured numerical (0–5) scale and semantic descriptors (not perceptible, begins to be perceived, weak, moderate, strong, very strong) were used.

2.7 Discrimination testing

Discriminative tests are used to establish whether or not an overall difference exists between two or more samples. There are a large number of these types of tests but the triangle test (used in this work) is the most known. This test consists of an evaluation of three coded products. The taster must indicate which two are most similar and which one is the most different. It is a procedure of forced choice and is applicable when there are differences in a single sensory attribute or in several sensory attributes. The test was carried out according to ISO (2004). This regulation regulates general testing conditions, qualification level and number of judges, test procedures, and analysis and interpretation of results. Two samples were evaluated; one composed of 100% roasted coffee and another composed of roasted coffee containing 20% green coffee. The objective of this test was to examine whether the panelists were able to differentiate between the two samples. Panelists received a set of 3 samples: two being identical and one being different (panelists were informed about this arrangement). After testing the samples from left to right, each panelist indicated which one they considered to be different from the

others. The preparation of the samples was identical (same coffee machine, same cups and equal amounts of coffee) and was carried out in the absence of the tasters. The plastic cups containing the coffee samples were coded uniformly using 3-digit combinations which were chosen at random for each test. A form was given to panelists to describe the differences/attributes found in each sample.

For both tests (descriptive analysis and discrimination test), results were expressed following evaluation of the samples using proper administration of the SCAA Evaluation Form (Association of America, 2003).

2.8 Statistical analyses

Statgraphics Plus software (Statpoint Technologies, Inc., The plains, USA), version 5.1 (2001) was used to check normal distribution of the results through the Kolmogorov Simirnov test, with a significance level of 95%. The Levene test was used to check homogeneity of variances, with significance being set at $p > 0.05$. Analysis of variance (ANOVA) was performed and the significance level was set at $p < 0.05$.

Statistical sensitivity of the triangle test is interpreted as a function of 3 values: risk α (probability of falsely concluding that a perceptible difference exists), risk β (probability of falsely concluding that there is no discernible difference) and pd (proportion of the population of judges capable of distinguishing between the two products). These aforementioned values were, therefore, adjusted before carrying out the test. Once values for pd, α and β had been established according to ISO (2004) (Table 1) guidelines regarding the number of judges needed to conduct the triangle test, it was concluded that at least 15 panelists would be necessary and, in the end, 18 panelists were selected.

alt-text: Table 1

Table 1

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Number of panelist needed for a triangle test.

α	P_D	β				
		0.2	**0.1**	**0.05**	**0.01**	**0.001**
0.20	50%	7	12	16	25	36
0.10		12	15	20	30	43
0.05		16	20	23	35	48
0.01		25	30	35	47	62
0.001		36	43	48	62	81

Multivariate statistical analysis was conducted to identify the key attributes of green and roasted coffee. Exploratory methodology (principal components analysis (PCA)), interpretative methodology (permutational multivariate analysis of variance (PERMANOVA), canonical correspondence analysis (CCA)) and

discriminatory methodology (Orthogonal projections to latent structures discriminant analysis (OPLS-DA)) were carried out. All analyses were carried out in R version 3.5.0.

3 Results and discussion

3.1 Antioxidant activity

Antioxidant capacity was estimated through ABTS and FRAP methods. This also involved the Folin-Ciocalteu assay in order to measure total phenolic content as it is based on antioxidant reactions.

According to the present results shown in Table 3, roasted coffee tended to have greater antioxidant properties and to have higher total phenolic content than green coffee (Fig. 1**).** However, no significant ($P < 0.05$) differences were found for any of the tests mentioned. Comparisons between green and roasted coffee antioxidant capacity have been previously reported. However, the results reported in such research studies are contradictory. Some authors have found green coffee to have greater antioxidant properties than roasted coffee due to the loss of bioactive compounds during roasting (Perrone, Farah, & Donangelo, 2012). On the other hand, Liang, Xue, 2016 found that roasted coffee, in fact, had greater antioxidant capacity than green coffee. Such disagreement could come from the complexity of the chemical reactions involved in the roasting process. During roasting, some green coffee compounds are degraded. Degraded compounds are mostly phenolic compounds such as chlorogenic acids, although these can also be incorporated into melanoidins, which in turn could reduce antioxidant capacity (Perrone et al., 2012). On the other hand, such degradation also involves a corresponding release of hydroxycinnamates and quinic acid (Wei & Tanokura, 2015, pp. 83–91). Moreover, the Maillard reaction takes place due to the high temperatures applied, giving rise to a plethora of compounds which can also contribute to antioxidant capacity (Pastoriza & Rufián-Henares, 2014). Accordingly, all of the compounds that appear during roasting could compensate for the loss of some other substances or even increase antioxidant capacity (Ludwig, Bravo, De Peña, & Cid, 2013).

alt-text: Table 3

Table 3

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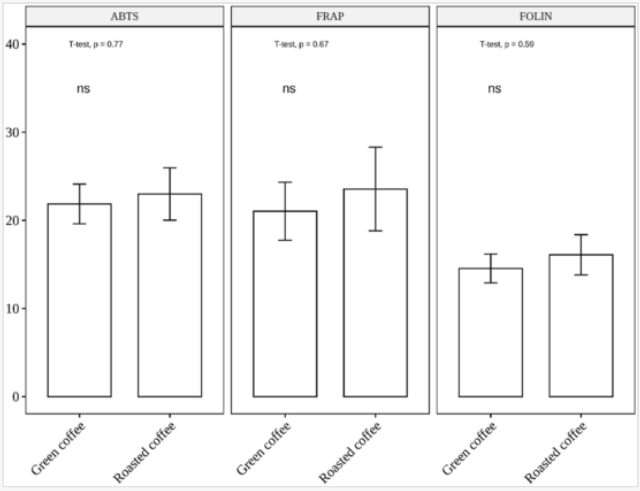
Statistically data to antioxidant activity by ABTS, FRAP and Folin assays in green and roasted coffee.

Antioxidant capacity	Green Coffee (n = 12)		Roasted Coffee (n = 12)	
	Mean (SD)	Range	Mean (SD)	Range
ABTS (mmol Trolox/L)	21.87 (7.78)	7.41–31.44	22.98 (10.28)	6.76–33.28
FRAP (mmol Trolox/L)	21.04 (11.43)	6.26–43.66	23.55 (16.43)	6.13–62.37
Folin (mg Gallic acid/L)	2473.21 (968.38)	990.07–3527.43	2737.14 (1348.58)	884.09–4854.91

SD: standard deviation.

alt-text: Fig. 1

Fig. 1



Bar charts showing antioxidant capacity (ABTS and FRAP) and total phenolic (Folin-Ciocalteu) content. ABTS and FRAP values are expressed as mmol of Trolox/L, and FOLIN values are expressed as mmol of Gallic acid/L. Statistical significance was examined using t-tests with green coffee acting as the reference group. ns - non-significant.

3.2 Individual phenolic compounds

The content of hydroxybenzoic acids, hydroxycinnamic acids, tyrosols and other phenolic compounds determined in the samples it is show in Table 4 and it is depicted in Fig. 2.

alt-text: Table 4

Table 4

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Content of individual phenolic compounds of green and roasted coffee (mg/L).

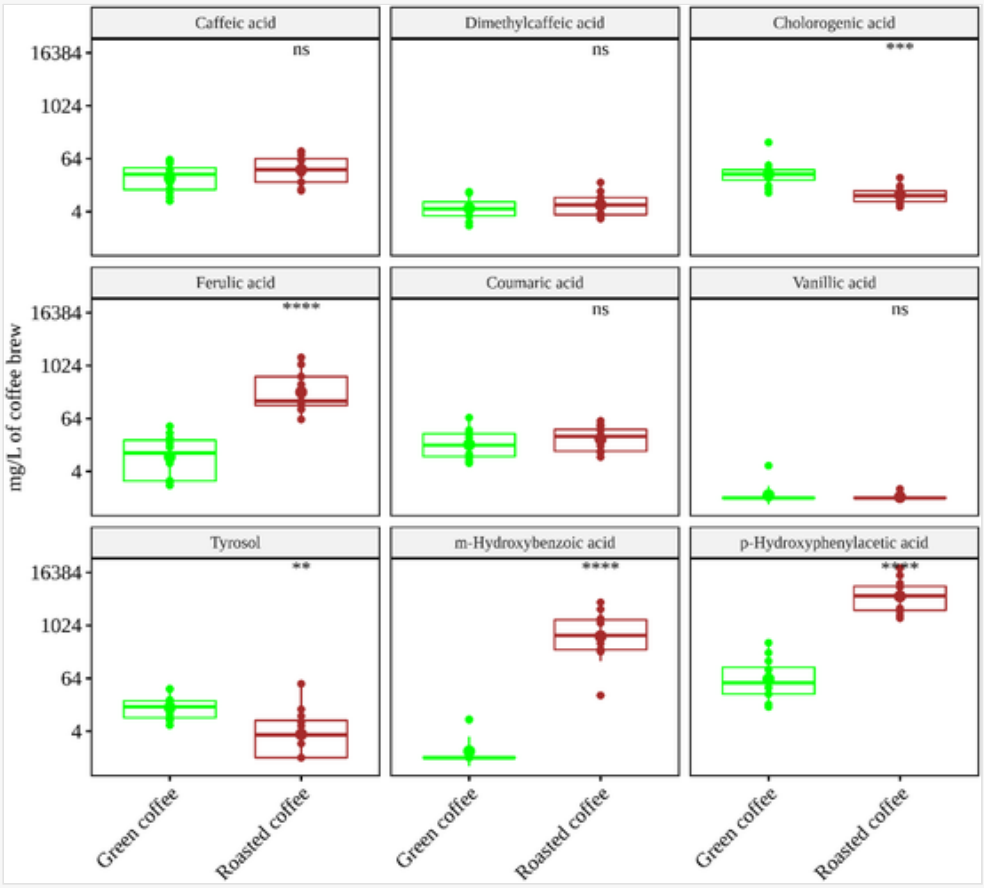
Phenolic compounds	Green Coffee (n = 12)		Roasted Coffee (n = 12)	
	Mean (SD)	Range	Mean (SD)	Range
Hydroxybenzoic acids				
m-Hydroxybenzoic acid	1.06 (2.49)	0.00–6,50	1020.47 (1017.01)	25.19–3428.53
Vanillic acid	0.37 (1.27)	0.00–4.40	0.05 (0.17)	0.00–0.59
Hydroxycinnamic Acids				
Caffeic acid	28.11 (18.93)	5.99–60.34	44.50 (30.19)	10.95–93.64
Dimethyl caffeic acid	4.63 (3.41)	0.89–10.25	5.84 (4.62)	1.76–17.41
p-cumaric acid	20.33 (17.42)	5.17–65.83	25.22 (15.95)	7.51–55.68
Ferulic acid	13.16 (13.03)	1.25–41.69	421.81 (470.38)	60.15–1568.85

Chlorogenic acid	26.28 (40.11)	1.45–149.75	9.50 (5.23)	4.12–22.62
Tyrosols				
Tyrosol	15.58 (10.69)	4.46–36.15	6.91 (13.21)	0.00–47.05
Hydroxyphenylacetic acids				
p-Hydroxyphenylacetic acid	102.86 (118.50)	13.28–410.83	6585.21 (5809.53)	1502.24–20543.40

SD: standard deviation.

alt-text: Fig. 2

Fig. 2



Concentration of individual phenolics found in green and roasted coffee brews. Statistical significance was examined using t-tests with green coffee acting as the reference group. ns – not-significant, * -$p < 0.05$, ** -$p < 0.01$, *** -$p < 0.001$, **** -$p < 0.0001$. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

According to the present results, roasted coffee tended to contain more hydroxycinnamic acids than green coffee, although differences were only significant ($p < 0.05$) in the case of ferulic acid. On the other hand, chlorogenic acid was found in significantly ($p < 0.05$) higher concentrations in green coffee. As mentioned above, during roasting, quinic acid and hydroxycinnamates concentrations increase due to the degradation of chlorogenic acids. This has also been seen in previously reported findings (Wei & Tanokura, 2015, pp. 83–91). However, excessive roasting could also lead to a decrease in such hydroxycinnamates, resulting in the formation of lactones (Wei & Tanokura, 2015, pp. 83–91).

In relation to hydroxybenzoic acids, m-hydroxybenzoic acid was found in significantly larger concentrations in roasted coffee than in green coffee ($p < 0.05$). Vanillic acid was more abundant in green coffee, although this was not seen to be a significant finding. In the case of p-hydroxyphenylacetic acid, significantly greater concentrations were detected in roasted coffee.

3.3 Sensory evaluation

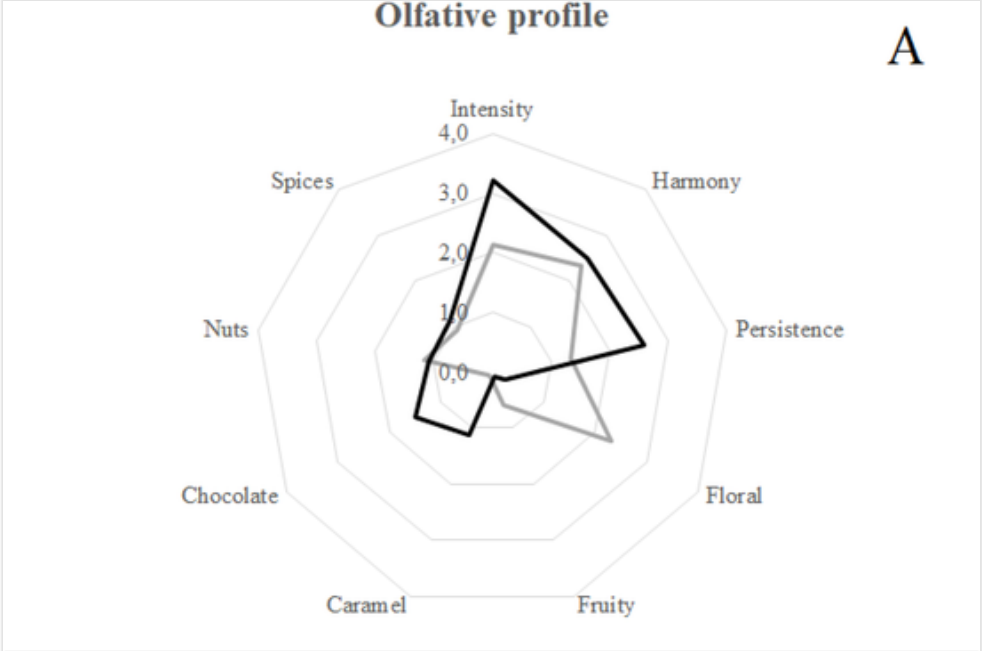
3.3.1 Sensory profiles

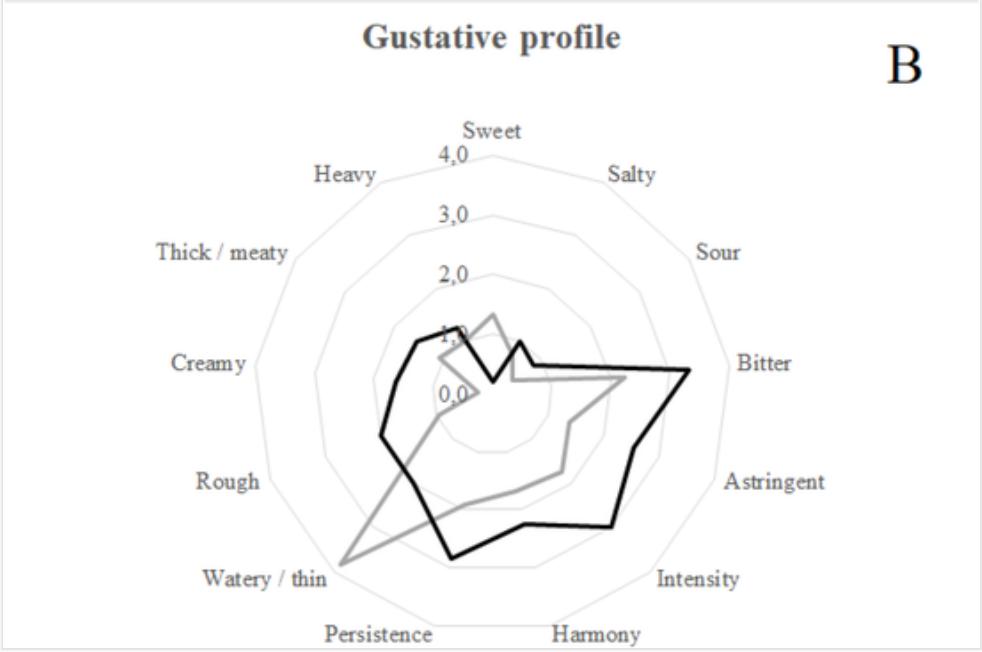
Authors such as Feria-Morales (2002), argue that a number of essential aspects should be considered in order to improve current procedures from a sensory point of view. These aspects include mandatory use of trained sensory panels, totally blind tasting, identifying the key attributes of different types of coffee products and expanding the approach to include evaluation of the acidity and body of green coffee. Some of these aspects will be discussed in the present article.

Mean values for each attribute of the olfactory and gustative profile are shown in Fig. 3.

alt-text: Fig. 3

Fig. 3


Olfative profile
A
Intensity
4,0
3,0
2,0
1,0
0,0
Harmony
Persistence
Floral
Fruity
Caramel
Chocolate
Nuts
Spices


Gustative profile
B
Sweet
4,0
3,0
2,0
1,0
0,0
Salty
Sour
Bitter
Astringent
Intensity
Harmony
Persistence
Watery / thin
Rough
Creamy
Thick / meaty
Heavy

Descriptive sensory analysis of A) olfactory and B) gustative profiles.

With regards to olfactory perception, green coffee samples recorded higher scores than roasted coffee samples for floral, fruity and nutty aromas. However, green coffee also achieved lower scores for caramel and chocolate aromas. As was expected, green coffee was characterized by aromas related to the plant origin, such as flowers, fruits and vegetables. This is corroborated by other authors (Preedy, 2014). In consideration of the gustative profile, green coffee brews achieved higher scores for watery/thin and sweet attributes. However, they achieved lower scores for roughness, persistence and intensity. Roasted coffee samples were characterized by the attributes of flavor persistence, intensity and bitterness.

On the other hand, roasted coffee brews were found to have higher scores for attributes such as caramel and chocolate, despite these being aromas related to roasting. Roasting is a very complex process, involving high temperatures and different physicochemical reactions which prompt deep changes in coffee composition. Thus, roasting has been pointed out as the main factor to influence coffee flavor (Toledo, Pezza, Pezza, & Toci, 2016). Some volatile compounds appear during this process which are responsible for aromas of caramel, chocolate and spice, whilst non-volatile compounds also appear which are responsible for gustative attributes such as astringency, bitterness and sweetness. The main reactions involved during roasting are the Maillard reaction and pyrolysis reactions. During roasting many different compounds appear: pyrazynes, furans, volatile phenolic compounds, etc. Pyrazynes are responsible for roasted and nutty flavors, whilst furans are responsible for sweet/almond, caramel, spicy flavors, and volatile phenolics are responsible for phenolic/cravo/astringent flavors (Toledo et al., 2016).

Further, the relationship between the presence of chlorogenic acid and the increase in astringency has been previously described (Di Donfrancesco, Gutierrez Guzman, & Chambers, 2014). During roasting, quinic acid and caffeic acid increase due to the degradation of chlorogenic acids. If the roasting process is excessive, higher amounts of such compounds are formed, resulting in excessive bitterness and astringency (Rostagno, Celeghini, Debien, Nogueira, & Meireles, 2015; Wei & Tanokura, 2015, pp. 83–91). Accordingly, roasted coffee was evaluated as being more acidic, bitter, rough, creamy, thick and heavy.

Correspondingly, green coffee brews showed significantly ($p < 0.05$) higher floral, sweetness, and aqueous attributes, whereas roasted coffee brews showed significantly ($p < 0.05$) higher scores for intense, persistent, caramel, chocolate, astringent, rough, and creamy attributes.

3.4 Discrimination test

Analysis of the data obtained in the triangle test was carried out according to the table provided by the ISO, 2008 (2004) regulation (Table 2). Given that there is a minimum requirement for the number of correct answers necessary to conclude that two samples are similar, when the number of correct answers given was less than or

equal to the number indicated (corresponding to the number of evaluators, risk level β and the pd value chosen for the test), it was concluded that there was no significant difference between the samples.

alt-text: Table 2

Table 2

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Maximum number of correct answers necessary to conclude that two samples are similar.

N	B	P_D				
		10%	20%	30%	40%	50%
18	0.001	0	1	2	3	5
	0.01	2	3	4	5	6
	0.05	3	4	5	6	8
	0.10	4	5	6	7	8
	0.20	4	6	7	8	9

In the present trial, a total of 7 correct answers were obtained. This is lower than the number (8) required by the table of the ISO regulation (for 18 panelists β = 0.10 and pd = 50%), therefore, it was concluded that there were no significant differences between the samples.

Similarly, the upper confidence limit (0.1086) was calculated and, alongside the 90% confidence level, it was deemed that no more than 11% of tasters could distinguish between the samples. This mixture of roasted and green coffee could, therefore, be used interchangeably, even replacing, 100% roasted coffee.

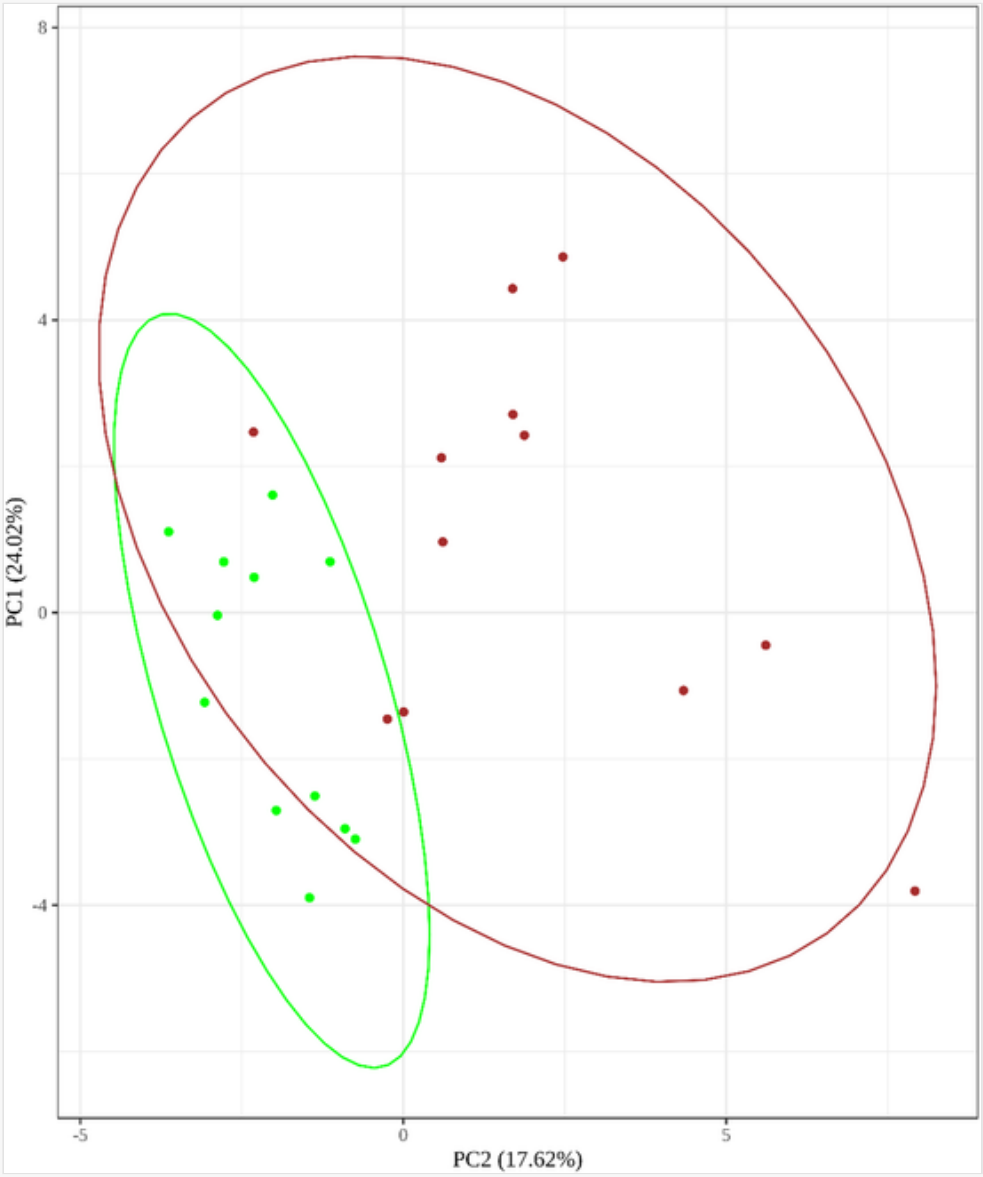
3.5 Multivariate statistical analysis

The statistical analysis conducted aimed to unravel whether green coffee and roasted coffee were significantly different from each other, and to discover which sensory attributes and phenols were more characteristics of each type of coffee brew. Statistical analysis involved exploratory methodology (principal components analysis (PCA)), interpretative methodology (permutational multivariate analysis of variance (PERMANOVA), canonical correspondence analysis (CCA)), and discriminatory methodology (orthogonal projections to latent structures discriminant analysis (OPLS-DA)).

PCA analysis allowed us to explore similarities between samples (Fig. 4). PCA showed some degree of separation between green and roasted coffee samples, explaining 41.64% of the variance with two principal components. PCA told us that green and roasted coffee could in fact be significantly different in relation to sensory attributes, and phenolic and antioxidant profiles.

alt-text: Fig. 4

Fig. 4

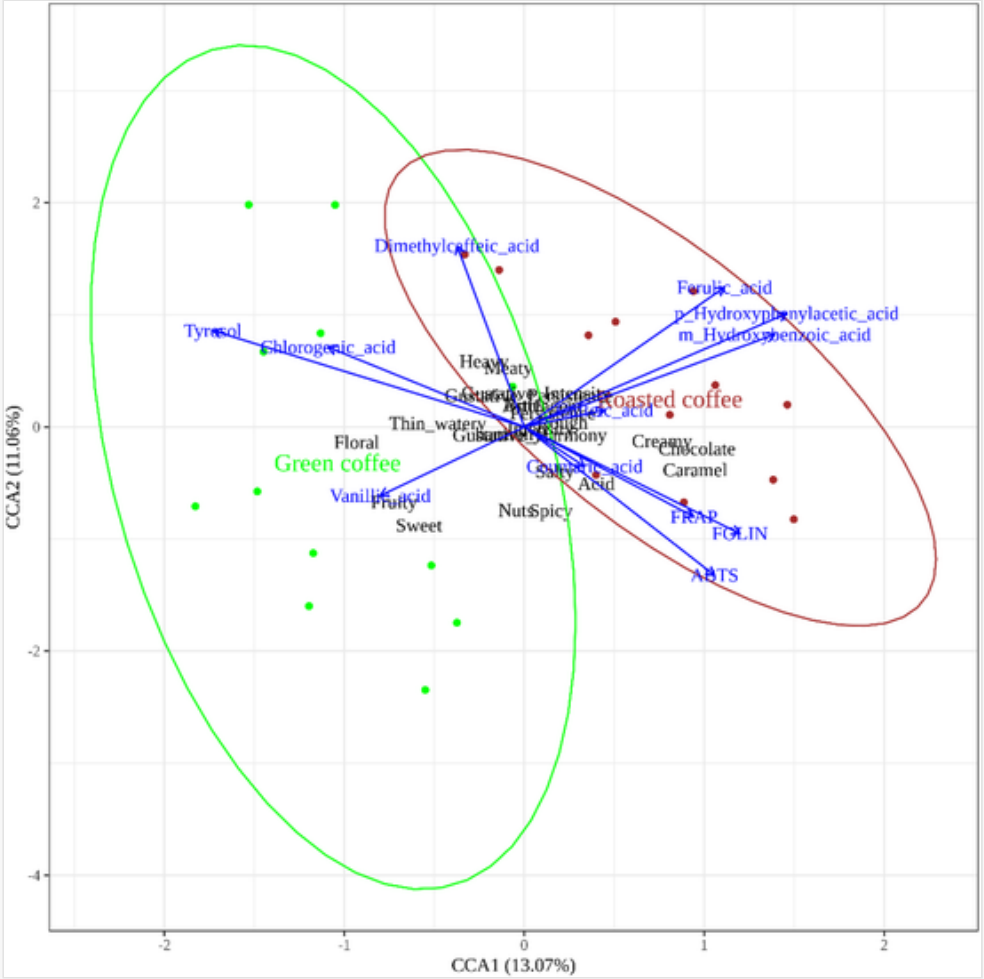


Principal component analysis of green and roasted coffee brews. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

Interpretative multivariate approaches were then applied to examine significance. PERMANOVA showed that green and roasted coffee were, in fact, significantly different ($P < 0.05$) in relation to their sensory and phenolic profiles. CCA was also applied, resulting in similar results to those seen with PERMANOVA. This analysis allowed us to explain the extent to which variation found between green and roasted coffee brews can be explained by differences in sensory attributes and the phenolic profile. Moreover, CCA allowed us to graphically interpret possible relationships between the samples and the variables (Fig. 5). Accordingly, we observed that floral, sweet, fruity and thin aqueous (taste) sensory attributes, and the phenolics tyrosol, vanillic acid and chlorogenic acid were more related to green coffees.

alt-text: Fig. 5

Fig. 5



Canonical correspondence analysis (CCA) of green and roasted coffee brews. Green dots represent green coffee samples and brown dots represent roasted coffee samples. Black letters represent sensory attributes, and blue letters represent antioxidant capacity and phenolic compounds. The direction indicated by the arrows depicts the direction of changes in the variable. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

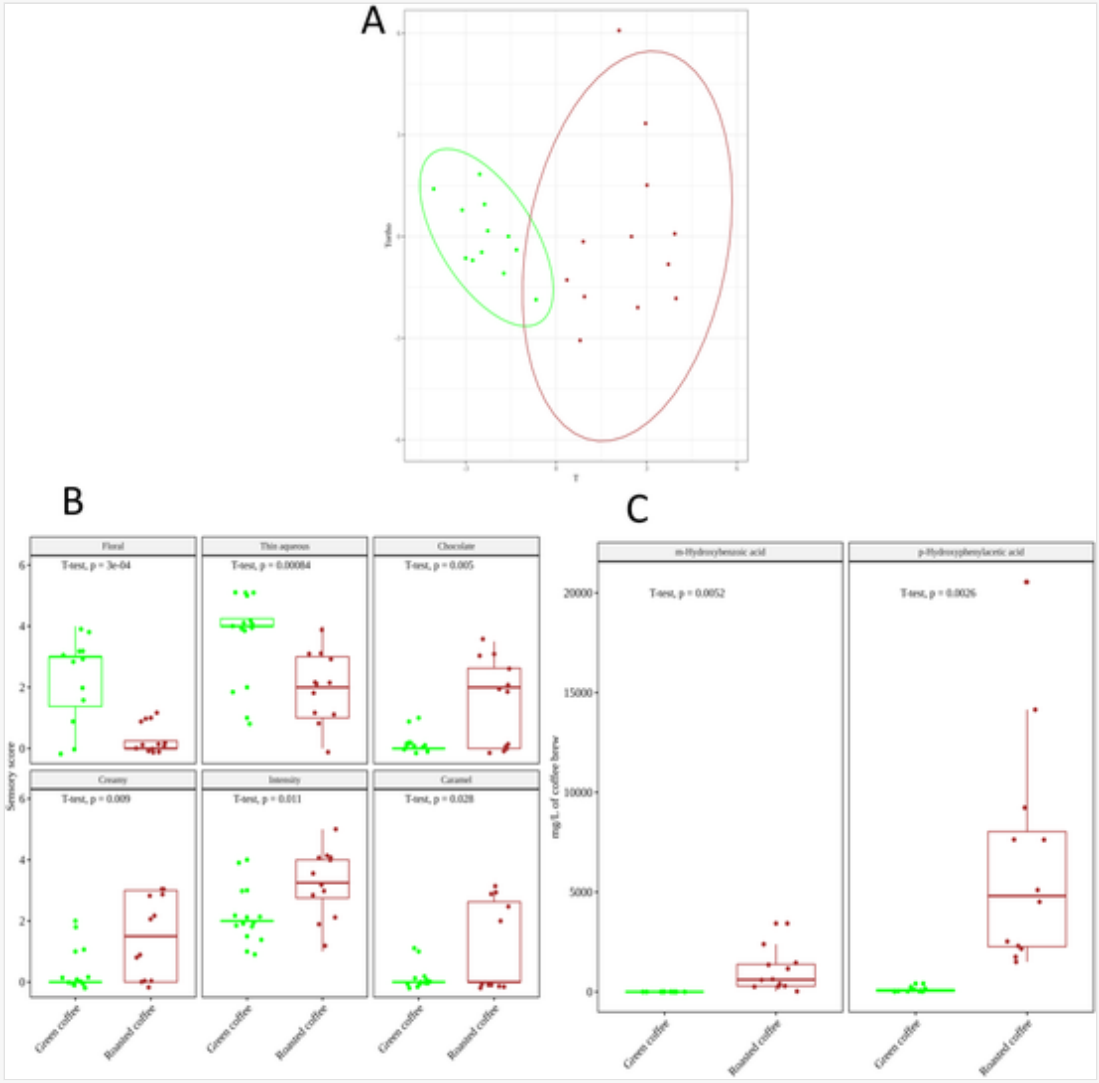
On the other hand, creamy, chocolate and caramel sensory attributes, and the phenolics p-hydroxyphenylacetic acid, m-hydroxybenzoic acid and ferulic acid were more related to roasted coffee. As has been previously described, aromas naturally present in green coffees can disappear during roasting (Ossenblok, 2016; Preedy, 2014). During roasting, not only are some polymers and phenolic compounds degraded into smaller volatile compounds, but the Maillard reaction also takes place. This has a great influence on sensory attributes. These compounds are responsible for some roasted coffee flavors such as spice, caramel, bitterness, astringency, etc. Moreover, during roasting, quinic acid and caffeic acid concentrations increase due to chlorogenic acid degradation. If the roasting process is excessive, higher amounts of such compounds are formed resulting in an excessive bitterness and astringency (Perrone et al., 2012; Rostagno et al., 2015; Wei & Tanokura, 2015, pp. 83–91).

Finally, we applied OPLS-DA, a discriminatory method aiming to maximize the separation of objects amongst different classes and predict response variables from a set of predictor variables. OPLS-DA separated the samples well (R2 = 0.825) achieving a predictive power of Q2 = 0.576 (Fig. 6A). This test allowed us to identify the variables that had a stronger influence on the separation of green and roasted coffee, and thus, the main variables responsible for classifying coffee brews as either green or roasted. Accordingly, creamy,

chocolate, thin aqueous, floral, intense and caramel sensory attributes, and the phenolics p-hydroxyphenylacetic acid and m-hydroxybenzoic acid emerged as the main discriminant variables (Fig. 6B–C).

alt-text: Fig. 6

Fig. 6



A. Orthogonal projections to latent square discriminant analysis (OPLS-DA). Panel A shows the score plot. **B.** Orthogonal projections to latent square discriminant analysis (OPLS-DA). Panel B shows the top six discriminant sensory attributes. **C.** Orthogonal projections to latent square discriminant analysis (OPLS-DA). Panel C shows the top discriminant phenolic compounds. Statistical significance testing using t-tests with green coffee acting as the reference group. ns - non-significant, * -$p < 0.05$, ** -$p < 0.01$, *** -$p < 0.001$, **** -$p < 0.0001$. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

The statistical analysis allowed us to corroborate that green and roasted coffee are, in fact, significantly different ($P < 0.05$) in relation to their sensory attributes and phenolic profile. This analysis also allowed us to identify the most influential variables in this separation of green and roasted coffees.

4 Conclusions

Sensory attributes, antioxidant capacity and phenolic compound content of green and roasted coffee brews were evaluated. Under the extraction conditions, a large number of phenolic compounds and high antioxidant capacity were observed in green coffee. The different phenolic profiles showed green coffee to be a better source of tyrosol and chlorogenic acid, whereas roasted coffee provided higher amounts of ferulic acid, m-hydroxybenzoic

acid and p-hydroxyphenylacetic acid. On the other hand, green coffee brews are characterized by floral and thin aqueous flavors, whereas roasted coffee brews are characterized by chocolate, caramel, creamy and intense flavors. Finally, using multivariate analysis we were able to identify the sensory attributes and phenolic profiles that were most characteristic of each type of coffee. Hence, a multivariate analytical approach could be better than an individual statistical data analysis approach with primitive methods. Thus, the present research shows that identification of the antioxidant properties of both types of coffees and linking them with their sensory qualities, can lead to more satisfying outcomes.

Uncited References

Gotteland and de Pablo, 2007; Jeszka-Skowron et al., 2016; Rufián-Henares and Morales, 2007.

CRediT authorship contribution statement

Adelaida Esteban Muñoz: Conceptualization, Methodology, Validation, Investigation, Data curation, Writing - original draft, Writing - review & editing. **Silvia Sánchez Hernández:** Data curation, Writing - original draft, Writing - review & editing. **Alba Recio Tolosa:** Investigation. **Sergio Pérez Burillo:** Software. **Manuel Olalla-Herrera:** Resources, Supervision, Project administration.

Declaration of competing interest

Conflicts of Interest: No potential conflict of interest was reported by the authors.

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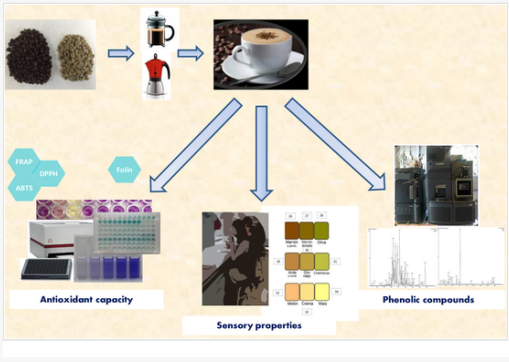
Graphical abstract

alt-text: Image 1



Highlights

- Roasted coffee has a higher antioxidant capacity than green coffee.
- Roasted coffee has a higher total content of phenolic compounds.
- In the gustatory profile, roasted coffee scored higher in 7 descriptors.
- An 80/20% blend of roasted/green coffee is proposed.
- Coffee making conditions its use as a functional food.

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