

APPLICATION OF CHEMOMETRIC METHODS IN THE COFFEE BLENDS EVALUATION

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Consumers approves a product when it is produced with a certain quality standard. The manufacturer must therefore make sure that the quality of his product is controlled. In coffee, an important part of this control is the coffee specie used. There are approximately eighty coffee species however only two are of commercial importance¹, *arabica* and *robusta*. *Arabica* coffee presents more pronounced and refined flavor, and *robusta* generally is mixed with *arabica* to make the product cheaper.

Our work proposes a evaluation of coffee blends with several proportions this species. The information about the extracted components in a cup of coffee is obtained through ¹H NMR spectra and, then it is analysed by chemometric methods.

The ¹H NMR spectra were recorded on a Bruker DRX400 spectrometer, in triplicate. In 0.6 mL of coffee solution we added three drops of D₂O for lock signal and the temperature was maintained constant, 303K. For chemometric analysis the Pirouette[®] software package was used. An exploratory study from spectroscopic data was done using the Principal Components Analysis (PCA) and Hierarchical Clusters Analysis (HCA) methods. Classification and calibration models also were built from k-Nearest Neighbor (KNN) and Partial Least Squares (PLS)² methods, respectively. After to build the models they were validated with external samples, doing the prediction of class (more *arabica* content/more *robusta* content) or of coffee specie amount into a unknown sample.

This work shows that ¹H NMR spectroscopy together with the chemometric methods can be used in a “easy way” to identify and quantify the *arabica* and *robusta* contents in coffee blends.

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