



Minority compounds and sensory analysis evaluation of *Coffea arabica* var. caturra cultivated in three different altitudinal ranges

Evaluación de los compuestos minoritarios y análisis sensorial de *Coffea arabica* var. caturra cultivado en tres diferentes rangos altitudinales

Jennifer Tatiana Cruz Bolívar¹, Wilson Rodríguez Pérez¹, Juan Carlos Suárez Salazar^{1*}, Claudia Mercedes Ordoñez Espinosa² and Gustavo Adolfo Vega Cano²

¹Universidad de la Amazonia, Florencia – Caquetá, Colombia. ²Centro de Gestión y Desarrollo Sostenible Surcolombiano. Tecnoparque Agroecológico Yamboro, SENA. Pitalito-Huila, Colombia. Author for correspondence: juansuarez1@gmail.com

Rec.: 14.06.2016 Acep.: 29.09.2016

Abstract

The composition of minority compounds in samples of roasted and ground coffee (*Coffea arabica* var. caturra) cultivated in three altitudinal ranges 1300-1400, 1400-1600, 1600-1800 m. a. s. l., in the Huila department of Colombia were determined. The samples were collected in July of 2012. pH, total acidity and total lipids were measured. Subsequently, the composition of total lipids after esterification and gas chromatography analysis coupled to high resolution mass spectrometry (GC-MS) was established. Quality cup test considering the following attributes: fragrance/aroma, taste, residual flavor, acidity, body, uniformity, balance, clean cup, sweetness, quality and note, were performed. No statistically significant difference ($p < 0.05$) in pH, titratable acidity, total time of roasting and cracking time was determined. Significant difference was found in% humidity range: 1300-1400 m relative to the ranges: 1400-1600 and 1600-800 meters. As for the major compounds are predominantly: stigmaterol, sitosterol, 4-methylpentanamide and 2- (2-hydroxyphenyl) buta-1,3-diene, in the altitudinal ranges evaluated. No significant difference ($p > 0.05$) was found in the evaluated attributes at the quality cup test at different altitudinal range.

Keywords: Attributes, GC-MS, pH, quality cup test, total acidity, total lipids.

Resumen

Se determinó la composición de compuestos minoritarios en muestras de café tostado y molido (*Coffea arábica* var. caturra), cultivado en tres rangos altitudinales 1300-1400, 1400-1600, 1600-1800 m. s. n. m., en el departamento del Huila. Se colectaron muestras en Julio de 2012 para analizar características como pH, acidez total titulable y composición de compuesto minoritarios previa esterificación y análisis por cromatografía de gases de alta resolución acoplado a espectrometría de masas. Así mismo, se realizó prueba de calidad de taza considerando los siguientes atributos: fragancia/aroma, sabor, sabor residual, acidez, cuerpo, uniformidad, balance, taza limpia y dulzor. El contenido de humedad para los diferentes rangos de altitud solamente presentó diferencia significativa ($p < 0.05$) a nivel de rango altitudinal. Se identificaron doce compuestos de la fracción insaponificable de café tostado y molido predominando estigmaterol, beta sitosterol, 4-metilpentanamida y 2-(2-Hidroxifenil) buta-1,3-dieno, en los rangos altitudinales evaluados. En la prueba de calidad de taza no se encontró diferencia significativa ($p > 0.05$) en los atributos evaluados variando el rango altitudinal.

Palabras clave: Acidez total, atributos, CG-EM, lípidos totales, pH, prueba de calidad de taza.

Introducción

Coffee is one of the most commercialized agricultural products in the world and consumed by its pleasant aroma that together with its stimulating effect generate great acceptability in the population (Yener *et al.*, 2015). When making a coffee infusion, a variety of chemical compounds responsible for their sensorial quality are extracted, including lipids, which are rich in diterpenes, sterols, tocopherols, phosphatides and waxes (Tryptamine derivatives (Villarreal *et al.*, 2012; Ferrari *et al.*, 2010)). The extraction depends on the temperature, water chemistry and the accessible coffee surface area (Uman *et al.*, 2016). In the coffee non-saponifiable fraction, the diterpenes (Kahweol & cafestol Dias *et al.*, 2013).

Among the methods to obtain the roasted coffee lipid fraction, are the extraction with solvent and supercritical fluid (Hurtado *et al.*, 2016). The coffee lipid fraction constitutes 11 to 20% of green grain, depending on the variety (Al-Hamamre *et al.*, 2010). Intake of lipids from coffee infusions is not a significant source of fat in the human diet, 0.4 g has been reported in five unfiltered daily infusions (Budryn *et al.*, 2012).

These variations in quality are influenced by the availability of oxygen, moisture, exposed surface and temperature in the roasting processes (Pérez-Martínez *et al.*, 2008).

During the coffee grain roasting, these formed carbonyl compounds can react with amino groups and form Schiff bases (Maillard reaction), besides reactions such as depolymerization, pyrolysis, Strecker reaction among others. Some coffee lipid compounds have been used as chemotaxonomic markers. Fatty acids have become chemical descriptors used to differentiate among coffee varieties. Sterols have been used as suitable markers for coffee blending studies (Speer & Kölling-Speer, 2006).

It has been shown that arabica coffee grains cultivated at altitudes between 1020-1200 m. a. s. l., have a positive effect on the final beverage quality, although there is a great dependence on the crop site of origin (Avelino *et al.*, 2005). The chlorogenic acid and fatty acid contents in seeds depend on air temperature, contrary to total lipids, total soluble sugars and polysaccharides in coffee seed, which were not influenced by the climate (Joët *et al.*, 2010). Thus, continuing studies on vegetable lipids (Murcia *et al.*, 2013), The aim of the present research was to Characterize chemically, physically and sensorially samples of coffee (*Coffea arabica var. caturra*) Roasted and ground cultivated in three altitudinal ranges (1300-1400, 1400-1600, 1600-1800 m. a. s. l.)

in coffee farms of the municipality of Pitalito, department of Huila, Colombia.

Materials and methods

Sample collection and treatment

Samples of cherry coffee (*Coffea arabica var. Caturra*), were supplied by farmers from nine farms with commercial coffee plantations in the rural area of the municipality of Pitalito, south side of Huila department, Colombia, in the corregimientos of Brussels and Palestine. The coffee farms were coded as J1, J2 and J3 for the altitudinal range of 1300-1400 m. a. s. l., J4, J5 & J6 for the altitudinal range of 1400-1600 m. a. s. l. and J7, J8 & J9 for the altitudinal range of 1600-1800 m. a. s. l. and selected according to availability of coffee grain for the present study. The samples were pulped using a mechanical demucilaginator and sun-dried on terraces at an ambient temperature between 25-28 ° C, obtaining the dried Pergamino coffee grains. Samples of dried Pergamino coffee, were stored at a temperature of 18-21° C in dark plastic bag. The husk was extracted to the Pergamino coffee grains with the Quantik C-200 thresher and they were toasted in a Quantik TC150AR kiln following the protocol of the Association of Special Coffees of America up to a medium roasting level with an L value of 21, 43 (obtained from the mixture of nine J1-J9 replicates), corresponding to a degree of clear-medium roasting.

Physical, chemical and sensory analysis

In samples of dry Pergamino coffee grains, moisture was measured by the Quantik MH-302 hygrometer before and during roasting, initial temperature (°C), final temperature (°C), cracking time (seconds), total time (seconds) and color, using Quantik IR800 digital colorimeter. Titratable acidity was determined (NTC 5247), pH (Potentiometry, Pereira *et al.*, 2007) and lipid fraction (Soxhlet, Martín *et al.*, 2001). Subsequently, this lipid fraction was mixed with KOH/2N MeOH. The reaction mixture was extracted with benzene and dried with anhydrous sodium sulfate prior to GC-MS analysis considering the methodology suggested by Díaz & Vásquez (2011).

Sensory analysis was performed with the application of the SCAA protocol (Toledo *et al.*, 2016), by Q-grader tasting panel and sensorial attributes were determined as follows: fragrance/aroma, taste, residual taste, acidity, body, uniformity, balance, clean cup, sweetness and final score. Tasting table was composed by twelve coffee samples (two cups per sample)

and were presented only with their codes. The tasting results were recorded in the SCAA format. The final score was calculated by summing the individual scores given for each of the aforementioned attributes and using the quality classification of coffee according to the total score as follows: 90-100% (exceptional), 85-89,99% (excellent), 80-84,99 (very good) y <80,0% Lower than the special quality.

Gas chromatography of high resolution - Mass spectrometry of electronic impact (GC-EI)

GC-EI analysis of the extracted organic phase with benzene was carried out on a gas chromatograph with mass selective detector (Shimadzu QP-2010) in scan mode. The automatic injector system AOC-20i, autosampler with injection AOC-20s *splitless*, direct injection system controlled by computer software. An Agilent HP-5 (5% of fenilmetilsiloxan) capillary column was used with 30 m length and 320 μm of internal diameter and 0.25 μm of film thickness. The entrainment gas used was high purity Helium with a constant flow of 1 mL.min⁻¹. The temperature in the injector and the detector was 350 ° C in each case.

Statistic analysis

For each of the chemical compounds identified by (GC-EI) and sensory attributes of cup quality were performed descriptive statistics (means and variable frequencies) and a means analysis using the Tukey test $P < 0.05$). A principal component analysis was performed (PCA) and Partial least squares regression PLS (*Partial Least Squares*) using the graphic option of Scatterplot Matrix to find the relationships between the compounds identified in the lipid fraction of *Coffea arabica* var. caturra and sensory attributes using the R software version 3.2.3.[®], Throughout the independent platform for statistical analysis R Commander, based on the package FactoMineR[®].

Results and discussion

Physical and chemical characteristics of coffee samples

Table 1, shows the results of physicochemical analysis of ground and roasted Caturra coffee variety samples. The average moisture contents of the dried Pergamino coffee before roasting to different altitudinal ranges studied were as follows: $16.1 \pm 4.90\%$ (Coefficient of variation: 30.4) in the altitudinal range of 1300-1400 m. a. s. l. 7.97 ± 2.67 (33.5) in the altitudinal range of 1400-1600 m. a. s. l. and 8.9 ± 1.0 (11.2) in the altitudinal range of 1600-1800 m. a. s. l., there was a significant difference ($P < 0.05$) among moisture values of the dry Pergamino coffee

samples of the altitudinal range 1300-1400 m. a. s. l. with respect to the other two evaluated altitudinal ranges: 1400-1600 and 1600-1800 m. a. s. l. (which did not present significant difference ($p > 0.05$) each other). The moisture content of the ground and roasted coffee samples from the three altitudinal ranges evaluated in the present study ranged from 0.773 to 1.031%, with no significant difference ($p < 0.05$) among altitudinal ranges. These moisture values are below the maximum allowable moisture value for roasted and ground coffee (<5%) Given by the Colombian technical standard NTC 3534.

Table 1. Physical and chemical variables determined in samples of *C. arabica* var caturra ground and roasted at different altitudinal range

Parameter	Altitude (m. a. s. l)		
	1300-1400	1400-1600	1600-1800
Initial roasting temperature (°C)	200.3±2.08(1.0)	200.7±3.06(1.5)	200.7±1.15(0.6)
Final roasting temperature (°C)	162.3±0.58(0.4)	166.0±3.61(2.2)	162.7±2.52(1.5)
Cracking time(s)*	321.0±50.47(15.7)	275.0±25.98(9.5)	293.3±11.15(3.8)
Total roasting time (s)	487.0±72.79(14.9)	390.6±21.01(5.4)	468.0±10.82(2.3)
pH	5.3±0.04(0.8)	5.3±0.18(3.4)	5.2±0.08(1.5)
Titrateable acidity (mg clorogenic acid. g of coffe ⁻¹ (db)	21.5±1.57(7.3)	21.8±1.75(8.0)	23.9±3.39(14.2)
% total lipid (db)	11.9±0.87(7.3)	11.5±0.14(1.2)	12.1±0.90(7.4)

*Cracking time: Period of time in which the grain begins to grow and begins to take brown color during the roasting. ** Roasting with open doors. ^a Different lowercase letter to the right of the coefficient of variation (CV) in the same row indicates significant difference ($p < 0.05$).wb: Wet basis; db: Dry basis.

The sensorial attributes evaluated in the cup test of samples of roasted and ground coffee evaluated here, presented total scores between 82.8 & 83.4, which are associated with very good qualification regardless of the considered altitude (Table 3). Budryn *et al.* (2012), indicated the roasting range of 190 to 216°C, Provides acceptable sensory properties to coffee. In this research was verified the decreasing values of the roasting range to values of 162.3- 200.7°C (Table 1), also a product of very good quality is achieved considering the total scores obtained (Table 3).

The range found for the total lipid content of roasted and ground coffee was 11.5 and 12.1 % on a dry basis (Table 1), lower than found for other coffee growing areas in Brazil (13.5% accordingly to Ferrari *et al.*, 2010), 15% in accordance with Calligaris *et al.* (2009), and India (15.28% accordingly to Al-Hamamre *et al.*, 2010; 16.5-16.4% in accordance with Ferrari *et al.*, 2010), these variations are largely due to

differences in geographical conditions (Avelino *et al.*, 2005).

The pH values found here were as follows: 5.2-5.3 (Table 1) and are among the optimum range for ground and roasted grains worldwide (5.1-5.8). The cause of the decrease in pH values is due to the increase of organic acids (formic, acetic, glycolic and lactic acid) produced by thermooxidation processes.

The acidity values found were as follows: 21.5 ± 1.57 to 23.9 ± 3.39 mg of clorogenic acid. g of coffee⁻¹ (Table 1) Being greater than those described for medium dark roasted coffee *C. arabica* cv. Bourbon in Brazil (10.8), *C. arabica* cv. Long Berry in Etiophy (9.4) and *C. canephora* cv. robusta in Uganda (13.34) (Farah *et al.*, 2005).

Composition of the unsaponifiable fraction of *Coffea arabica* var. caturra

According to the analysis of GC-EI mass spectra, twelve compounds were identified in the non-saponifiable lipid fraction of roasted and ground coffee (Table 2), predominating stigmasterol, beta-sitosterol and 4-methylpentanamide in the three evaluated altitudinal ranges. On the other hand, it was observed that as the altitudinal range increases, the content of 4-methylpentanamide and phytol decreases, as well as the content of 2-ethenyl-1,3,5-trimethylbenzene, allyl-tolil ether and 4-methyl-2H-benzopyran (Table 2). Alil or-tolil eter only showed significant difference between the altitudinal ranges of 1400-1600 and 1600-1800 m. a. s. l. These compounds found, for the most part, are products of lipid degradation in this type of sample (Caldeira & Bassoli, 2007).

4-Methyl-2H-benzopyran was identified at altitudes 1400-1600 and 1600-1800 m. a. s. l., this type of compound has been registered in roasted coffee, whose nucleus is part of the flavonoids structure and it is common to find it in samples of roasted coffee (Farah, 2005). In roasted coffee, nitrogenous rings such as pyridine, pyrazine and pyrrole are more common when working at roasting temperatures between 210-230°C (Toledo *et al.*, 2016).

In the present research, stigmasterol and beta-sitosterol were registered, two common sterols in coffee samples, which coincides with studies of sterols in roasted and ground *Coffea arabica* cultivated in United States (γ -sitosterol 53% and estigmasterol 21%). The stigmasterol contents of the present research (Table 2) Are higher than the values reported in tasting coffee lipids and consumption type of *C. arabica* var. Colombia (6.5%) obtained by supercritical fluid (Días & Vásquez, 2011). In addition, 2-propenamide (acrylamide), a nitrogen compound which occurs

during the Maillard reaction, is identified in the coffee roasting process (Alves *et al.*, 2009).

Butanal has been described as the product of the oxidative thermo-degradation of linoleic acid found in coffee samples. Finally, the presence of phytol, diterpene, which is part of the chlorophyll structure and found in lipid fractions of this type of samples (Siriamornpun *et al.*, 2014).

Chromatographic profile comparison of the unsaponifiable fraction according to the altitudinal range

According to the non-saponifiable fraction chromatography profiles of ground and roasted coffee lipids of *C. arabica* (Figure 1), the relative abundances of some compounds, which varied were analyzed according to the altitudinal range. To 1300-1400 and 1400-1600 m. a. s. l., predominance of the 4-metilpentanamide (4), 2-(2-Hidroxifenil) buta-1,3-dieno (7), and beta sitosterol (12) compounds. Contrary to what was found for the altitudinal range of 1600-1800 m. a. s. l., in repetitions J7 and J8, where there was a slight predominance of 2-etenil-1,3,5-trimetilbenzene (6), estigmasterol (11) and beta-sitosterol (12) compounds.

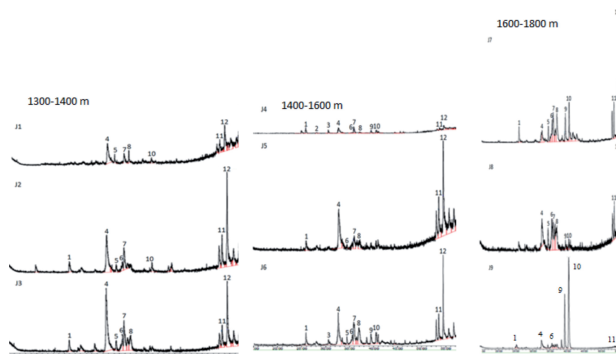


Figure 1. Chromatographic profiles of samples of roasted and ground coffee *Coffea arabica* var. Caturra, from each altitudinal range, three replicates of ground and roasted coffee samples were used as follows: 1300-1400 m (J1, J2 and J3), 1400-1600 m. a. s. l., (J4, J5 and J6) and 1600-1800 m. a. s. l. (J7, J8 and J9). Chromatographic peaks: (1) 2-propenamide, (2) Butanal, (3) 1-propenilaziridine, (4) 4-metilpentanamide, (5) 3-fenil-2-propenal, (6) 2-etenil-1,3,5-trimetilbenzene, (7) 2-(2-hidroxifenil)buta-1,3-dieno, (8) alil o-tolil eter, (9) 4-metil-2H-benzopyrane, (10) fitol, (11) estigmasterol and (12) beta sitosterol.

The J9 sample of ground coffee roasted from the altitudinal range of 1600-1800 m. a. s. l., performed a different chromatographic profile compared to J7 and J8 and with respect to repetitions (J1 to J6) from other altitudinal ranges considered (Figure 1). It is likely the J9 repetition has been contaminated with another species or coffee variety, for example, *Coffea canephora* var. robusta, cultivar preferred by some coffee growers in the study area. It is to denote the physical and chemical variables determined in samples of *C.*

arabica var *caturra* ground and roasted including J9 repetition at different altitudinal range 1600-1800 m. a. s. l., showed no significant difference with the altitudinal ranges of 1300-1400 and 1600-1800 m. a. s. l. (Table 1). Likewise, similar values were presented in attributes of the cup quality test (Table 3), Varying the altitudinal range and within the range of 1600-1800 m. a. s. l., including J9 repetition. It is noteworthy that differences were observed with respect to qualities and notes between repetitions J2 to J9 in the tasting test (Table 4) Indicating the relative abundance of the same compound in different replicates (J2 to J9), generates different sensory attributes (notes and qualities) in tasting test (Table 4). In conclusion, the chromatographic profiles of the non-saponifiable fraction of ground coffee and roasted coffee *C. arabica* are very similar between replicates and the three evaluated altitudinal ranges (Figure 1), except for J9 repetition, which is most likely according to the respective chromatographic profile to be contaminated with another variety of coffee as suggested above.

Sensorial analysis

The sensory attributes of the evaluated samples (replicates) from *C. arabica* var. *Caturra*, did not vary between different altitudinal ranges (Table 3), but there were different and specific notes and qualities for each J2-J9 repetition (Table 4). Butanal, found in the present research and its derivatives have been associated with negative

earthy notes, which decrease the drink quality. Butanal derivatives, generally of San Salvador carbonyl compounds are associated with aromas described as fatty, dairy and greenish.

The presence of butanal and alkylbenzenes (i.e. metilbenzene, 1,3-bis-1,1-dimetilbenzene (possibly 2-etenil-1,3,5-trimetilbenzene), are associated with crude defective seeds (Toledo *et al.*, 2016). The butanal presence could be related to the very good qualification of coffee quality evaluated in the present research according to total score (Table 3). In the attributes quantitative descriptive analysis, was evidenced that uniformity, clean cup and sweetness were the attributes which obtained the highest score in the cup quality test independent of the evaluated altitudinal range (Figure 2). On the other hand, a slightly higher total score was observed in the cup quality test (total score 83.4%), in samples of *C. arabica* var *caturra* cultivated to 1600-1800 m. a. s. l. with notes of papaya and qualities like raspberry, blackberry, lemon malt, panela and melon (Table 4), which showed higher allyl-tolyl ether and 4-methyl-2H-benzopyran contents compared to the other evaluated altitudinal ranges (Table 2).

Table 2. Compounds tentatively identified by GC-El of the non-saponifiable fraction of *Coffea arabica* var. *caturra*, cultivated at different altitudinal range using HP-5 5% column of fenilmetilsiloxane

Peak	Retention time (min)	Compound name	MM	CAS	Relative abundance (%) according to altitude (m. a. s. l.)		
					1300-1400	1400-1600	1600-1800
1	25.917	2-propenamida	72	79-06-1	2.9±2.4(85.5)	27.9±5.2(18.9)	12.3±3.51(28.5)
2	28.014	Butanal	72	123-72-8	0.9±2.6(288.9)	1.3±4.9(376.9)	nd
3	30.516	1-Propenilaziridina	83	80839-91-4	0.8±1.8(225.0)	3.6±20.0(555.5)	nd
4	32.588	4-metilpentanamida	115	1119-29-5	32.4±4.1(12.7) ^a	23.3±2.7(11.6) ^b	8.6±3.6(41.9) ^c
5	34.393	3-fenil-2-Propenal	132	104-55-2	3.9±1.4(35.9)	0.8±1.4(175.0)	5.1±0.5(9.8)
6	35.484	2-etenil-1,3,5-trimetilbenzena	146	000769-25-5	3.6±3.4(94.4)	3.7±1.2(32.4)	10.5±3.4(32.4)
7	35.862	2-(2-Hidroxifenil)buta-1,3-diene	146	1000245-56-3	10.4±0.9(8.7)	12.0±4.7(39.2)	14.1± 1.2(8.5)
8	36.945	Alil o-tolil eter	148	936-72-1	5.1±4.5(88.2) ^a	7.7±3.3(42.9) ^b	15.8±0.5(3.2) ^b
9	39.421	4-Metil-2H-benzopirane	146	1000245-56-4	nd	3.8±3.5(92.1)	6.9±5.2(75.4)
10	40.891	Fitol	296	150-86-7	3.0±2.7(90.0)	2.3±2.0(87.0)	1.8±2.5(138.9)
11	53.595	Estigmasterol	412	83-48-7	9.2±2.9(31.5)	8.5±7.1(83.5)	9.5±2.4(25.3)
12	54.523	Beta-sitosterol	414	83-46-5	27.8±7.0(25.2)	25.1±13.3(53.0)	25.5±0.5(2.0)

m±ds(cv)= Mean ± standard deviation (coefficient of variation). MM: molar mass, CAS: *chemical abstract service*. ^a different lowercase letters to the right of the standard deviation (sd) In the same row indicates significant difference (p<0.05)

Table 3. Results of the cup quality test performed on the samples of *Coffea arabica* var. caturra (Quantitative analysis)

Attributes	Altitude (m. a. s. l.)		
	1300-1400	1400-1600	1600-1800
Fragrance/ Arome	8.2±0.21(2.6)	7.9±0.12(1.5)	8.2±0.25(3.0)
Taste	7.6±0.57(7.5)	7.6±0.79(10.4)	7.7±0.29(3.8)
Residual taste	7.3±0.35(4.8)	7.5±0.50(6.7)	7.3±0.29(4.0)
Acidity	7.5±0.71(9.5)	7.5±0.40(5.3)	7.6±0.17(2.2)
Body	7.5±0.00(0.0)	7.4±0.51(3.8)	7.6±0.17(2.2)
Uniformity	10.0±0.0(0.0)	10.0±0.0(0.0)	10.0±0.0(0.0)
Balance	7.4±0.57(7.7)	7.4±0.51(6.9)	7.5±0.00(0.0)
Clean cup	10.0±0.0(0.0)	10.0±0.0(0.0)	10.0±0.0(0.0)
Sweetness	10.0±0.0(0.0)	10.0±0.0(0.0)	10.0±0.0(0.0)
Tasting score	7.5±0.71(9.5)	7.6±0.79(10.4)	7.5±0.25(3.3)
Total score	82.9±3.04(3.7)	82.8±3.62(4.4)	83.4±0.93(1.1)

m±sd (c.v)=mean ± standard deviation (coefficient of variation).

Table 4. Sensory attributes of tasting score to samples of *Coffea arabica* var. caturra. J2-J9: Sample repetitions of ground and roasted coffee of different altitudinal range

Qualities	Altitude (m. a. s. l.)								
	1300-1400			1400-1600			1600-1800		
	J2	J3	J4	J5	J6	J7	J8	J9	
	nut, peatnut, vainilla	clove, cedral, floral	Bitter chocolate	raisins, plum, hazelnut	cereal, peatnut, panela	raspberry, blackberry, lemon	panela, floral, malta	floral, melon	
Notes	mango, chocolate	caramel malta			raspberry, blackberry, lemon			papaya	

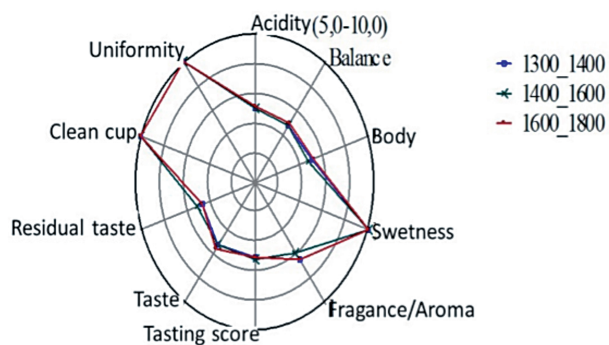


Figure 2. Diagram of the quantitative descriptive analysis from the evaluated attributes varying the altitudinal range

Relationship between chromatographic profile and sensory analysis

The first two components of PCA explains (3-phenyl-2-propenal, 2-ethenyl-1,3,5-trimethylbenzene, 3-phenyl-2-propenal), the main relationship

was presented for fragrance/aroma and body, Allyl-tolyl ether, Figure 3). The relationships between compounds identified in the lipid fraction of *Coffea arabica* var. caturra and sensorial attributes, which were obtained from different groupings in relation to the coefficients of correlation magnitude with fragrance/aroma between 3-fenil-2-Propenal, ($r^2:0.81$ $P<0.01$, Figure 4a), 2-etenil-1,3,5-trimetilbenzene ($r^2:0.6743$ $P<0.01$, Figure 4b) and alil o-tolil eter ($r^2:0.6343$ $P<0.01$, Figure 4c). The body showed correlation with 2-etenil-1,3,5-trimetilbenzene ($r^2:0.5409$ $P<0.01$, Figure 4d), 2-(2-Hidroxifenil)buta-1,3-dieno ($r^2:0.5363$ $P<0.01$, Figure 4e) and alil o-tolil eter ($r^2:0.5014$ $P<0.01$, Figure 4f).

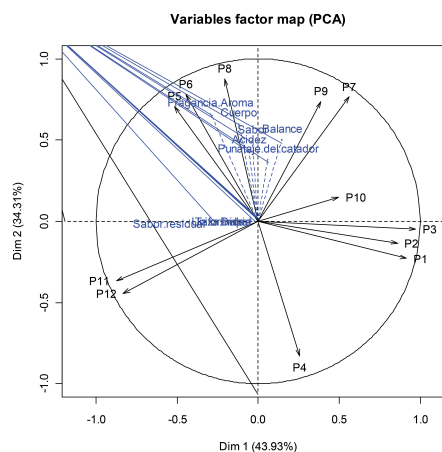


Figure 3. Biplot plain with the relationships between the identified compounds in the non-saponifiable fraction of *Coffea arabica* var. caturra and the sensorial attributes.

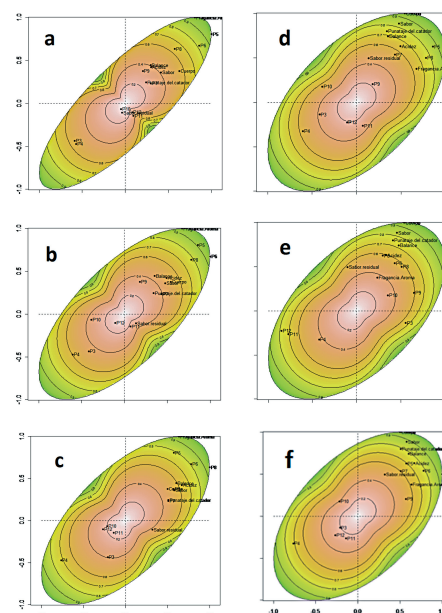


Figure 4. Partial least squares regression PLS. a-c Fragrance/aroma. d-f body. a.3-fenil-2-propenal b-d. 2-etenil-1,3,5-trimetilbenzene. c- f Alil o-tolil eter. e. 2-(2-Hidroxifenil)buta-1,3-dieno.

Conclusion

In the non-saponifiable fraction of *C. arabica* var. Caturra, to three altitudinal ranges, was tentatively determined: 2-propenamida, Butanal, 1-propenilaziridine, 4-metilpentanamida, 3-fenil-2-propenal, 2-etenil-1,3-5-trimetilbenzene, 2-(2-hidroxifenil)buta-1,3-dieno, alil o-tolil eter, 4-metil-2H-benzopirane, fitol, estigmasterol and beta sitosterol. The sensorial attributes evaluated in the cup test of samples of roasted and ground coffee evaluated here, presented very good qualification regardless of the considered altitude. Chromatographic profiles of the unsaponifiable fraction of ground and roasted coffee *C. arabica* are very similar between replicates and the three evaluated altitudinal ranges. The butanal presence and 3-phenyl-2-propenal, could explain the low grade obtained by coffee samples in the cup quality test in the group of special coffees.

References

- Alves R. C., Soares C., Casal S., Fernandes J. O., & Oliveira M. B. (2009). Acrylamide in espresso coffee: Influence of species, roast degree and brew length. *Food Chem*, 119(3), 929-934. <http://dx.doi.org/10.1016/j.foodchem.2009.07.051>
- Al-Hamamre, Z., Foerster, S., Hartmann, F., Kröger, M., & Kaltschmitt, M. (2010). Oil extracted from spent coffee grounds as a renewable source for fatty acid methyl ester manufacturing. *Fuel*, 96, 70-76. <http://dx.doi.org/10.1016/j.fuel.2012.01.023>
- Avelino, J., Barboza, B., Araya, J.C., Fonseca, C., & Davrieux, F. (2005). Effects of slope exposure, altitude and yield on coffee quality in two altitude *terroirs* of Costa Rica, Orosi and Santa Maria de Dota. *Sci Food Agric*, 22, 51-42. <http://dx.doi.org/10.1002/jsfa.2188>
- Budryn, G., Nebesny, E., Zyzelewics, D., Oracz, J., Miskiewicz, K., & Rosicka-Kaczmarek, J. (2012). Influence of roasting conditions on fatty acids and oxidative changes of Robusta coffee oil. *Eur J Lipid Sci Technol*, 114, 1052-1061. <http://dx.doi.org/10.1002/ejlt.201100324>
- Caldeira M. V. & Bassoli G. D. (2007). Utilização do índice de retenção linear para caracterização de compostos voláteis em café solúvel utilizando gc-ms e coluna hp-innowax. *Quim Nova*, 30(8), 2031-2034. <http://dx.doi.org/10.1590/S0100-40422007000800040>
- Calligaris, S., Munari, M., Arriguetti, G., & Barba, L. (2009). Insights into the physicochemical properties of coffee oil. *Eur J Lipid Sci Technol*, 111(12), 1270-1277. <http://dx.doi.org/10.1002/ejlt.200900042>
- Dias, R. C. E., de Faria, A. F. Mercadante, A. Z., Bragagnolo, N., & Benass, M. de T. (2013). Comparison of extraction methods for kahweol and cafestol analysis in roasted coffee. *J Braz Chem Soc*, 24 (3), 492-499. <http://dx.doi.org/10.5935/0103-5053.20130057>
- Farah, A., de Paulis, T., Trugo, L. C., & Martin, P. R. (2005). Effect of roasting on the formation of chlorogenic acid lactones in coffee. *J Agric Food Chem*, 53(5), 1505-1513. <http://dx.doi.org/10.1021/jf048701t>
- Ferrari M., Ravera, F., De Angelis E., Suggi Liverani F., & Navarini L. (2010). Interfacial properties of coffee oils. *Colloid Surface A*, 365(1-3), 79-82. <http://dx.doi.org/10.1016/j.colsurfa.2010.02.002>
- Hurtado, B. A., Dorado, A. D., & Sánchez, C. A. P. (2016). Study of the fatty acid profile and the aroma composition of oil obtained from roasted Colombian coffee beans by supercritical fluid extraction. *J Supercrit Fluid*, 113, 44-52. <http://dx.doi.org/10.1016/j.supflu.2016.03.008>
- Joët, T., Laffargue, A., Descroix, F., Doulebeau, S., Bertrand, B. Kochko, A., & Dussert, S. (2010). Influence of environmental factors, wet processing and their interactions on the biochemical composition of green Arabica coffee beans. *Food Chem*, 118(3), 693-701. <http://dx.doi.org/10.1016/j.foodchem.2009.05.048>
- Murcia, O. B., Chaves, L. C., Rodriguez, P. W., Murcia, M. A., Alvarado, E. R. (2013). Caracterización de biodiesel obtenido de aceite residual de cocina. *Rev Colom Biotecnol*, 15 (1), 61-70.
- Pereira B. H., Nascimento E. A., Tôres F. J., Chang R. & Lemos S. A. (2007). Composição química de cafés torrados do cerrado e do sul de minas gerais. *Ciência & Engenharia*, 16(1-2), 9-15
- Pérez-Martínez, M., Sopelana, P., Paz de Peña, M., & Cid, C. (2008). Changes in volatile compounds and overall aroma profile during storage of coffee brews at 4 and 25°C. *Agric Food Chem*, 56, 3145-3154. <http://dx.doi.org/10.1021/jf703731x>
- Toledo, P. R.A.B., Pezza, L., Pezza, H. R., & Toci, A. T. (2016). Relationship between the different aspects related to coffee quality and their volatile compounds. *Compr Rev Food Sci F*, 15(4), 705-719. <http://dx.doi.org/10.1111/1541-4337.12205>
- Siriamornpun S., Sriket, C., & Sriket, P. (2014). Phytochemicals of Thai local edible herbs. *Int Food Res*, 21(3), 1045-1052.
- Speer, K. & Kölling-Speer, I. (2006). The lipid fraction of the coffee bean. *Braz J Plant Physiol*, 18(1), 201-216. <http://dx.doi.org/10.1590/S1677-04202006000100014>
- Uman, E., Colonna, D. M., Colonna, D. L., Perger, M., Klatt, C., Leighton, S., Miller, B., Butler, K. T., Melot, B. C., Speirs, R. W., & Hendon, C. H. (2016). The effect of bean origin and temperature on grinding roasted coffee. *Sci Rep*, 18(6), 24483. <http://dx.doi.org/10.1038/srep24483>
- Villarreal, D., Baena, L., & Posada, H. (2012). Análisis de lípidos y ácidos grasos en café verde de líneas avanzadas de *Coffea arabica* cultivadas en Colombia. *Cenicafé*, 63(1), 19-40
- Yener, S., Romano, A., Cappellin, L., Granitto, P. M., Aprea, E., Navarini, L., Märk, T. D., Gasperi, F. & Biasioli, F. (2015). Tracing coffee origin by direct injection headspace analysis with PTR/SRI-MS. *Food Res Int*, 69, 235-243. <http://dx.doi.org/10.1016/j.foodres.2014.12.046>