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Identification of nutritional descriptors of roasting intensity in beverages of Arabica and Robusta coffee beans

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Abstract
Arabica and Robusta coffee beans were roasted at 220 ± 10°C for 7, 9 and 11 min to identify chemical descriptors in the beverages. The pH of the beverages showed the lowest value in the medium roasting level. In each degree of browning, the soluble solids content remained slightly higher in Arabica drinks. The contents of caffeine did not vary, but trigonelline decreased with burning up intensity. Chlorogenic acids also decreased with increasing roasting time. The 5-*O*-caffeoylquinic acid prevailed in Arabica and Robusta beverages, but the isomers of dicaffeoylquinic and feruolilquínic acids remained higher in Robusta. It was concluded that trigonelline and total caffeoylquinic, fatty dicaffeoylquinic and fatty feruolilquínic acids detached the beverages according to roasting intensity. Caffeine and pH allowed drinks separation between both species. Soluble solids take apart Arabica and Robusta drinks in each degree of roasting. All the individual groups of chlorogenic acids also explained 90% of the variance among samples.

Keywords: *Arabica coffee, caffeine, chlorogenic acids, Robusta coffee, roasting intensity, trigonelline*

Introduction

During a classic roasting, green coffee beans usually are subjected the temperature intervals (180–190°C and 220–230°C) are related with the indicated temperatures 12 or 15 minutes (Correia 1995; Bicho 2005). Tissues structure of coffee beans starts changing at 50°C and with temperature elevation protein denaturation and water evaporation increase. Above 100°C beans undergo browning due to thermal decomposition and organic compounds pyrolysis. Gaseous substances, namely water vapour, carbon dioxide and carbon monoxide, are released and the bean volume increases at 150°C. At 180–200°C, with the disruption of the endosperm, caramelization starts, bean cracking occurs, bluish smoke appears and aroma develops (Blitz and Grocsh 1988). Thereafter, to prevent excessive browning and the loss of aroma, coffee beans are cooled with a stream of cold air or with water spray (Blitz and Grocsh 1988; Smith 1989).

Depending on roasting intensity and time of exposure, the chemical composition might change significantly in coffee beans and beverages (Correia 1995; Bicho 2005). The amount of caffeine, trigonelline and chlorogenic acids decreases during roasting (Nestlé 1991; Viani 1993; Bicho 2005, 2009). Trigonelline degradation further triggers nicotinic acid, pyridine, 3-methyl-pyridine and methyl ester of nicotinic acid synthesis (Bicho 2005, 2009). Roasting mediated the decrease of chlorogenic acids contents due to numerous reactions, such as isomerization, hydrolysis, oxidation, fragmentation, polymerization

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Table I. Levels of pH, soluble solids, caffeine and trigonelline in beverages of Arabica and Robusta coffee beans roasted at 220 ± 10°C, for 7, 9 and 11 min (T_1, T_2 and T_3), respectively.

	Arabica	Robusta
pH		
T_1	5.12 ± 0.02^{ar}	5.27 ± 0.02^{as}
T_2	4.98 ± 0.01^{br}	5.24 ± 0.01^{as}
T_3	5.39 ± 0.03^{cr}	5.47 ± 0.03^{br}
Soluble solids (mg cm^{-3})		
T_1	24.23 ± 0.54^{abr}	23.88 ± 0.22^{ar}
T_2	21.50 ± 0.95^{br}	20.17 ± 0.94^{br}
T_3	25.53 ± 0.17^{ar}	23.21 ± 0.94^{abr}
Caffeine (mg cm^{-3})		
T_1	1.274 ± 0.040^{ar}	2.163 ± 0.057^{as}
T_2	1.127 ± 0.109^{ar}	1.955 ± 0.095^{as}
T_3	1.330 ± 0.008^{ar}	2.065 ± 0.092^{as}
Trigonelline (%)		
T_1	1.274 ± 0.025^{ar}	0.912 ± 0.017^{as}
T_2	1.107 ± 0.034^{br}	0.790 ± 0.034^{bs}
T_3	0.566 ± 0.007^{cr}	0.485 ± 0.021^{cr}

Notes: Each value is the mean ± SE ($n = 3$). Different letters indicate significant differences in a multiple range analysis, for 95% confidence level, among roasting for the same species (a, b and c) or between coffee types for the same roasting (r and s).

and association of these compounds with denatured proteins (Clifford 1989). A large number of aromatic compounds, namely phenol esters, carbonyl compounds and esters, and polycyclic compounds also result due to thermal decomposition of chlorogenic acids (Clifford 1987). Hydroxycinnamic acids, especially chlorogenic acid in the double form of caffeine and potassium chlorogenate (Viani 1993; Clifford 1999), are significantly destroyed with the release of alkaloids (Correia 1990, 1995).

Following international standard regulations and considering the intensity of temperature and time of beans roasting, this work aims to identify, at a chemical level, descriptors in beverages of Arabica and Robusta coffees from Brazil and India.

Materials and methods

Sampling of *Coffea arabica* (from Brazil) and *Coffea canephora* (from India) was carried out according to Normativa Instrução N° 8 (2003), NP 1666 (1980) and ISO 4072 (1982), as recommended by International Coffee Organization for sampling green coffee in bags. The sampling process began with the selection of green coffee bags (PSCB N° 36/02 2002; Bicho et al. 2011), at random (a minimum of 10% of the lot). The selected bags were separated from the lot and 30 ± 6 g of coffee was collected (in triplicate from the top, middle and bottom of the bag). After extraction and homogenization, the portions were mixed together, for an overall take of green coffee, with a minimum mass of 1.5 kg (Bicho et al. 2011). Arabica and Robusta green coffee samples were, therefore, roasted using the highest temperature (220 ± 10°C) applied in classical coffee burning and considering three browning times (7, 9 and 11 min). These roasted samples were used for all the subsequent studies.

Following the criteria of Lingle (1996) and ABIC (2007), for the preparation of coffee drinks, samples of roasted beans were ground to a medium level. Coffee beverages were prepared according to ISO 6668 (1991) using coffee filters no. 4. Roasted ground coffee (10 ± 0.01 g) was mixed with 100 ± 0.01 ml of mineral water and subjected to a temperature of 95–98°C for 4 min. The process was performed in triplicate for each roasted coffee sample and the fractions were collected and mixed together to get a replicate for subsequent analysis. The above procedure was repeated to obtain triplicates of each drink.

Soluble solids and pH were measured according to AOAC (1996a,b). After calibration of the electrode with pH 4.0 and 7.0 buffer solutions, pH was measured at 25°C. For quantification of soluble solids, 25 ml of the coffee drink was dried in a water bath until dryness and then placed in an oven at 105°C. After cooling in a desiccator, the residue was weighted until the mass remained constant. Data are the average of triplicate for each sample of roasted coffee.

Caffeine and trigonelline contents were measured according to ISO 10095 (1992). Coffee drinks were prepared and cooled to room temperature. Samples were, therefore, water diluted 1:4 (w/v), homogenized and filtered with a 0.45 μm filter. Caffeine quantification was carried out in an integrated high-performance liquid chromatography system (Waters, equipped with UV–VIS detector, model 440, column Lichrosorb 100 RP-18/Merck, with 5 μm in pore size, 4 μm in diameter and 250 mm in length), using the

Table II. Levels of 3-CQA, 4-CQA, 5-CQA and CQA_{total} in beverages of Arabica and Robusta coffee beans roasted at 220 ± 10°C, for 7, 9 and 11 min (T_1, T_2 and T_3), respectively.

		3-CQA	4-CQA	5-CQA	CQA_{total}
Arabica (mg cm^{-3})	T_1	0.889 ± 0.012^{ar}	1.092 ± 0.017^{ar}	1.958 ± 0.024^{ar}	3.939 ± 0.052^{ar}
	T_2	0.503 ± 0.015^{br}	0.676 ± 0.022^{br}	1.053 ± 0.036^{br}	2.232 ± 0.073^{br}
	T_3	0.196 ± 0.001^{cr}	0.247 ± 0.001^{cr}	0.351 ± 0.001^{cr}	0.794 ± 0.002^{cr}
Robusta (mg cm^{-3})	T_1	0.937 ± 0.018^{ar}	1.147 ± 0.024^{ar}	1.913 ± 0.035^{ar}	3.997 ± 0.077^{ar}
	T_2	0.577 ± 0.013^{bs}	0.742 ± 0.017^{br}	1.118 ± 0.026^{br}	2.437 ± 0.055^{br}
	T_3	0.251 ± 0.002^{cr}	0.316 ± 0.003^{cr}	0.410 ± 0.030^{cr}	1.004 ± 0.009^{cr}

Notes: Each value is the mean ± SE ($n = 3$). Different letters indicate significant differences in a multiple range analysis, for 95% confidence level, among roasting for the same species (a, b and c) or between coffee types for the same roasting (r and s).

Table III. Levels of 3,4-diCQA, 3,5-diCQA, 4,5-diCQA and $diCQA_{total}$ in beverages of Arabica and Robusta coffee beans roasted at 220 ± 10°C, for 7, 9 and 11 min (T_1, T_2 and T_3), respectively.

		3,4-diCQA	3,5-diCQA	4,5-diCQA	$diCQA_{total}$
Arabica ($mg\,cm^{-3}$)	T_1	0.100 ± 0.001^{ar}	0.075 ± 0.001^{ar}	0.099 ± 0.001^{ar}	0.274 ± 0.003^{ar}
	T_2	0.038 ± 0.001^{br}	0.026 ± 0.001^{br}	0.029 ± 0.002^{br}	0.093 ± 0.004^{br}
	T_3	0.008 ± 0.000^{cr}	0.005 ± 0.000^{cr}	0.004 ± 0.000^{cr}	0.017 ± 0.000^{cr}
Robusta ($mg\,cm^{-3}$)	T_1	0.181 ± 0.020^{as}	0.134 ± 0.004^{as}	0.134 ± 0.006^{as}	0.479 ± 0.011^{as}
	T_2	0.095 ± 0.002^{bs}	0.058 ± 0.001^{bs}	0.058 ± 0.002^{bs}	0.219 ± 0.005^{bs}
	T_3	0.023 ± 0.000^{cs}	0.013 ± 0.000^{cs}	0.013 ± 0.000^{cs}	0.050 ± 0.001^{cs}

Notes: Each value is the mean ± SE ($n = 3$). Different letters indicate significant differences in a multiple range analysis, for 95% confidence level, among roasting for the same species (a, b and c) or between coffee types for the same roasting (r and s).

32 Karat Software (version 7.0, build 1048, 1998–2003 Copyright Beckman Coulter, Inc.). The mobile phase, at a flow rate of $1\,ml\,min^{-1}$, consisted of phosphate buffer ($0.02\,mol\,l^{-1}$ and acetonitrile, 9:1). The column temperature was maintained at 25°C, a wavelength of 254 nm was applied and aliquots of 20 μl were injected. A standard curve was constructed for caffeine using eight solutions with concentrations ranging between 7.813 and $1.000\,g\,ml^{-1}$. Seven solutions with concentrations ranging between 7.813 and $500\,\mu g\,ml^{-1}$ were also used for the standard curve of trigonelline. Data were within the detection limits of the method. All extractions and chromatographic analysis were performed in triplicate.

Chlorogenic acids analysis followed Correia (1990). To 10 ml of coffee drink, and 1 ml of Carrez solution II (aqueous solution of zinc acetate dihydrate and glacial acetic acid, 10.95 g and 1.5 ml, respectively, to a final volume of 50 ml) and Carrez solution II (aqueous solution of 5.3 g of potassium hexacyanoferrate II trihydrate in a final volume of 50 ml) were added for clarification and thereafter methanol:water (40:60) was added to a final volume of 100 ml. After 15 min, the mixture was filtered through a Whatman filter no. 1 and an aliquot of 10 ml was removed and filtered again with a 0.45 μm filter. For quantification, an integrated high-performance liquid chromatography system (Beckman System Gold, equipped with diode array detector, model 168, and a reverse-phase column Spherisorb S5 ODS2/Waters, with 4.6 mm diameter and 250 mm in length) with a 32 Karat Software (version 7.0, build 1048, 1998–2003 Copyright Beckman Coulter, Inc.) was used. To the mobile phase, a gradient elution program was applied (solvent A tripotassium citrate buffer solution $0.01\,mol\,l^{-1}$, pH 2.5 and solvent B methanol 100%, at a flow rate of $1\,ml\,min^{-1}$; starting 80% solvent A and 20% solvent B to a final of 30% solvent A and 70% solvent B; each run 45 min), detection was made at wavelengths of 325 and 330 nm, and a sample volume of 20 μl was injected.

For isomerization of chlorogenic acids, 200 mg of 5-caffeoylquinic acid was diluted in 20 ml of distilled water and the pH was adjusted to 8 with ammonium hydroxide ($4\,mol\,l^{-1}$). The solution was boiled for 30 min in a water bath, cooled and then the pH was adjusted to 2.5 with HCl ($4\,mol\,l^{-1}$). After filtration, the samples were used for quantification. The identification and quantification of chromatographic peaks was carried out using standard solutions of 5-*O*-caffeoylquinic acid (5-CQA). To identify the isomers 3-*O*-caffeoylquinic acid (3-CQA) and 4-*O*-caffeoylquinic acid (4-CQA), the standard 5-CQA was subjected to isomerization as described. The peaks appeared in the following sequence: 3-CQA, 3-*O*-feruolilquínic acid (3-FQA), 4-CQA, 5-CQA, 4-*O*-feruolilquínic acid, 5-*O*-feruolilquínic acid (5-FQA), 3,4-*O*-dicaffeoylquinic acid (3,4-diCQA), 3,5-*O*-dicaffeoylquinic acid (3,5-diCQA) and 4,5-*O*-dicaffeoylquinic acid (4,5-diCQA). The calibration curve was obtained from 5-CQA with readings at 325 and 330 nm. The quantification considered the peak areas and the standard 5-CQA. To quantify each compound, the following equation was used (Correia 1990; Farah et al. 2005): $c = [Fr \times \varepsilon_1 \times Mr_2 \times A]/[\varepsilon_2 \times Mr_1]$ (where c is the concentration of the isomer to be quantified, in $mg\,l^{-1}$; Fr is the response factor of the standard 5-CQA,

Table IV. Levels of 3-FQA, 5-FQA and FQA_{total} in beverages of Arabica and Robusta coffee beans roasted at 220 ± 10°C, for 7, 9 and 11 min (T_1, T_2 and T_3), respectively.

		3-FQA	5-FQA	FQA_{total}
Arabica ($mg\,cm^{-3}$)	T_1	0.061 ± 0.001^{ar}	0.133 ± 0.003^{ar}	0.194 ± 0.005^{ar}
	T_2	0.045 ± 0.002^{br}	0.087 ± 0.004^{br}	0.132 ± 0.006^{br}
	T_3	0.027 ± 0.000^{cr}	0.033 ± 0.001^{cr}	0.060 ± 0.001^{cr}
Robusta ($mg\,cm^{-3}$)	T_1	0.141 ± 0.004^{as}	0.324 ± 0.009^{as}	0.465 ± 0.013^{as}
	T_2	0.095 ± 0.003^{bs}	0.175 ± 0.008^{bs}	0.270 ± 0.011^{bs}
	T_3	0.060 ± 0.000^{cs}	0.097 ± 0.001^{cs}	0.158 ± 0.001^{cs}

Notes: Each value is the mean ± SE ($n = 3$). Different letters indicate significant differences in a multiple range analysis, for 95% confidence level, among roasting for the same species (a, b and c) or between coffee types for the same roasting (r and s).

Table V. Correlation coefficients between the first, second and third principal components (CP_1, CP_2 and CP_3) with 3-CQA, 4-CQA, 5-CQA, 3,4-diCQA, 3,5-diCQA, 4,5-diCQA, 3-FQA and 5-FQA.

Variables	CP_1	CP_2	CP_3
pH	0.600	0.746	−0.185
Soluble solids	0.191	0.106	−0.970
Caffeine	−0.099	0.932	0.211
Trigonelline	−0.786	−0.583	−0.109
CQA_{total}	−0.978	0.012	−0.159
$diCQA_{total}$	−0.900	0.388	−0.129
FQA_{total}	−0.769	0.616	0.053
Eigenvalue	3.38	2.31	1.08
Variance (%)	48.28	32.96	15.37

in $mg\,l^{-1}$ per unit area; ε_1 is the molar absorption coefficient of the standard 5-CQA, in $l\,mol^{-1}\,cm^{-1}$; ε_2 is the molar absorption coefficient of the isomer to be quantified, in $l\,mol^{-1}\,cm^{-1}$; Mr_2 is the molecular weight of the isomer under study – caffeoylquinic acids $= 354.31\,g\,mol^{-1}$, fatty feruolilquínic acids $= 368.28\,g\,mol^{-1}$, fatty dicaffeoylquinic acids $= 516.44\,g\,mol^{-1}$; Mr_1 is the molar mass of acid 5-CQA; A is the peak area of the isomer to be quantified). The molar absorption coefficients (3-CQA = 18,400, 4-CQA = 18,000, 5-CQA = 19,500, 3,4-diCQA = 31,800, 3,5-diCQA = 31,600, 4,5-diCQA = 33,200, with $\lambda = 330$ nm; 3-FQA = 19,000, 4-*O*-feruolilquínic acid = 19,500, 5-FQA = 19,300, with $\lambda = 325$ nm) indicated by Correia (1990) and Farah et al. (2005), in $l\,mol^{-1}\,cm^{-1}$, were used. Data were within the detection limits of the method. All extractions and chromatographic analysis were performed in triplicate.

Data were statistically analysed using a one-way ANOVA ($p \leq 0.05$). On the basis of the ANOVA results, a Tukey's test was performed for mean comparison, for a 95% confidence level. Different letters indicate significant differences. Multivariate analysis was carried out with STATISTICA software Copyright StatSoft, Inc., following Neto and Moita (1998), Alvarenga (2009), Chapman et al. (2001), Maeztu et al. (2001) and Da Silva et al. (2004).

Results and discussion

The soluble solid contents ranging between about 20 and 26 $mg\,cm^{-3}$ were slightly higher in Arabica beverages for the same degree of browning and showed the lowest value in the roasting at 220 ± 10°C, for 9 min (Table I). Accordingly, the soluble solid contents remained within reference values (Illy and Viani 1998; Maeztu et al. 2001). In Arabica and Robusta coffees, the pH of the beverages also showed the lowest value in the same roasting level and varied from 4.98 to 5.39 and from 5.24 to 5.47, respectively (Table I). In this context, according to Clifford (1987), only the Arabica coffee beverage after beans roasting at 220 ± 10°C for 11 min was not be palatable, because pH must vary between 4.90 and 5.20 or from 5.00 to 5.80 in Arabica and Robusta coffees, respectively. Nevertheless, considering that Brazilian Arabica coffees have a low acidity (Mendonça et al. 2005), according to the criteria of Maeztu et al. (2001) and Fujioka and Shibamoto (2008), regardless of the intensity of roasting, all the coffee beverages can be considered within limits of acceptance because the pH varied between 4.8 and 6.0. Following also the assumptions of Clifford (1987), the quality of Arabica (but not Robusta) beans roasted at 220 ± 10°C for 9 min further pointed to a gourmet rating. The caffeine contents varied between 1.2 and 2 $mg\,cm^{-3}$ and were lower in Arabica coffee drinks, but did not vary significantly with the degree of roast (Table I). Nevertheless, these data were below the reference values 2.09 and 2.88 $mg\,cm^{-3}$, as shown for Arabica and Robusta coffees by Maeztu et al. (2001), possibly because caffeine levels vary with the type of grinding

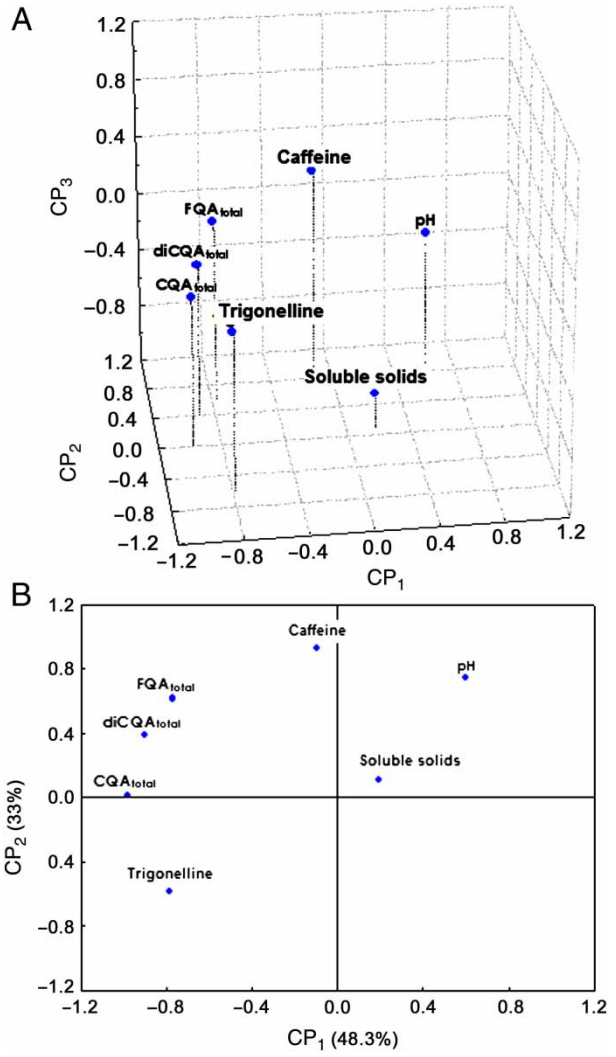

Figure 1. Projection of pH, soluble solids, caffeine, trigonelline, CQA_{total}, $diCQA_{total}$ and FQA_{total} in plans defined by (A) first, second and third components (CP_1, CP_2 and CP_3); (B) first and second components (CP_1 and CP_2).

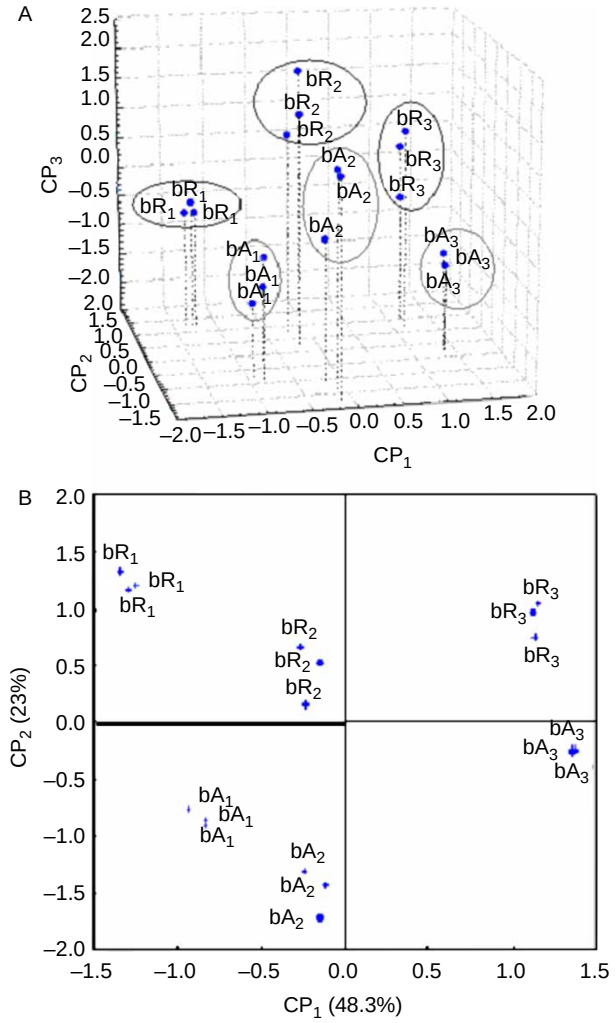

Figure 2. Projection of pH, soluble solids, caffeine, trigonelline, $diCQA_{total}$, $diCQA_{total}$ and FQA_{total} in plans defined by (A) first, second and third components (CP_1, CP_2 and CP_3); (B) first and second components (CP_1 and CP_2). The symbols have the following meaning: b = beverage; A_1, A_2, A_3 and R_1, R_2, R_3 = roasting of Arabica and Robusta green beans at 220 ± 10°C, for 7, 9 and 11 min, respectively.

and brewing and with the ratio between water and coffee mass used for the preparation of the beverages (Bell et al. 1997; Andueza et al. 2003). In the coffee beverages, trigonelline content also diminished with increasing roasting intensity, but remained higher in Arabica drinks (Table I). Reference levels of 1.15 and 1.14 mg cm^{-3} contents were shown for both coffee species (Maeztu et al. 2001) but similar values were obtained only in Arabica coffee beverages obtained from beans roasted at 220 ± 10°C for 9 min. The different patterns obtained for Arabica and Robusta beverages probably are linked to the different diffusion coefficients of caffeine, this being the result of the physical structure and particle size of the beans (Saldaña et al. 1997; Andueza et al. 2003) and to physical–chemical characteristics of each grain specie (Toci et al. 2006). In addition, these trends can further be linked to the chemical composition of the cell wall that also can influence the phenomenon of partition of different compounds during their extraction (Fischer et al. 2001).

The contents of 3-CQA, 4-CQA, 5-CQA and total caffeoylquinic acids ($diCQA_{total}$) in Arabica and Robusta coffee beverages also decreased with the intensity of roasting, but were not significantly different for the same degree of browning (Table II). As previously reported by Fujioka and Shibamoto (2008), isomer 5-CQA was quantitatively the most important in Arabica and Robusta beverages, followed by 4-CQA and 3-CQA (Table II). The levels of 3,4-diCQA, 3,5-diCQA, 4,5-diCQA and total fatty dicaffeoylquinic acids ($diCQA_{total}$) also decreased with increasing roasting intensity and remained significantly higher in Robusta coffee drinks for similar levels of roasting (Table III). The levels of 3,4-diCQA were also higher than those of 3,5-diCQA and 4,5-diCQA (Table III), therefore, following a pattern also shown by Fujioka and Shibamoto (2008). The levels of 3-FQA, 5-FQA and total fatty feruolilquínic acids (FQA_{total}) sharply decreased with increasing roasting, but remained significantly higher in Robusta coffee for the same browning degree (Table IV). Overall, the content of total chlorogenic acids was significantly higher in Robusta coffee beverages due to the higher levels of $diCQA_{total}$ (Tables II–IV). The percentage ratio of 5-CQA and $diCQA_{total}$ also remained at higher levels in Arabica coffee beverages in all roasting intensities, unlike the percentage ratio of FQA_{total} and $diCQA_{total}$, which showed a higher value in Robusta coffee drinks (Tables II–IV). The percentage ratio of $diCQA_{total}$ markedly decreased in Arabica and Robusta beverages, therefore, following an antagonistic pattern relative to the ratio and percentage of $diCQA_{total}$ and FQA_{total} (Tables II–IV). Thus, the relative importance of FQA_{total} for $diCQA_{total}$

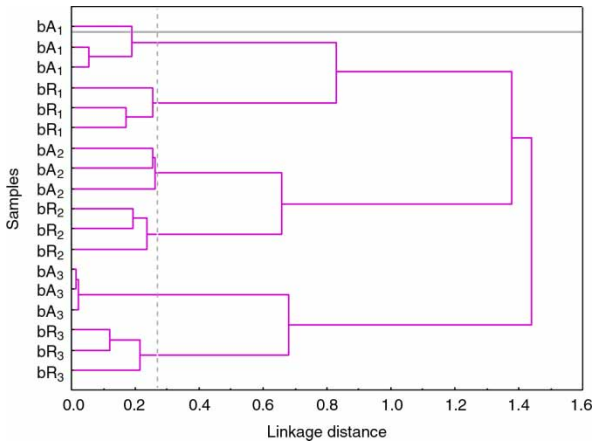

Figure 3. On the basis of Euclidean distances, dendrogram of coffee samples, considering pH, caffeine, trigonelline, $diCQA_{total}$, $diCQA_{total}$ and FQA_{total} between them. The symbols have the following meaning: b = beverage; A_1, A_2, A_3 and R_1, R_2, R_3 = roasting of Arabica and Robusta green beans at 220 ± 10°C, for 7, 9 and 11 min, respectively.

Table VI. Correlation coefficients between the first and second principal components (CP_1 and CP_2) with 3-CQA, 4-CQA, 5-CQA, 3,4-diCQA, 3,5-diCQA, 4,5-diCQA, 3-FQA and 5-FQA.

Variables	CP_1	CP_2
3-CQA	−0.953	−0.301
4-CQA	−0.945	−0.314
5-CQA	−0.924	−0.382
3,4-diCQA	−0.970	0.112
3,5-diCQA	−0.992	0.072
4,5-diCQA	−0.992	0.018
3-FQA	−0.878	0.465
5-FQA	−0.932	0.354
Eigenvalue	7.20	0.69
Variance (%)	90.05	8.67

increased in drinks prepared with more intense roasted coffee.

Equating the concentration of caffeine, trigonelline, soluble solids, pH, $diCQA_{total}$, $diCQA_{total}$ and FQA_{total}, three principal components were defined in the coffee beverages, comprising 96.6% of the total variance (Table V). The levels of $diCQA_{total}$, $diCQA_{total}$, trigonelline and FQA_{total} significantly correlated with the first principal component (Table V; Figure 1), being higher in lower roasted coffee drinks. Therefore, the first principal component detached the beverages according to coffee roasting intensity. Caffeine and pH were identified as variables of the second principal component (Table V; Figure 1), allowing the separation of drinks according to the species, and rising higher for drinks of Robusta coffee. To explain the variation among the coffee samples, the third principal component had a minor importance. Moreover, the content of soluble solids correlated with this component, allowing the separation Arabica and Robusta coffee drinks having the same degree of roasting (Table V; Figure 1). Although these variables were important as chemical descriptors, the most relevant were $diCQA_{total}$, $diCQA_{total}$ and caffeine.

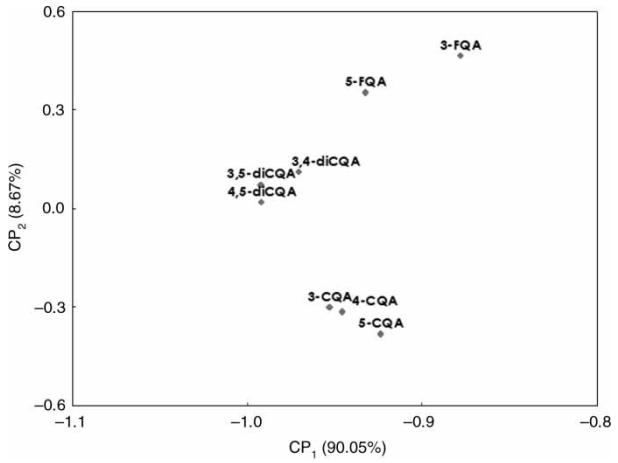

Figure 4. Projection of 3-CQA, 4-CQA, 5-CQA, 3,4-diCQA, 3,5-diCQA, 4,5-diCQA, 3-FQA and 5-FQA plans designed by the first and second principal components (CP_1 and CP_2).

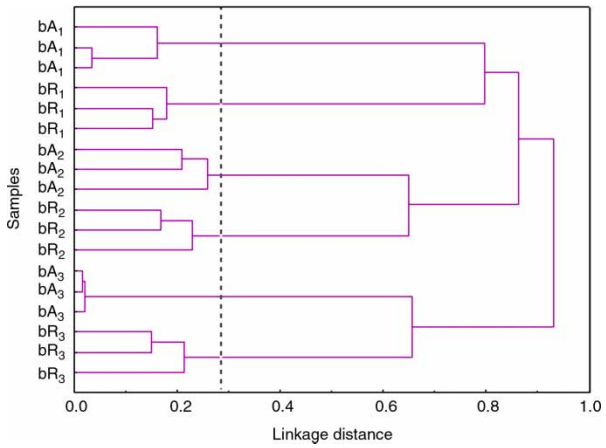

Figure 5. Dendrogram of samples beverages based on Euclidean distances, considering the variables pH, caffeine, trigonelline, 3-CQA, 4-CQA, 5-CQA, 3,4-diCQA, 3,5-diCQA, 4,5-diCQA, 3-FQA and 5-FQA. The symbols have the following meaning: b = beverage; A_1, A_2, A_3 and R_1, R_2, R_3 = roasting of Arabica and Robusta green beans at 220 ± 10°C, for 7, 9 and 11 min, respectively.

Consequently, the coffee drinks parameters formed six groups (Figure 2). The soluble solids content persisted with lower importance to explain the variance among samples of coffee drinks. The remaining parameters (pH, caffeine, trigonelline, $diCQA_{total}$, $diCQA_{total}$ and FQA_{total}) enabled by itself a discrimination between samples, as was further seen through its hierarchical classification for a distance connection around 0.3 (Figure 3). The total content of each group of chlorogenic acids was relevant for the separation of beverages (Table VI; Figure 4). The analysis of the principal components showed that all the individual groups of total chlorogenic acids (3-CQA, 4-CQA, 5-CQA, 3,4-diCQA, 3,5-diCQA, 4,5-diCQA, 3-FQA and 5-FQA) could explain 90% of the variance among samples of coffee drinks (Table VI; Figure 4). Thus, the individual groups of chlorogenic acids in the coffee drinks are highly correlated with the first principal component, which may constitute an axis for samples separation by the roasting degree. In general, the individual fractions are highly correlated with the first principal component, whereas the fraction 3-FQA becomes less important although significant. Considering the patterns of 3-CQA, 4-CQA, 5-CQA, 3,4-diCQA, 3,4-diCQA, 4,5-diCQA, 3-FQA and 5-FQA, as well as the other parameters (caffeine, trigonelline and pH), and since the soluble solids have not proved to be a good discriminator, again it is concluded that the coffee drinks parameters might constitute six individual groups (Figure 5).

Conclusion

The chemical composition of the beverages of Arabica and Robusta coffee beans from Brazil and India subjected to increasing roasting intensity might vary at

different levels. Total soluble solids and pH had lower values when beans are roasted at 220 ± 10°C, for 9 min. The contents of caffeine did not vary significantly but trigonelline and chlorogenic acids sharply decreased with higher burning up. Considering all the patterns of these variables, the beverages can therefore be discriminated following the intensity of coffee roasting, the kind of coffee and, under the same degree of roasting, the coffee type.

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