Characterization of Espresso Coffee Aroma by Static Headspace GC−MS and Sensory Flavor Profile

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The aromas of three espresso coffee (EC) samples from different botanical varieties and types of roast (Arabica coffee, Robusta natural blend, and Robusta Torrefacto blend (special roast by adding sugar)) were studied by static headspace GC−MS and sensory flavor profile analysis. Seventy-seven compounds were identified in all of the EC samples. Among them, 13 key odorants have been quantified and correlated with their flavor notes by applying multivariate statistical methods. Some correlations have been found in the EC samples: some aldehydes with fruity flavors, diones with buttery flavors, and pyrazines with earthy/musty, roasty/burnt, and woody/papery flavors. By applying principal component analysis (PCA), Arabica and Robusta samples were separated successfully by principal component 1 (60.7% of variance), and Torrefacto and Natural Robusta EC samples were separated by principal component 2 (28.1% of total variance). With PCA, the aroma characterization of each EC sample could be observed. A very simple discriminant function using some key odorants was obtained by discriminant analysis, allowing the classification of each EC sample into its respective group with a success rate of 100%.

Keywords: *Espresso coffee; key odorants; sensory flavor profile; multivariate analysis; principal component analysis; discriminant analysis; brew coffee; Arabica coffee; Robusta coffee; Torrefacto roast*

INTRODUCTION

Brew coffee is the second-most popular beverage in the world, after tea (*1*). It is consumed for its pleasant aroma assessable directly through the nostrils of the nose, or as the aroma on drinking a brew.

Espresso coffee (EC) has a peculiar aroma characteristic mainly produced by the presence of foam, which traps the volatilized aromas and doses their emission into the atmosphere (*2*). A lot of papers have been written about the aroma of ground roasted coffee and coffee brews. However, only a few works about EC aroma have been found (*3*).

The flavor of coffee brew depends on the type of coffee used to prepare it. From Arabica and Robusta ground roasted coffees, different aromatic profiles in coffee brews were obtained (*4*−*7*). The influence of the roast degree on the aroma profile has been studied in ground roast coffee (*8, 9*) and in EC (*3*). However, no work about Torrefacto roast coffee has been found. Torrefacto is a special roasting process in which sugar is added to low-quality Robusta coffees in order to brown the coffee brew and mask some negative flavors.

The composition of the volatile fraction of roasted and brew coffee has been studied for years, and several hundreds of compounds have been reported as constituents of coffee aroma (*2, 8, 10*−*11*). Although the volatile fraction in coffee is very complex, only the bioactive substances (called key odorants) are responsible for coffee flavor (*12*). Recently, studies about the character impact odorants of coffee have been carried out, and 28 volatile compounds have been identified as important contributors to the flavor (*4*−*7, 13*).

Headspace sampling has progressively replaced techniques such as steam-distillation or solvent extraction because it is the most suitable for studying very volatile compounds (*3, 11, 14*−*16, 17, 18*), and because its composition better represents the aroma perceived by the consumer (*19*).

Gas chromatography−olfactometry has been used to determine the potency and sensory attribute of each key odorant (*6, 19*). Other studies used an aroma model by dissolving the standard key odorants in water to obtain a solution with a flavor profile similar to that of coffee brew (*5, 7, 20*).

In EC, the foam plays an important role in the sensory flavor perception. Therefore, the sensory descriptive analysis, by means of a panel of judges, could be the most suitable method to describe the real aroma profile of EC. Furthermore, in the past few years, the development of different multivariate statistical methods has progressed immensely. The application of one of them could be a good way to relate instrumental and sensory flavor results.

The aim of this paper was to establish a correlation between key odorants and flavors in different ECs by the application of multivariate statistical methods. Therefore, the influence of the botanical varieties (Arabica and Robusta) and the types of roasting (natural and Torrefacto) on EC flavor were studied in order to characterize each EC, and discriminant analysis was applied to classify the EC samples by their aroma profiles.

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MATERIALS AND METHODS

Materials. Three roasted coffee samples, Arabica (pure *Coffea arabica* from Colombia, 2.0% water content), Robusta natural blend (80:20 blend of *Coffea canephora* and *Coffea arabica*, 2.0% water content), and Robusta Torrefacto blend (50% Robusta natural blend previously defined, and 50% Robusta Torrefacto roast, 1.8% water content), were provided by a local factory. Two batches for each coffee sample were used.

Pure reference standards of 2-methylpropanal, 2-methyl-1-propanol, 2-butanone, 3-methylbutanal, 2,3-butanedione, and 2,3-pentanedione were purchased from Acros (Springfield, NJ); 3-penten-2-one, 2-methylfuran, thiophene, propionaldehyde, and dimethyl sulfide were obtained from Aldrich (Steinheim, Germany), and hexanal was obtained from Sigma (Steinheim, Germany).

EC Sample Preparation. The EC samples were prepared, just before each analysis, from 7.5 g of finely ground roasted coffee for a volume of 40 mL, using an experimental EC prototype. EC preparation conditions were fixed at relative water pressure of 9 atm, water temperature of 96 °C (erogation temperature 90±2 °C), extraction time of 21±3 s, and holder filter diameter of 38 mm.

Volatile Compound Analysis. The profiles of volatile compounds were obtained with the method described by Sanz et al. (2001), adapted to EC, using static headspace gas chromatography−mass spectrometry (SHGC−MS). SHGC analysis was performed with an HP 6890 gas chromatograph (Hewlett-Packard) equipped with a static headspace sampler (Hewlett-Packard model 7694).

A 6-mL portion of a homogenized cup of EC was introduced into a 10-mL vial which was immediately sealed with a silicone rubber Teflon cap. Each vial was equilibrated at 60 °C during 20 min in the static headspace sampler. Each vial was pressurized with carrier gas for 12 s, and 3 mL of the coffee headspace sample was injected into a capillary column HP-Wax (60 m × 0.25 mm × 0.5 μm film thickness; Hewlett-Packard). Each EC sample was analyzed in triplicate, using three EC cups.

The injector temperature was set at 180 °C, and helium (10 mL/min linear speed) was the carrier gas. The oven temperature was maintained at 40 °C for 6 min and programmed to 190 °C at 3 °C/min.

Mass spectrometry analysis was carried out using a Hewlett-Packard mass selective detector (model 5973) coupled to the gas chromatograph. The mass spectrometer operated in the electron impact ionization mode (70 eV), with a scan range of 33 to 300 amu. The ion source temperature was set at 230 °C.

Identification of the Volatile Compounds. The volatile compounds studied were identified by comparing their mass spectra to those of the Wiley library and in addition, by comparison of their retention times with those of standard compounds. The kovats indexes were also calculated according to Tranchant (1982) and compared with available literature data (*22*).

Quantitative Measurements. The total content of the volatiles of each headspace analysis was defined by integrating the peak areas of the 13 key odorants identified. The relative percentages of individual compounds were calculated from the total contents of volatiles on the chromatograms.

Sensory Flavor Profile. The sensory flavor profile was made using a selected and trained panel of judges. The judges were recruited among members of the Food Science and Technology Department at the University of Navarra. The selection criteria were good health, time availability, no aversion to coffee, and willingness to participate. The preselected judges were submitted to preliminary tests to investigate their ability to identify and differentiate the five basic tastes, using UNE 87-003-95 and UNE 87-024-1-95 (*23*). Then 10 judges were selected.

Judges were trained over eight 1.5-h sessions. First, during four sessions, descriptive terms about EC flavor were generated and defined through group discussion by selected judges. For the most common flavors in coffee, including off-flavors, some reference substances were prepared and used. Second, in four other sessions, individual evaluations of three reference or sample ECs (30 min) were carried out. During training, a scorecard was developed. The odor/flavor attributes most frequently described by judges during the training process were written on the scorecard in two columns: one for positive and the other for negative flavor attributes. In both columns, one line for "other flavors" was added.

Sensory flavor profile evaluation of the EC samples was then carried out in triplicate over six sessions. Three ECs were analyzed per session. Each EC was prepared immediately before taste and served in a white porcelain coffee cup labeled with a 3-digit code. Each judge was served only one cup at a time. The order of presentation was randomized among judges and sessions. All evaluations were conducted in isolated sensory booths illuminated with white light in the sensory lab under standardized conditions as described by UNE 87-004-79 (*23*). Rinse water was provided for the judges between individual samples.

The flavor profile of each EC sample was defined by the percentages of judges that perceived each of the positive and negative flavor attributes.

Statistical Analysis. Analysis of variance (ANOVA) was applied to the volatile compounds and sensory data. The source

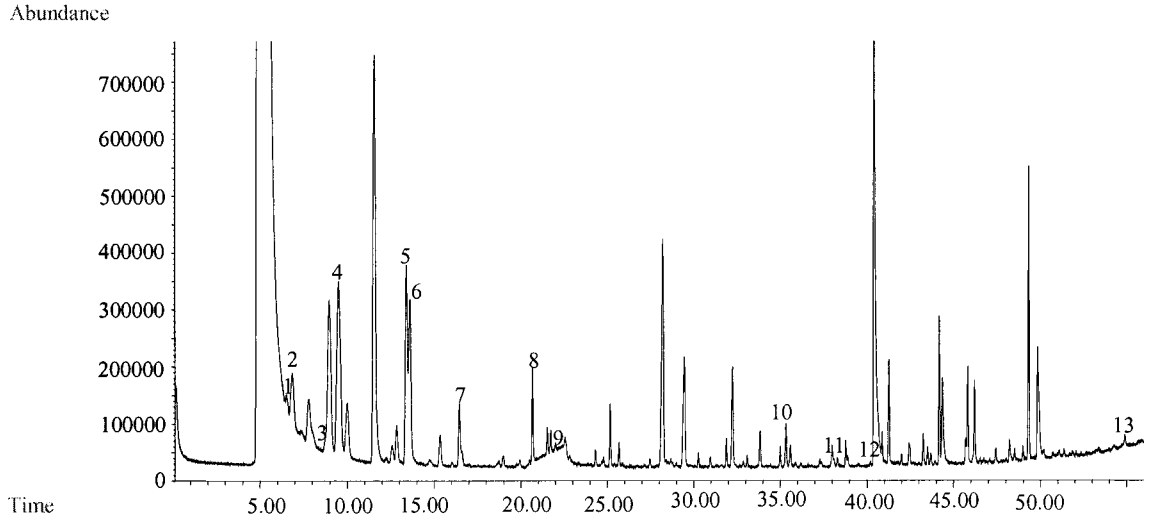

Figure 1. GC−MS Chromatogram of Arabica EC. Peaks: (1) methanethiol; (2) acetaldehyde; (3) propanal; (4) 2-methylpropanal; (5) 2-methylbutanal; (6) 3-methylbutanal; (7) 2,3-butanedione; (8) 2,3-pentanedione; (9) hexanal; (10) 2-ethylpyrazine; (11) 2-ethyl-6-methylpyrazine; (12) 2-ethyl-3,5-dimethylpyrazine; (13) guaiacol.

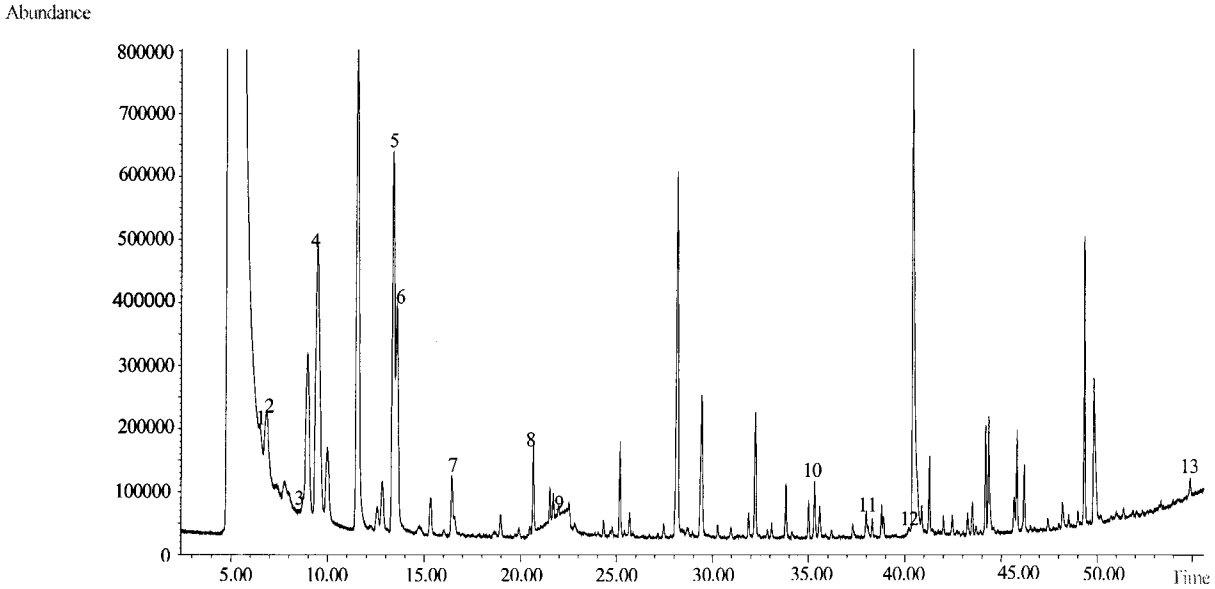

Figure 2. GC−MS Chromatogram of Robusta natural blend EC. Peaks: (1) methanethiol; (2) acetaldehyde; (3) propanal; (4) 2-methylpropanal; (5) 2-methylbutanal; (6) 3-methylbutanal; (7) 2,3-butanedione; (8) 2,3-pentanedione; (9) hexanal; (10) 2-ethylpyrazine; (11) 2-ethyl-6-methylpyrazine; (12) 2-ethyl-3,5-dimethylpyrazine; (13) guaiacol.

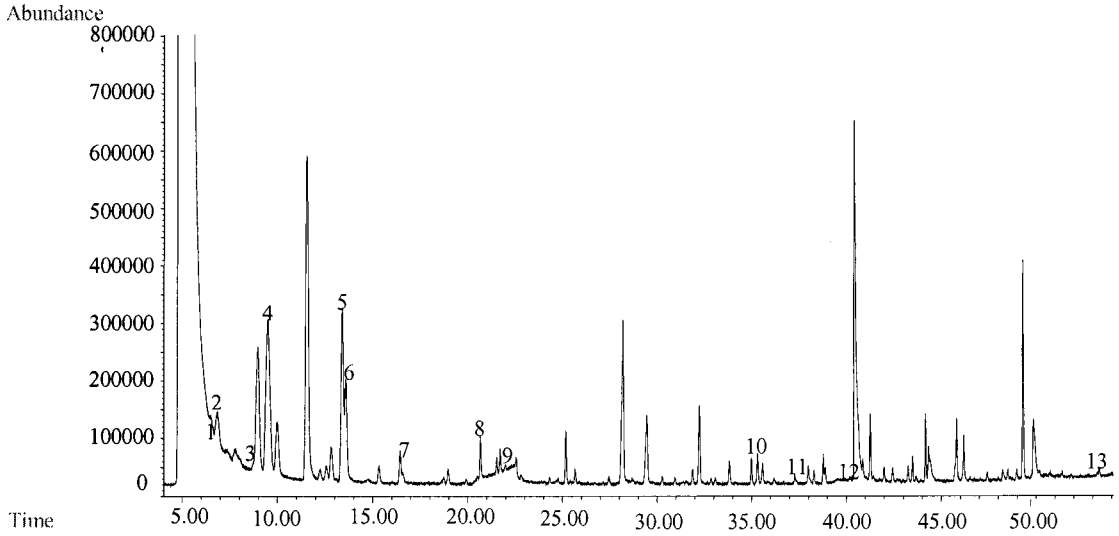

Figure 3. GC−MS Chromatogram of Robusta Torrefacto blend EC. Peaks: (1) methanethiol; (2) acetaldehyde; (3) propanal; (4) 2-methylpropanal; (5) 2-methylbutanal; (6) 3-methylbutanal; (7) 2,3-butanedione; (8) 2,3-pentanedione; (9) hexanal; (10) 2-ethylpyrazine; (11) 2-ethyl-6-methylpyrazine; (12) 2-ethyl-3,5-dimethylpyrazine; (13) guaiacol.

of variation was the type of coffee. T-Tukey was applied as the test a posteriori with a level of significance of 95%.

Pearson's correlation was applied among all the parameters.

Principal component analysis (PCA) was applied to the volatile compounds and sensory ratings (based on the Pearson correlation matrix) in order to determine relationships among variables and differences among EC samples. Principal components (PC) that explained a total variance greater than 85% were selected. The varimax rotation method was applied.

Discriminant analysis (DA) was performed with key odorant results to obtain an easy equation by which EC samples could be classified. Wilks' Lambda stepwise method was used. The criteria were 0.05 for maximum significance of F to enter and 0.10 for minimum significance of F to remove.

All statistical analyses were performed using the SPSS v. 10.0 software package.

RESULTS AND DISCUSSION

The gas chromatograms obtained for the three types of EC samples are shown in Figures 1−3. Seventy-seven volatile compounds were identified by headspace analysis of the EC samples (Table 1): 16 furans, 13 pyrazines, 9 ketones, 8 aldehydes, 6 alcohols, 6 pyrrols, 5 esters, 3 pyridines, 3 sulfur compounds, 2 thiazoles, 2 thiophenes, 1 acid, 1 alkene, 1 lactone, and 1 phenolic compound. Thirteen of these have been considered as key odorants in coffee by other authors (*4*, *6*, *13*, *24*) and they have been quantified (Table 2). Seven positive and eight negative flavors were detected by the panel of judges in the EC samples (Table 3).

All key odorants and flavor sensory results were included in PCA, and two PCs that explained 88.8% were selected (Figure 4).

Among the sulfur compounds identified, methanethiol was reported as one of the key odorants responsible for the freshness aroma in ground roasted coffee (*8*). Also, this compound has been related to sulfurous flavor in brew coffee (*6*). In our study, methanethiol in EC

Table 1. Volatile Compounds Identified in EC Samples by SHGC−MS

KI[a]	ID[b]	compound[c]	KI[a]	ID[b]	compound[c]	KI[a]	ID[b]	compound[c]
		ALKENES	1516	C	2-furfuryl methyl sulfide	1542	A	1H-pyrrole
624	C	1,3-pentadiene	1519	C	furfuryl formate	1661	C	2-formyl-1-methylpyrrole
		SULFUR COMPOUNDS	1536	B	2-acetylfuran		C	N-furfurylpyrrole
635	C	methanethiol*	1559	C	furfuryl acetate			PYRIDINES
671	A	dimethyl sulfide	1605	C	5-methylfurfural	1203	B	pyridine
1077	B	dimethyl disulfide	1636	C	2-furfurylfuran	1239	C	2-methylpyridine
		ALDEHYDES	1686	C	furfuryl alcohol	1413	C	3-ethylpyridine
645	A	acetaldehyde*			KETONES			PYRAZINES
712	A	propanal*	753	A	2-propanone	1231	B	pyrazine
747	A	2-methylpropanal*	866	A	2-butanone	1288	B	2-methylpyrazine
839	C	butanal	962	A	2,3-butanedione*	1347	B	2,5-dimethylpyrazine
880	C	2-methylbutanal*	1053	C	3-hexanone	1353	B	2,6-dimethylpyrazine
884	A	3-methylbutanal*	1058	A	2,3-pentanedione*	1359	B	2-ethylpyrazine*
1084	A	hexanal*	1138	A	3-penten-2-one	1372	C	2,3-dimethylpyrazine
1102	C	2-methyl-2-butenal	1143	C	3,4-hexanedione	1411	C	2-ethyl-6-methylpyrazine*
		ESTERS	1323	C	1-hydroxy-2-propanone	1419	C	2-ethyl-5-methylpyrazine
682	C	formic acid, methyl ester	1554	C	1-acetyloxy-2-butanone	1432	C	2-ethyl-3-methylpyrazine
782	C	acetic acid, methyl ester			ALCOHOLS	1447	C	N-propylpyrazine
850	B	acetic acid, ethyl ester	913	C	ethanol	1467	C	2-vinylpyrazine
872	C	propanoic acid, methyl ester	1103	A	2-methyl-1-propanol	1475	C	2-ethyl-3,5-dimethylpyrazine*
1484	C	1-hydroxy-2-propanone acetate	1220	C	3-methylbutan-1-ol	1521	C	2-methyl-6-vinylpyrazine
		FURANS	1264	C	3-methyl-3-buten-1-ol			THIAZOLES
716	A	furan	1337	C	3-methyl-2-buten-1-ol	1270	C	1,3-thiazole
832	C	3-methylfuran	1509	C	2-ethyl-1-hexanol	1304	C	4-methylthiazole
858	A	2-methylfuran			THIOPHENES			ACIDS
930	B	2,5-dimethylfuran	1021	A	thiophene	1480	B	acetic acid
1075	C	2-vinylfuran	1097	B	2-methylthiophene			LACTONES
1160	B	2-vinyl-5-methylfuran			PYRROLS	1673	C	γ-butirolactone
1251	B	2-(methoxymethyl)furan	1149	B	1-methylpyrrole			PHENOLIC COMPOUNDS
1283	B	2-methyltetrahydrofuran-3-one	1194	C	1-ethyl-1H-pyrrole		C	2-methoxyphenol (guaiacol)*
1490	C	2-furancarboxaldehyde	1225	D	2,5-dimethylpyrrole			

[a] KI, Kovats index calculated for the HP-Wax capillary column. [b]ID, Identification. Reliability of the identification proposal is indicated by the following: A, mass spectrum, retention time, and Kovats index according to standards; B, mass spectrum and Kovats index according to literature data; C, mass spectrum, compared with Wiley mass spectral databases. [c]Asterisks denote key odorants quantified in this work.

Table 2. Relative Percentages of Key Odorants in EC Samples[a]

KI[b]	ID[c]	key odorant	Arabica ($n = 6$) $\bar{X} \pm$ SD	Robusta natural blend ($n = 6$) $\bar{X} \pm$ SD	Robusta Torrefacto blend ($n = 6$) $\bar{X} \pm$ SD
		SULFUR COMPOUNDS			
635	C	methanethiol	0.13 ± 0.01^{c}	0.08 ± 0.01^{a}	0.11 ± 0.02^{b}
		ALDEHYDES			
645	A	acetaldehyde	0.36 ± 0.02^{b}	0.35 ± 0.04^{b}	0.25 ± 0.01^{a}
712	A	propanal	0.52 ± 0.07^{b}	0.50 ± 0.07^{b}	0.35 ± 0.04^{a}
747	A	2-mehylpropanal	1.80 ± 0.25^{a}	2.55 ± 0.35^{b}	1.93 ± 0.17^{a}
880	C	2-methylbutanal	1.25 ± 0.11^{a}	2.33 ± 0.34^{b}	1.43 ± 0.19^{a}
884	A	3-methylbutanal	2.61 ± 0.29^{b}	3.33 ± 0.56^{c}	1.92 ± 0.24^{a}
1084	A	hexanal	0.05 ± 0.00^{b}	0.06 ± 0.00^{c}	0.03 ± 0.00^{a}
		KETONES			
962	A	2,3-butanedione	0.42 ± 0.04^{c}	0.36 ± 0.04^{b}	0.27 ± 0.02^{a}
1058	A	2,3-pentanedione	0.63 ± 0.04^{c}	0.42 ± 0.03^{b}	0.33 ± 0.03^{a}
		PYRAZINES			
1359	B	2-ethylpyrazine	0.10 ± 0.02^{a}	0.17 ± 0.01^{c}	0.13 ± 0.02^{b}
1411	C	2-ethyl-6-methylpyrazine	0.06 ± 0.01^{a}	0.13 ± 0.02^{c}	0.08 ± 0.01^{b}
1475	C	2-ethyl-3,5-dimethylpirazine	0.04 ± 0.01^{a}	0.07 ± 0.01^{b}	0.06 ± 0.01^{b}
		PHENOLIC COMPOUNDS			
	C	guaiacol	0.11 ± 0.01^{c}	0.09 ± 0.01^{b}	0.07 ± 0.01^{a}

[a] In each row, different superscripts indicate significant difference ($p < 0.05$) among EC samples. [b] KI, Kovats index calculated for the HP-Wax capillary column. [c] The reliability of the identification proposal is indicated by the following: A, mass spectrum, retention time, and Kovats index according to standards; B, mass spectrum and Kovats index according to literature data; C, mass spectrum, compared with Wiley mass spectral databases.

samples had significant correlation with freshness (0.567; $p < 0.05$), both included in PC1, but not with sulfurous flavor, which was included in PC2.

Among the aldehydes identified, many of them have been quantified as key odorants. Acetaldehyde and propanal may be responsible for the fruity flavor in brew coffee (*6*). In EC samples, fruity flavor was very significantly correlated ($p < 0.01$) with acetaldehyde (0.627) and propanal (0.594). However, although these key odorants were included in PC2, fruity flavor was in PC1 but with a high loading in PC2 (Figure 4). Mayer et al. (*20*), in an aroma model for the coffee brew, observed that methanethiol produced a synergistic effect with acetaldehyde, increasing fruity flavor. This fact might explain the correlation found between methanethiol and fruity (0.616; $p < 0.01$), both included in PC1.

2-Methylpropanal, 2-methylbutanal, and 3-methylbutanal, which are the Strecker degradation products of Valine, Isoleucine, and Leucine, were proposed as responsible for malty flavor in brew coffee (*6*, *7*).

Table 3. Sensory Profile of EC Samples

flavor attributes[a]	Arabica ($n = 6$) $\bar{X} \pm$ SD	Robusta natural blend ($n = 6$) $\bar{X} \pm$ SD	Robusta Torrefacto blend ($n = 6$) $\bar{X} \pm$ SD
POSITIVE			
fruity/winey	28.5 ± 1.6^{c}	4.9 ± 1.8^{b}	0.0 ± 0.0^{a}
malty/cereal	23.5 ± 3.8^{c}	18.3 ± 1.8^{b}	8.3 ± 1.9^{a}
freshness	18.5 ± 1.6^{b}	10.0 ± 0.0^{a}	8.3 ± 1.9^{a}
buttery	15.2 ± 2.0^{b}	8.3 ± 1.9^{a}	8.3 ± 1.9^{a}
spicy	3.3 ± 0.0^{b}	0.0 ± 0.0^{a}	0.0 ± 0.0^{a}
caramel-like	11.7 ± 1.8^{b}	0.0 ± 0.0^{a}	0.0 ± 0.0^{a}
chocolate-like	8.3 ± 1.8^{b}	0.0 ± 0.0^{a}	0.0 ± 0.0^{a}
NEGATIVE			
woody/papery	15.2 ± 2.0^{a}	33.3 ± 7.7^{b}	41.5 ± 1.6^{c}
roasty/burnt	33.0 ± 0.0^{a}	51.8 ± 5.7^{b}	55.0 ± 2.2^{b}
acrid	13.0 ± 0.0^{a}	53.3 ± 7.3^{b}	68.5 ± 1.6^{c}
fermented	0.0 ± 0.0^{a}	15.0 ± 1.8^{c}	11.6 ± 1.8^{b}
earthy/musty	8.3 ± 1.8^{a}	15.0 ± 1.8^{c}	11.6 ± 1.8^{b}
rancid	0.0 ± 0.0^{a}	0.0 ± 0.0^{a}	3.3 ± 0.0^{b}
burnt rubbery	0.0 ± 0.0^{a}	6.7 ± 0.0^{b}	25.0 ± 5.5^{c}
sulfurous	0.0 ± 0.0^{a}	0.0 ± 0.0^{a}	8.3 ± 1.8^{b}

[a] Results are expressed as the percentage of judges that perceived each flavor attribute. In each row, different superscripts indicate significant difference ($p < 0.05$) among EC samples.

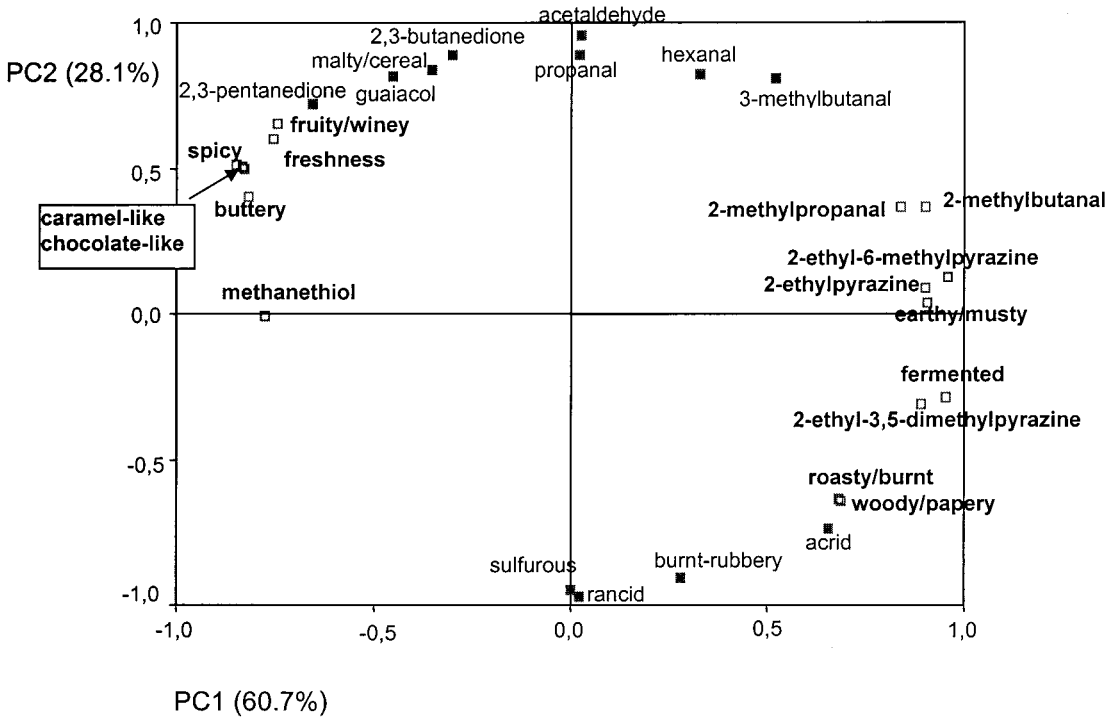

Figure 4. Principal component loadings for the EC variables: □ **PC1**; ■ PC2.

Furthemore, in ground roasted coffee, 2-methylbutanal was described as fermented by Holscher et al (*8*). In our work, no correlation between malty flavor and Strecker aldehydes was found; possibly because of masking by other more potent odorants in the EC samples. On the other hand, a highly significant correlation between fermented flavor and 2-methylbutanal was found (0.754; $p < 0.001$); both were included in PC1.

From the nine ketones identified, 2,3-butanedione and 2,3-pentanedione were quantified as key odorants. Blank et al. (*4*) associated these compounds with buttery flavor in ground coffee and coffee brew. In our EC samples, this flavor was also correlated with 2,3-butanedione (0.503; $p < 0.05$) and 2,3-pentanedione (0.839; $p < 0.001$). However, in PCA (Figure 4), both ketones were unexpectedly included in a PC different from that of the buttery flavor, but the three variables were included in the Arabica EC area (Figure 5). Semmelroch and Grosch (*7*) obtained higher concentrations of diones than Strecker aldehydes in coffee brew by filtering. By contrast, EC percolation seems to contribute to the extraction of Strecker aldehydes as opposed to diones, obtaining less mild aroma brews.

Many pyrazines are recognized as the volatile contributing to roasted aromas of cooked foods (*25*). In ground roast coffee and coffee brew, the pyrazines have been associated with roasty and earthy/musty flavors (*4, 24*). Among the 13 pyrazines identified, three have been quantified as key odorants. 2-ethyl-3,5-dimethylpyrazine, one of the most potent odorants in coffee (*4*), has been correlated with woody/papery (0.832; $p < 0.001$), roasty/burnt (0.789; $p < 0.01$), and earthy/musty flavors (0.699; $p < 0.01$) in EC samples. Also, in our work, the other two pyrazines quantified, 2-ethylpyrazine and 2-ethyl-6-methylpyrazine, have been associated

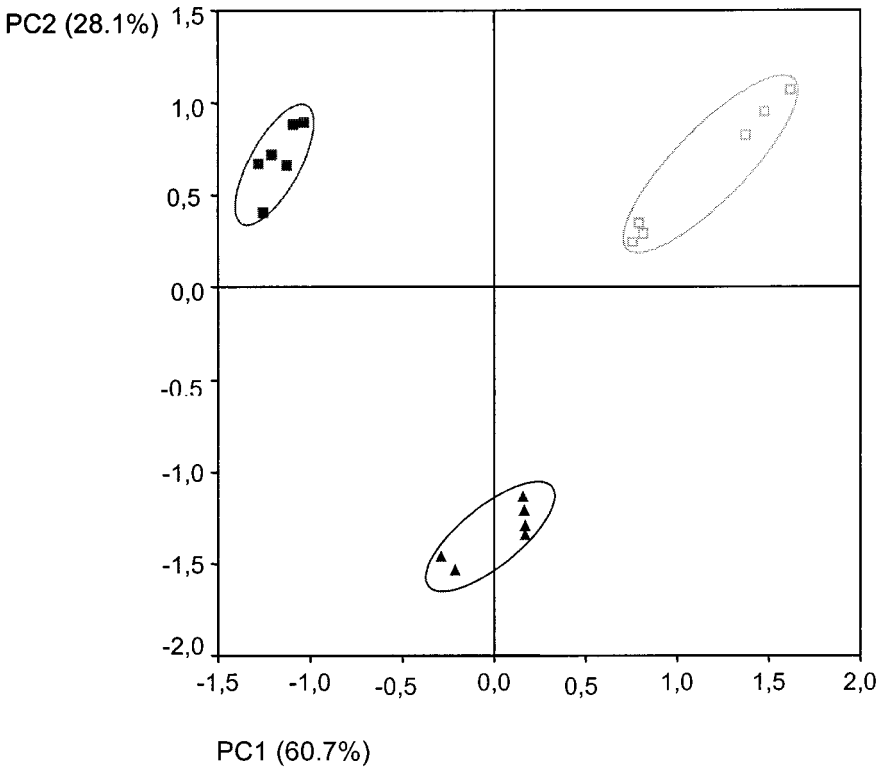

Figure 5. Normalized PCA scores of the EC samples: ▲ Robusta Torrefacto blend; □ Robusta natural blend; ■ Arabica.

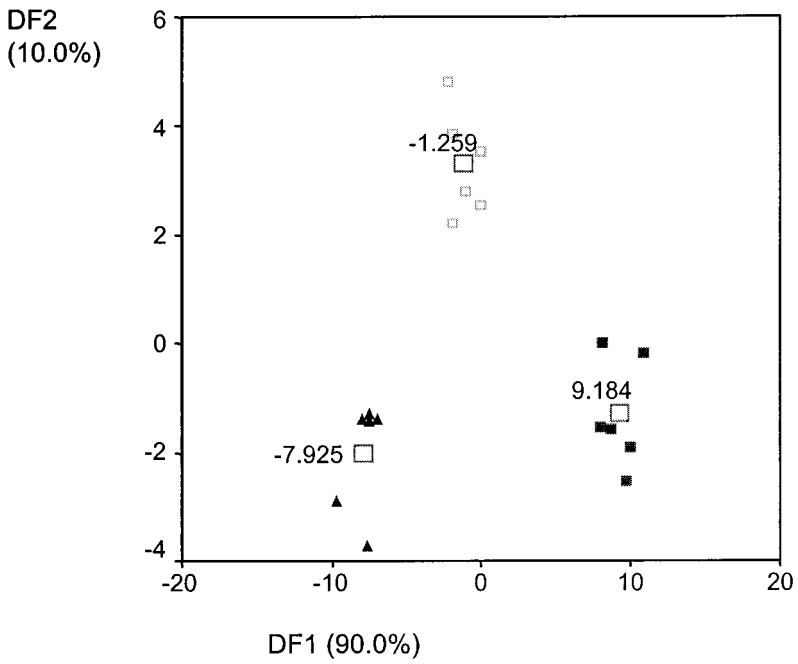

Figure 6. Discriminant scores and centroid values of the EC samples: ▲ Robusta Torrefacto blend; □ Robusta natural blend; ■ Arabica.

with woody/papery (0.593, $p < 0.01$; 0.604, $p < 0.01$, respectively), roasty/burnt (0.551, $p < 0.05$; 0.552, $p < 0.05$), and earthy/musty (0.681, $p < 0.01$; 0.816, $p < 0.001$). Woody/papery and roasty/burnt might be mainly produced by 2-ethyl-3,5-dimethylpyrazine, and earthy/musty flavor seems to be more influenced by 2-ethyl-6-methylpyrazine in EC samples. These three pyrazines and flavors were included in PC1.

The guaiacol, a phenolic compound, is responsible for phenolic and spicy aromas (*4*) and phenolic and burnt flavors (*6*). In EC samples, a highly significant correlation ($p < 0.001$) was found only between this compound and spicy flavor (0.792).

Arabica and Robusta EC samples were separated by PC1 (60.7% of the total variance). Arabica EC samples were defined by parameters with negative loading in PC1 and positive loading in PC2. So, Colombian EC could be described as mild and sweet (caramel-like, chocolate-like, and buttery), fruity and fresh flavors, and some malty/cereal notes. In the same area methanethiol, some aldehydes, and diones were included. Although guaiacol was in the Arabica area, it could be due to a

Table 4. Classification Results of EC Samples with DF1

	experimental group (count, percentage)					
real group $n = 6$	Arabica		Robusta natural blend		Robusta Torrefacto blend	
Arabica	6	100.0%	0	0.0%	0	0.0%
Robusta natural blend	0	0.0%	6	100.0%	0	0.0%
Robusta Torrefacto blend	0	0.0%	0	0.0%	6	100.0%

higher degree of roast in commercial Colombian coffee so as to decrease the acidity and increase the body of brew coffee (*26*).

Robusta natural and Robusta Torrefacto EC were separated by PC2 (28.1%). Robusta natural EC samples seem to be defined by Strecker aldehydes and less potent pyrazines smelling earthy/musty, and in addition, compared with Arabica EC, other negative notes tended to increase. The higher amount of Strecker aldehydes in Robusta than in Arabica coffee have been reported by some authors (*6*), also in EC by Liardon and Ott (*3*). Robusta Torrefacto EC samples were clearly defined by the most negative flavors and 2-ethyl-3,5 dimethylpyrazine.

The separation of three EC samples by aroma characteristic allowed us to think of the possibility of discriminating them by a few key odorants. Then, discriminant analysis was applied and two discriminant functions (DF) were obtained. Figure 6 shows the different sample results for DF1 and DF2, and the DF1 centroids values. The DF1 which explained 90.0% of the total variance is

$$y = -5.303 \cdot (\text{2-methylpropanal}) + 58.705 \cdot (\text{2,3-butanedione}) + 218.234\ (\text{hexanal}) - 156.202 \cdot (\text{2-ethyl-3,5-dimethylpyrazine}) - 10.799$$

The DA proposed a function which was very easy to apply. DF1 allowed the classification of the EC samples into their respective groups, with a success rate of 100% (Table 4). This procedure might be considered a first valuable approach that should be validated by other EC samples.

In conclusion, the key odorants and the sensory flavor profile combined by means of PCA allowed the separation and aroma characterization of EC samples with different botanical varieties (PC1) and types of roast (PC2). Furthemore, some correlations between key odorants and flavor characteristics were obtained. Some of them were similar to those proposed by different authors for ground roast coffee and coffee brew. But new, different correlations were obtained for EC samples.

A very simple discriminant function, which included four key odorants, was obtained allowing the classification of each EC sample into its respective group, with a success rate of 100%.

ABBREVIATIONS USED

EC, espresso coffee; PCA, principal component analysis; PC1, first principal component; PC2, second principal component; DA, discriminant analysis; DF1, first discriminant function; DF2, second discriminant function.

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