

## Application of Exploratory Analysis to the Differentiation of Brazilian Coffees

Andréa P. Fernandes<sup>a</sup>, Mirian C. Santos<sup>a</sup>, Sherlan G. Lemos<sup>a,b</sup>, Márcia M.C. Ferreira<sup>c</sup>, Ana Rita A. Nogueira<sup>b</sup>, Joaquim A. Nóbrega<sup>a</sup>

<sup>a</sup>*Grupo de Análise Instrumental Aplicada (GAIA), Departamento de Química, Universidade Federal de São Carlos, São Carlos, SP, Brasil.*

<sup>b</sup>*Embrapa Pecuária Sudeste, São Carlos, SP, Brasil.*

<sup>c</sup>*Instituto de Química, Universidade Estadual de Campinas, Campinas, SP, Brasil.  
[deapfernandes@yahoo.com.br](mailto:deapfernandes@yahoo.com.br)*

Coffee is one of the most popular drinks in the world and its huge commercial and social importance is obvious. In terms of international trade, coffee is the world second product in value, putting in motion approximately 35 billion US\$ per year, being supplanted only by petroleum. Brazil continues to be the greatest producer and exporter of this product. Taking into account these aspects, the characterization of the essential and toxic elements in coffee samples is of great interest. The developed work investigated the application of statistical methods to the analysis of samples of Brazilian coffee. Forty-three samples of coffee from different geographic origins were selected and analyzed by Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA) with relation to its mineral content. Data analysis was performed using the software Pirouette 2.7 (Infometrix, Seattle, WA).

The determination of Al, Ba, Ca, Cu, Fe, K, Mg, Mn, Na, Pb, S, Si, Sr and Zn was carried out in the samples by axial viewing inductively coupled plasma optical emission spectrometry (ICP OES, Vista Varian, Mulgrave, Australia). Prior to analysis, 1.0 g of sample was added to 10 ml of boiling deionized water and mixed for extraction. After that, the slurries were centrifuged during 6 min (4000 rpm) and 5 ml of supernatant in 0.1% v/v nitric acid solution were utilized for emission measurements.

The multivariate approach of PCA and HCA allowed us to distinguish between the industrialization type (roasted and ground coffee and instant soluble coffee) and the production mode (organically or conventionally produced) and determine which are the most important parameters to characterize them. All the variables were auto scaled to avoid misjudges on data analysis. The results demonstrated that K, Mg, Na and S were the principal elements for discrimination among samples. Three principal components were accounted for explain 78% of the total data variance. With relation to the distinction between organic and conventional type coffee, the PCA analysis pointed out to the parameters Al, Mg, Cu, Ba and Sr as the responsible for the separation, being the elements Al and Mg more easily extractable in organic type coffee. Three PCs were accounted for explain 71% of the total data variance in this case.