Metabolomic approach and data analysis: mass spectrometry in green coffee beans of Paraná

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Key words: *coffee, metabolomics, data analysis.*

Introduction

Brazil is the largest producer of green coffee beans, as *Coffea arabica* L. and *C. canephora* var. *Robusta* around 72 and 28%, respectively. Among the growing states are Paraná with important participation in the Brazilian economy. Several state producers aims recognition of the region to obtain a seal quality. The study of the particular characteristics of coffee beans searches for information on production and cultivars related to chemical profile. Analysis of a large amount of samples such as used in this work, from different regions of the State of Paraná, needs a metabolomics approach, here performed by mass spectrometry and data analysis by chemometrics that enable information on the differences and similarities between the coffee beans.

Results and discution

The green coffee beans were provided by IAPAR. Twenty-four (60repetitions) samples were milled and subjected to extraction with methanol:deionised water (70:30, v / v) in ultrasonic bath. The extract was filtered, subsequently diluted to mass spectrometry analysis by ion cyclotron resonance and Fourier transform (FT- ICRMS) in negative mode ion (ESI). It was possible to identify 15 substances including phenolic compounds, fatty acids, sucrose and glycosylated diterpenes, as described in the literature[2]. Mass spectra obtained from samples showed similar profile for all regions. The data was processed with statistical tools, principal component analysis(PCA), and to observe the behavior of the 15 substances in the ratio *m/z* with their relative intensities(RI). From this it was suggest a differentiation between the post-harvest treatment groups(natural and peeled coffee) and between the producing regions (North Central and Pioneiro).

In relation to post-harvest treatment, the class of atractylosides was responsible for the classification of the samples: natural coffee (green color) and peeled coffee (yellow in Figure 1).

The ions with higher contribution to this grouping are the *m/z* 727.3546 (Atractyloside I); 565.3018 (Atractyloside III); 771.3444 (carboxyatractyloside I).

For most samples the process to which coffee was submitted could also be observed. However, it was not possible to define which ions were responsible for this similarity.

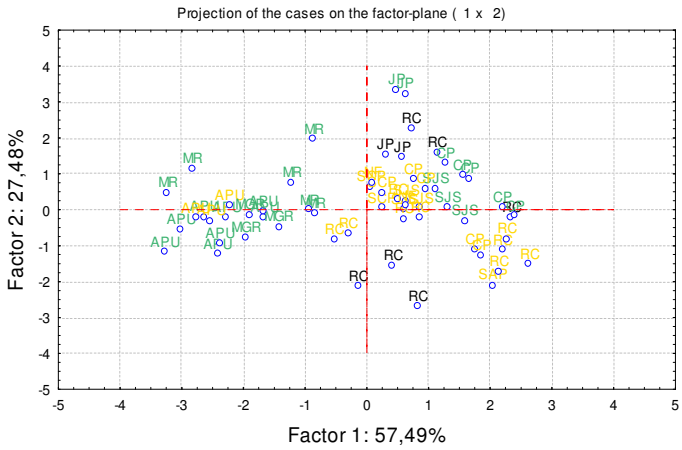

Figure 1. Separation of green coffee samples from Paraná [27 samples of natural coffee (green color) and 25 samples of peeled coffee (yellow color) and 8 micro lots of natural and peeled].

Conclusion

The metabolomic approach on the analysis by ESI (-) FT-ICRMS identified 15 metabolites present in green coffees, such as phenols compounds, fatty acids, sucrose and glycosylated diterpenes. With support of multivariate data analysis, we observed differentiation between North Central and North Pioneiro regions and among post-harvest treatments, where atractylosides were mainly responsible for the grouping.

Ackonowledgements

CNPq, CAPES, IAPAR, Embrapa Café, Laboratório ThoMSon e Faperj.

[1] CONAB: Página na *internet* da Companhia Nacional de Abastecimento, http://www.conab.gov.br/, acessada em maio de 2014.
[2]Garrett, R.; Schimdt, E.M.; Pereira, L.F.P.; Kitzberger, C.S.G.; Scholz, M.B.S.; Eberlin, M.N.; Rezende, C.M. *Food Sci. Technol.*,**2013**, 50, 496.