Exploratory data analysis of commercial coffees with different roasting degrees using chromatograms obtained from SPME-GC-FID

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Keywords: Coffee, gas chromatography, SPME

The characteristic flavor of coffee results from the sensorial impact of the complex combination of volatile and non-volatile chemicals present in different concentrations. Most of those compounds are formed during the roasting process of the green coffee beans[1], especially by the so-called Maillard reactions. Due to the obvious importance of flavor on consumer acceptance and quality perception, the coffee's chemical composition has been intensively studied[2]. However, due to its complex nature, the association of the quality of roasted coffee to its volatile composition demands the use of chemometrics methods for data treatment. In the present work, we demonstrate that Principal Component Analysis (PCA) allied to gas chromatographic data, obtained after isolation and pre-concentraction of the volatile fraction of roasted coffee by using Solid Phase Microextraction (SPME), could be an alternative for chemical classification of coffee samples.

Samples and experimental conditions: Triplicates of eighteen different Brazilian commercial coffees were analyzed (seven of them were medium roasted and decaffeinated; other six had normal roasting and the other five were extra roasted – all of them from different production batches). The extraction and chromatographic conditions were optimized according to the literature. Two fibers, SPME coated with Carboxen/PDMS and PDMS/DVB were employed. Therefore, two data sets were obtained ([54 x 7501] and [54 x 5100]). Data processing was carried out with Matlab 6.5 software. The raw chomatograms for both SPME fibers were aligned using COW (correlation optimized warping)[3]. The data was meancentered and variable selection was performed for better discrimination.

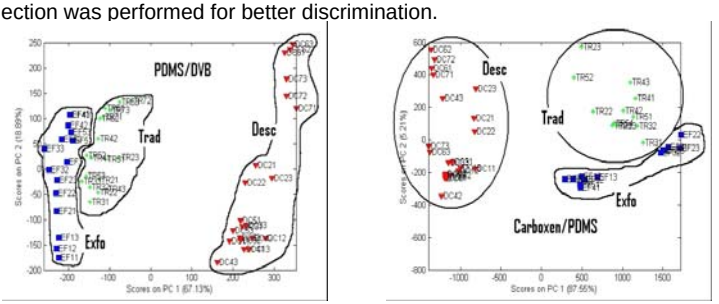

Fig. 1 – Scores Plots – (A) Carb/PDMS, (B) PDMS/DVB

The selected regions were: **PDMS/DBV**- 1486-1822, 2237-2443, 2798-3004 and 3350-4040 (**X** = [54 x 1442]), **Carb/PDMS** – 1548-2020, 2190-2480 and 3313-3800 (**X** = [54 x 1252]). PCA was applied and revealed clusters according to the coffee roasting process. In the PC1xPC2 score plot **(Figure 1)**, three groups of coffees could be clearly distinguished as follows: The decaffeinated coffee **(Desc)** samples formed one separated cluster, probably not only due to roasting but also to the caffeine extraction process. The other two groups have a higher similarity degree and correspond to different roasting processes –Traditional **(Trad)** and extra roasted **(Exfo).** The exploratory data analysis clearly shows the potential of SPME-GC-FID coupled to chemometrics to differentiate commercial roasted coffees. According to the results, any of the two SPME fibers could be used separately simultaneously to discriminate the roasted coffees by their flavor compounds.

Acknowledgment. Capes, CNPq, FAPESP and Agronomic Institute of Campinas

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