

## Exploratory data analysis of commercial coffees with different roasted degrees and process using diffuse reflection mid-infrared spectroscopy

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Coffee is one of the most popular drinks around the world. Strategies used to authenticate certain of its characteristics have been traditionally relied on wet chemistry. These methods, however, are time-consuming and expensive, and consequently, demand for rapid and inexpensive controls is growing.

Infrared spectroscopy is regarded as a quick and reliable mean of investigating food quality and safety. The main advantages of mid-infrared (MIR) spectroscopy include its speed of analysis and potential selectivity, when coupled to chemometric data analysis techniques.

Despite the amount of research conducted to classify varieties of the same food product, there is no published work applying mid-infrared spectroscopy to discriminate different roasted degrees of coffee samples.

In the present work, Brazilian commercial coffees of different roasting degrees were analyzed by diffuse reflectance mid-infrared spectroscopy.

**Samples.** Twenty one samples of Brazilian commercial coffee were analyzed in triplicates (7 of them medium roasting and decaffeinated; 7 of normal roasting; and the remainder of extra roasting – all from different production batches).

**Data acquisition.** MIR spectra of each solid sample were recorded at room temperature and transformed to absorbance units with a background spectrum of ground KBr. Each spectrum was obtained by scanning the 400 – 4000  $\text{cm}^{-1}$  region 256 times at a nominal resolution of 4  $\text{cm}^{-1}$ . Spectral data were smoothed by a moving average filter with a window size  $n = 25$ , followed by a multiplicative signal correction (MSC). Principal Component analysis of meancentered pre-treated data (Fig. 1) was carried out with Pirouette 3.11 chemometrics software.

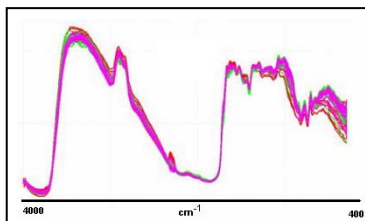


Fig. 1 – Pre-treated spectra

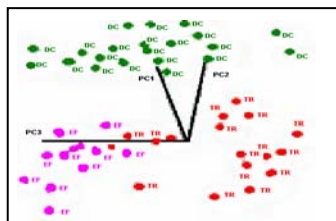


Fig. 2 – Scores plot - PC1x PC2 x PC3

Variable selection was performed to remove those regions of low discriminating and modeling power. Therefore, the spectral regions 4000 – 3500, 2500 – 2300 and 100 - 400  $\text{cm}^{-1}$  were excluded from data set.

Principal component analysis was applied to the selected variables. PC1xPC2xPC3 scores plot describing 84.92 % of the total variance (Fig. 2) shows that three clusters of coffee could be distinguished as follows: the upper group of decaffeinated coffee (green color) is clearly discriminated from the other two probably due to the roasting and caffeine extraction processes. The other two groups at the bottom of the plot correspond to the other roasting processes - traditional (red color) and extra roasting (violet).

This exploratory data analysis clearly shows that diffuse reflectance mid-infrared spectroscopy coupled to chemometrics has potential advantages to differentiate among commercial coffee samples of various roasting degrees.

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