Multivariate Methods for Characterization and Classification of Espresso Coffees from Different Botanical Varieties and Types of Roast by Foam, Taste, and Mouthfeel

Laura Maeztu, Susana Andueza, Carmen Ibañez, M. Paz de Peña, José Bello, and Concepción Cid*

Departamento de Bromatología, Tecnología de Alimentos y Toxicología, Facultad de Farmacia, Universidad de Navarra, E-31080 Pamplona, Spain

Three espresso coffee (EC) samples of different botanical varieties and types of roast were prepared in standard conditions using an experimental EC prototype: Arabica coffee, Robusta Natural blend, and Robusta Torrefacto blend (a special roast by adding sugar). The ECs were characterized with regard to the physical parameters, amount of total solids, total solids on filtrate, lipids, caffeine, trigonelline, and chlorogenic acids by HPLC, and sensory descriptive analysis related to foam appearance, taste, and mouthfeel. Principal component analysis (PCA) was applied to differentiate the EC samples. Arabica and Robusta samples were separated successfully by principal component 1 (55.3% of variance) including physicochemical and sensory parameters related to foam and taste of ECs. Torrefacto and Robusta Natural EC samples were separated by principal component 2 (20.7% of total variance) including mouthfeel and other attributes of color foam. Some interesting correlations among sensory and physicochemical variables were found. A very simple discriminate function was obtained by discriminate analysis allowing the classification of each EC sample into its respective group with a success rate of 100%.

Keywords: *Espresso coffee; sensory descriptive analysis; multivariate analysis; principal component analysis; discriminate analysis; brew coffee; Arabica coffee; Robusta coffee; Torrefacto roast*

INTRODUCTION

Espresso is an increasingly popular drink. Every day, more than 50 million cups of espresso coffee (EC) are consumed throughout the world (*1*, *2*). By definition, EC is a “poliphasic beverage prepared from roast and ground coffee and water alone, constituted by a foam layer of small bubbles with a particular tiger-tail pattern, on top of an emulsion of microscopic oil droplets in an aqueous solution of sugars, acids, protein-like material, and caffeine, with dispersed gas bubbles and solids” (*1*). These characteristics of EC are reponsible for their peculiar sensorial properties. A fine EC should have a great amount of persistent, consistent, and hazelnut foam with “tiger-skin” effect, a bitter/acid balance taste, and a strong body (*1*, *3*).

An important factor in the final quality of EC is the ground roasted coffee used which could be defined by the type of coffee and the roasting process. Comparison of EC from Arabica and Robusta varieties have been studied from a physicochemical point of view (*1*, *4*), but no sensory comparative studies in EC have been found.

In the roasting process, the influence of the degree of roast in the final quality of the EC has been reported by Nunes et al. (*4*), but another type of roast, such as “Torrefacto”, has not been studied. Torrefacto is a roasting process where sugar is added to Robusta coffees. This type of roast produces caramelization of sugar which contributes to the brownish color of the coffee brew and covers the negative sensory characteristics of low quality Robusta coffees. Usually, Torrefacto coffee is blended with Natural roast to be consumed. This technique of roast is used in some countries, such as Spain, Portugal, Costa Rica, and Argentina.

The aim of this paper was to differentiate and to classify ECs prepared from different botanical varieties (Arabica and Robusta) and types of roast (Natural and Torrefacto) according to the sensory and physicochemical characteristics related to visual foam appearance, taste, and mouthfeel, using multivariate analysis. Furthermore, the correlations among different parameters have been studied.

MATERIALS AND METHODS

Materials. Three roasted coffee samples, Arabica coffee (pure *Coffea arabica* from Colombia, 2.0% water content), Robusta Natural blend (80:20 blend of *Coffea canephora* and *C. 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 lots for each coffee sample were used.

EC Samples and Preparation for Analysis. The ECs were prepared 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: 9 atm, water temperature: 96 °C (erogation temperature: 90 ± 2 °C), extraction time: 21 ± 3 s, holder filter diameter: 38 mm. Twenty ECs of each coffee sample were prepared to be analyzed by triplicate.

pH, Density, Viscosity, and Surface Tension. The EC samples were rapidly cooled at 20 °C, and the pH (Orion 420 A Benchtop pH meter), density (densimeter), viscosity (Ostwald viscosimeter), and surface tension (Traube estalagmometer) were measured.

* Corresponding author. Phone: +34-948-425600 (Ext. 6264). Fax: +34-948-425659. E-mail: ccid@unav.es.

10.1021/jf010314l CCC: $20.00
Published on Web 09/13/2001

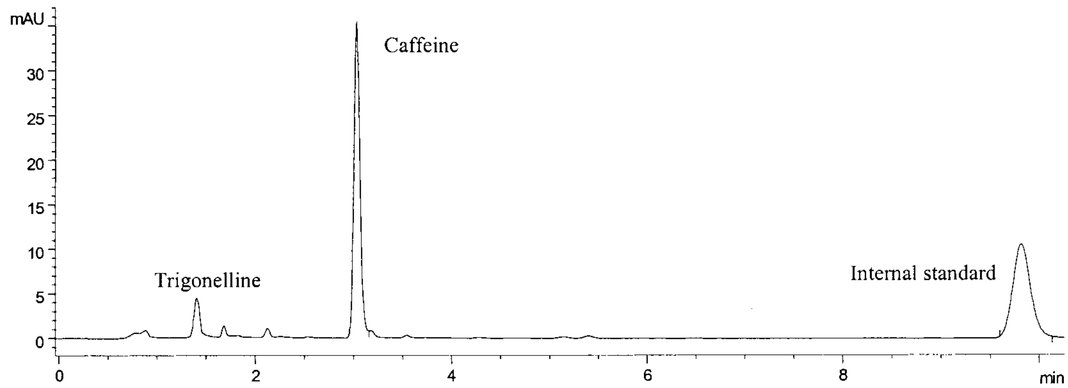

Figure 1. Chromatogram of caffeine and trigonelline analysis.

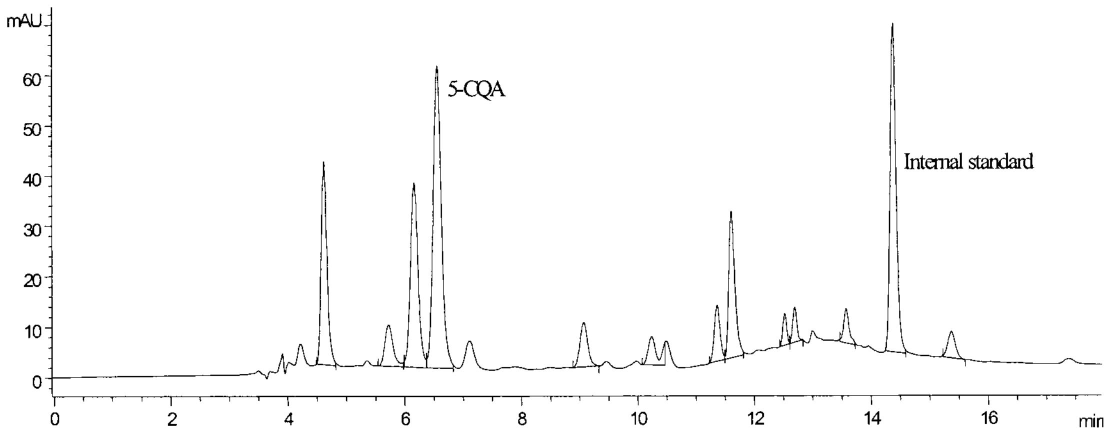

Figure 2. Chromatogram of 5-CQA analysis.

Foam Index and Persistence of Foam. The *foam index* was defined as the ratio, in percentage, of EC foam and liquid volumes measured inmediately after the extraction of EC using a 100-mL graduated cylinder. The *persistence of foam* was defined as the time (in minutes) that the liquid phase below the cream layer took to appear during cooling at room temperature.

Total Solids, Extraction, Concentration, Total Solids on Filtrate. The *total solids* were determined by oven drying 40 mL of EC to a constant weight (14 h, 102 ± 3 °C). The *extraction* was defined as the percentage of total solids with respect to ground roast coffee dose (7.5 g). The *concentration* was defined as the percentage of total solids with respect to the EC volume (40 mL). The *total solids on filtrate* were determined by oven drying 40 mL of EC after filtering with Whatman 1 to a constant weight (14 h, 102 ± 3 °C).

Lipids. The total lipids amount was determined by liquid–liquid extraction using trichloromethane. Twenty milliliters of EC were extracted by extracting with 20 mL of trichloromethane three times in a separating funnel. The organic fraction was washed with distillated water three times. Total lipids were quantified by weight after evaporation of the solvent.

Caffeine and Trigonelline. *Extract Preparation and Cleanup for HPLC Analysis.* For extraction of caffeine and trigonelline compounds, 2 mL of internal standard (pentoxiphylline, Sigma), 75 mL of distilled water, and 2 mL of lead 2-hydroxide acetate (Panreac) were added to 5 mL of EC in a 100-mL volume flask. After 10 min, the extract was diluted to 100 mL and filtered in Whatman 3. Solution cleanup was carried out on a C_{18} Sep-Pack cartridge 51910 (Waters Corp., Milford, MA). A total of 6 mL of extract was loaded onto the cartridge previously conditioned with 5 mL of acetonitrile and 3 mL of distilled water. The cartridge was eluted with 10 mL of acetonitrile/water (30:70). The eluate was diluted to 50 mL.

HPLC Analysis. HPLC analysis was achieved with an analytical HPLC unit (Hewlett-Packard 1100) equipped with a Rheodyne injector of 20 μL loop, a binary pump and a Diode-array detector. A reversed-phase Hypersil-ODS (5 μm particle size, 250 × 4.6 mm) column was used. The mobile phase was an acetonitrile/water (15:85) in isocratic condition at a constant flow rate of 2.0 mL min^{-1} at 25 °C. Detection was accomplished with a diode-array detector, and chromatograms were recorded at 280 nm (Figure 1). The method was validated obtaining a linear relationship between the concentration of both compounds and the UV absorbance ($r = 0.999$ and $r = 0.998$ for caffeine and trigonelline, respectively). The recovery values were 101.9 ± 2.4% for caffeine and 104.0 ± 5.7% for trigonelline. The precision and the accuracy were lower than 15% in all cases.

Chlorogenic Acids (5-CQA). The extraction of 5-CQA and cleanup were carried out according to Bicchi et al. (*5*). The HPLC equipment has been described previously. The conditions of the gradient solvent system used were 100% citrate–acetic acid buffer solution (pH = 3.0) for 2 min, 85:15 buffer/methanol for 8 min, both at a flow rate of 0.8 mL min^{-1}, and 85:15 buffer/methanol for 5 min at a flow rate of 1.2 mL min^{-1}, at 25 °C. The wavelength of detection was at 325 nm (Figure 2).

Sensory Descriptive Analysis. The sensory properties of the EC samples were measured using a variation of the quantitative descriptive analysis method (*6*). 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 the ability to identify and differentiate the five basic tastes, using UNE 87-003-95 and UNE 87-024-1-95 (*7*). Then, 10 judges were selected.

Table 1. Physicochemical Parameters of EC Samples[a]

physicochemical parameters	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
pH	5.4 ± 0.0^a	5.6 ± 0.1^b	5.6 ± 0.0^b
density (g/mL)	1.010 ± 0.000^a	1.010 ± 0.000^a	1.010 ± 0.000^a
viscosity ($\times 10^{-3}$ N/m^2 s)	1.34 ± 0.11^a	1.26 ± 0.04^a	1.29 ± 0.07^a
surface tension (mN/m)	49.68 ± 1.38^b	50.52 ± 0.21^b	45.76 ± 2.30^a
foam index (%)	12.3 ± 0.2^a	20.3 ± 0.5^b	22.3 ± 0.6^c
persistence of foam (min)	30.27 ± 4.49^b	24.50 ± 2.81^a	$28.36 \pm 1.14^{a,b}$
total solids (mg/mL)	41.69 ± 0.95^b	39.68 ± 1.38^a	43.65 ± 0.76^c
extraction (%)	22.2 ± 0.5^b	21.2 ± 0.7^a	23.3 ± 0.4^c
concentration (%)	4.2 ± 0.1^b	3.9 ± 0.1^a	4.4 ± 0.1^c
total solids on filtrate (mg/mL)	39.10 ± 1.27^a	38.49 ± 1.52^a	42.02 ± 0.82^b
total lipids (mg/mL)	5.85 ± 0.24^c	4.77 ± 0.42^b	4.35 ± 0.19^a
caffeine (mg/mL)	2.09 ± 0.10^a	2.88 ± 0.14^b	2.96 ± 0.10^b
trigonelline (mg/mL)	1.15 ± 0.07^a	1.14 ± 0.05^a	1.33 ± 0.11^b
chlorogenics acids (5-CQA) (mg/mL)	1.30 ± 0.04^a	1.50 ± 0.05^b	1.30 ± 0.02^a

[a] In each row, different superscripts indicate significant difference ($p < 0.05$) among EC samples.

Table 2. Sensory Attributes of EC Samples

sensory attributes	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
body	5.6 ± 0.7^a	5.5 ± 1.1^a	6.3 ± 1.4^b
acidity	5.9 ± 1.4^c	1.9 ± 0.4^b	0.8 ± 0.2^a
bitterness	6.6 ± 0.7^a	7.6 ± 1.2^b	7.4 ± 1.2^b
astringency	6.2 ± 0.8^a	6.6 ± 1.1^{ab}	6.9 ± 1.2^b
aftertaste intensity	5.3 ± 1.3^a	6.2 ± 1.0^b	6.9 ± 1.2^c

[a] In each row, different superscripts indicate significant difference ($p < 0.05$) among EC samples.

Table 3. 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 Sugar blend	0	0.0%	0	0.0%	6	100.0%

Judges were trained over eight 1.5-h sessions. First, during four sessions, descriptive terms about EC were generated and defined through group discussion by selected judges. Second, in four other sessions, individual evaluations of three reference or sample EC (30 min) and consensus about numerical position of every attribute of EC (1 h) was carried out.

During training, a scorecard was developed. The appearance of foam was determined by the percentage of judges that observed the color of foam as clear, hazelnut, or dark, and the consistency was determined as consistent or inconsistent. For attributes such as body, acidity, bitterness, astringency, and aftertaste intensities, 10-cm line scales, typically anchored with the words “none” (0) and “very high” (10) about 1 cm from each end and marked in the middle with “medium” (5) were used.

Descriptive evaluation of the EC samples was then carried out in triplicate over six sessions. Three EC were analyzed per session. Each EC was prepared immediately before taste and served in a white porcelain coffee cup labeled with 3-digit codes monadically. 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 standarized conditions by UNE 87-004-79 (*7*). Rinse water was provided between individual samples.

Statistical Analysis. Analysis of variance (ANOVA) was applied to the physicochemical and sensory data. The source of variation was the type of coffee. T-Tukey was applied as the test a posteriori with a level of significance of 95%.

Principal component analysis (PCA) was applied to the analytical and descriptive ratings (based on the Pearson correlation matrix) to determine relationships among attributes and differences among EC samples. Extraction and concentration were excluded because they are mathematically related to total solids. Factors with eigenvalues greater than 1 were selected. The varimax rotation method was applied.

Discriminant analysis (DA) was performed to obtain an easy equation by which EC samples could be classified. Wilks' Lambda stepwise method was used. The criteria were of 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

Table 1 shows the ANOVA results of the physicochemical parameters. Significant differences were obtained among the three groups of EC in all parameters, except in density and viscosity. The pH of all of our samples were included within the “limit of acceptance” (4.8−6.0) (*8*, *9*).

Table 2 shows the ANOVA results of sensorial parameters. Significative differences were obtained among the three groups of EC in all of the parameters.

Principal Component Analysis (PCA). Four principal components (PC) with eigenvalues higher than 1 were selected by PCA. PC1 and PC2 explained 76% of the total variance. In each PC, the correlated parameters among the variables were included. Figures 4 and 5 show bidimensional representations of PC1 and PC2 scores for all of the variables and samples, respectively.

Arabica and Robusta EC samples were perfectly separated by PC1 (Figure 5). It explained 55.3% of the total variance. This component included the main foam and taste characteristics of EC.

Highly significant ($p < 0.001$) correlations between the foam index and the total solids (0.988), total lipids (−0.902), and pH (0.943) were found. These results were also reported by Nunes et al. (*4*). Nevertheless, another foam characteristic, such as persistence, was not correlated with the foam index because coffee foamability is mainly influenced by the melanoidin type subfraction, whereas foam stability is mainly influenced by the polysaccharide subfraction (*4*, *10*).

With regard to taste characteristics, PC1 included all of the sensory taste parameters (acidity, bitterness, astringency, and aftertaste intensity) and some physicochemical taste parameters (total solids, caffeine, and pH) (Figure 4). The perception of acidity depends not only on pH, but also on the individual acids (*1*, *11*). Although pH was only poorly correlated with perceived

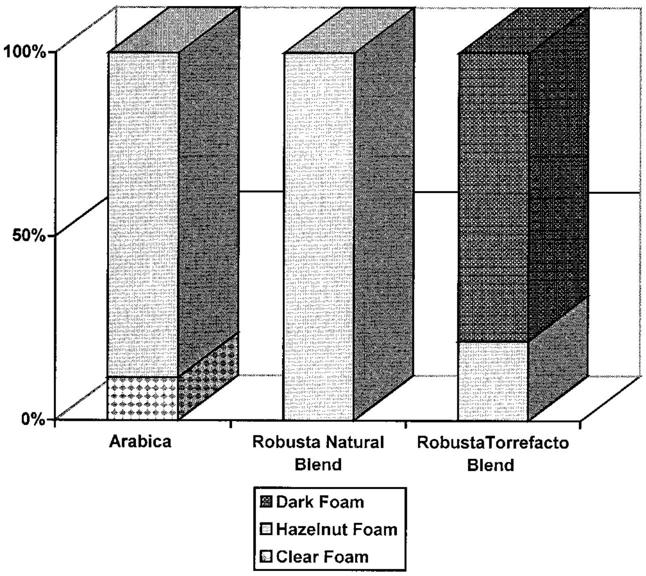

Figure 3. Color of foam of EC samples (percentage of judges who observed the foam as clear, hazelnut, or dark.

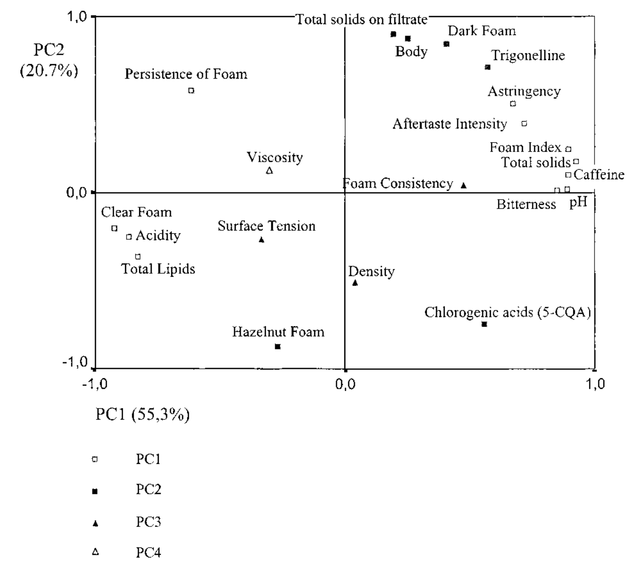

Figure 4. Principal component loadings for the EC variables.

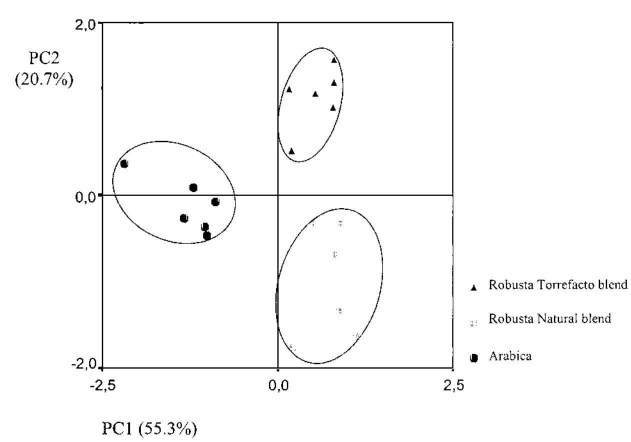

Figure 5. Normalized PCA scores of the EC samples.

acidity in other papers (*12*), a highly significant correlation between acidity and pH (−0.950) was found. Many substances and classes of compounds such as caffeine, 5-CQA, and trigonelline have been implicated as possible contributors to the overall bitter perception in coffee (*13*). In our study, bitterness of EC was significantly ($p < 0.001$) correlated with caffeine contents (0.723) but only poorly correlated ($p < 0.05$) with 5-CQA (0.560) and not correlated at all ($p > 0.05$) with trigonelline, which was included in PC 2 (Figure 4).

Our Arabica EC had a "tiger skin" effect that was identified as clear foam by 11.7% of the panel. Nevertheless, this typical foam effect did not exist in Robusta EC samples where the color of foam was darker (Figure 3). The foamability of Arabica EC samples were less than Robusta EC samples, but higher than 10%, a minimum percentage foam index for a good EC (*1*). Although the total solids of Arabica EC were higher than Robusta Natural EC (Table 1) in the PCA graph (Figure 4), the total solids were graphed in the Robusta EC score area (*1*), near the foam index. In addition, Arabica EC had higher total lipids scores than Robusta.

Arabica EC samples had the highest acidity values and the lowest bitterness values, which were associated with a good acid/bitter balance in comparison with Robusta EC samples (*1*).

Torrefacto and Natural Robusta EC samples were separated by PC2. It explained 20.7% of the total variance. Mouthfeel and other attributes of color foam were included (Figure 4).

The only difference between the two Robusta samples was the addition of sugar in the "Torrefacto" roast process. It may be the origin of the total solids on filtrate increase (which was defined by compounds soluble in water) in Torrefacto EC (Table 1). Furthermore, we found a significant difference in body perception between the Torrefacto EC and the other natural EC's (Arabica and Robusta) (Table 2) and a highly significant ($p < 0.001$) correlation between total solids on filtrate and body (0.802). In some papers, the body perception has been associated with oil droplets (*1*) and insoluble materials in brew coffee (*14*), but not with total solids on filtrate; however, these studies used only natural roast ground coffee. Also, the foam of Torrefacto EC samples were perceived as darker than Robusta Natural EC by 78.3% of the panel judges. The "tiger skin" effect was not perceived in any of the Robusta EC samples. A highly significant ($p < 0.001$) correlation of "dark foam" (percentage of judges who perceived dark color foam), (Figure 3) with total solids on filtrate was found (0.798). This fact also could be explained by the higher content of soluble caramelized sugars in Torrefacto coffee that have been extracted in the brewing process.

Therefore, the Torrefacto roasting process allows the use of low quality Robusta coffees to be added to a blend so as to obtain higher bodies, while EC with darker foams is also obtained.

Discriminant Analysis (DA). 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 99.3% of the total variance is shown:

$$y = -3.810 \bullet \text{astringent} + 0.114 \bullet \text{foam dark} + 49.129 \bullet \text{pH} + 1.919 \bullet \text{foam index} + 2.842 \bullet \text{total solids} - 364.593$$

The DA proposed a function that was very easy to apply because the physicochemical parameters selected in DF1 were very simple to analyze and the sensory attributes were very easy to detect. DF1 allowed the classification of the EC samples into their respective group with a success rate of 100%. This procedure might

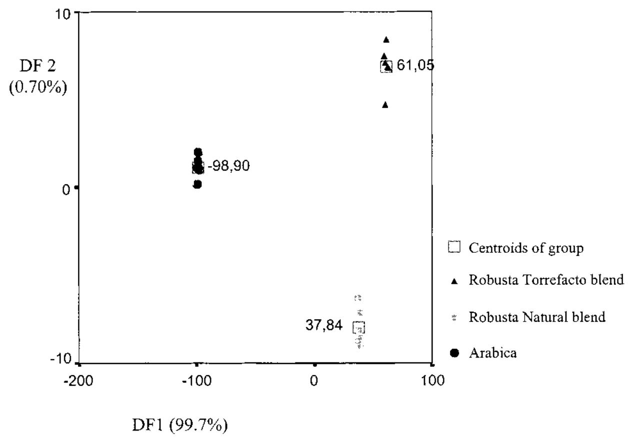

Figure 6. Discriminant scores and centroids values of the EC samples.

be considered as a first valuable approach that should be validated to other EC samples application.

In conclusion, the three EC samples were separated perfectly by PCA. The main differences between Arabica and Robusta coffees were the physicochemical and sensory parameters related to the foam and taste of espresso coffee. The addition of Torrefacto to the blend increased the body and produced dark foam.

A very simple discriminate function was obtained by discriminate analysis allowing the classification of each EC sample into their respective groups with a success rate of 100%.

ABBREVIATIONS USED

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

ACKNOWLEDGMENT

We thank the panel of judges as this study could not be carried out without them.

LITERATURE CITED

(1) Illy, A.; Viani, R. *Espresso Coffee: The Chemistry of Quality*; Illy, A. and Viani, R., Eds; Academic Press Limited 24-28 Oval Road: London, 1995.
(2) Butler, R. Solubles into the millenium. *Tea Coffee Trade J.* **1999**, *171*, 10, 70, 72−74, 76.
(3) Cipolla, M. Today's Espresso Bar: Common Problems and Relative Solutions. *Tea Coffee Trade J.* **1999**, *171*, 5, 32−39.
(4) Nunes, F. M.; Coimbra, M. A.; Duarte, A. C.; Delgadillo, I. Foamability foam stability, and chemical composition of espresso coffee as affected by the degree of roast. *J. Agric. Food Chem.* **1997**, *45*, 3238−3243.
(5) Bicchi, C. P.; Binello, A. E.; Pellegrino, G. M.; Vanni, A. C. Characterization of green and roasted coffees through the Chlorogenic Acid fraction by HPLC-UV and Principal Component Analysis. *J. Agric. Food Chem.* **1995**, *43*, 1549−1555.
(6) Sidel, J. L.; Stone, H. The role of sensory evaluation in the food industry. *Food Quality Pref.* **1993**, *4*, 65−73.
(7) AENOR. Análisis sensorial. Tomo1. Alimentación. Recopilación de Normas UNE, 1997
(8) Dalla Rosa, M.; Barbanti, D.; Lerici, C. R. Changes in Coffee Brews in Relation to Storage Temperature. *J. Sci. Food Agric.* **1990**, *50*, 227−235.
(9) Severini, C.; Giuliani, S.; Pinnavaia, G. G. Studio su diversi sistemi di estrazione della bevanda di caffè (Italian). *Indust. delle Bevande* **1994**, *23*, 6, 227−230.
(10) Petracco, M., Navarini, L., Abatangelo, A., Gombac, V., D'Agnolo, E., Zannetti, F. Isolation and Characterization of a Foaming Fraction from hot Water Extracts of Roasted Coffee. ASIC, 18° Colloque, Helsinki, 1999; pp 95−104.
(11) Woodman, J. S. Carboxylic Acids. In *Chemistry*, Vol. 1; Clarke, R. J., and Macrae, R., Eds. Elsevier Science Publishers LTD Crown House: Barking, Essex, England, 1985.
(12) Voilley, A.; Sauvageot, F.; Simatos, D.; Wojcik, G. Influence of some processing conditions on the quality of coffee brew. *J. Food Process. Preserv.* **1981**, *5*, 135−143.
(13) MacCamey, D. A.; Thorpe, T. M.; McCarthy, J. P. Coffee bitterness. In *Bitterness in Foods and Beverages. Developments in Food Science*; Vol. 25; Rouseff, R. L., Ed. Elsevier Science Publishing: New York, 1990.
(14) Lingle, T. R. Coffee brewing control chart. In *The Coffee Brewing Handbook. A Systematic Guide to Coffee Preparation*; Lingle, T. R., Ed.; Long Beach: Specialty Coffee Association of America, 1996.

Received for review March 7, 2001. Revised manuscript received July 12, 2001. Accepted July 12, 2001. We thank the Comisión Interministerial de Ciencia y Tecnología project (ALI-1999-0319) for their contribution to the financial support of this work. We also thank the Departamento de Industria del Gobierno de Navarra and the Ministerio de Ciencia y Tecnología Español for grants given to L.M. and S.A., respectively.

JF010314L