

Determination of the authenticity of commercial coffees by application of chemometrics to ^1H NMR and FT-IR spectra

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Coffee is one of the most widely consumed beverages in the world and Brazil is the first producer. Its quality control is difficult because depends of the weather, harvest conditions, species used, soil nutrients, etc and It can also adulterated with cheaper substitutes like barley, chicory, cereals, malt, maltodextrins, caramelised sugar, etc [1, 2].

Many techniques have been investigated to tackle the problem of coffee adulteration. Spectroscopic methods such as NMR and FT-IR that can monitoring a wide range of chemicals in a single spectrum have been a great success. However, the richness of this information makes the spectra too complex to be analysed one by one and require chemometric analysis to extract the useful information [3].

In order to verify which methodology is better to determine barley addition into the coffees, multivariate analysis methods were applied to ^1H NMR and FT-IR spectra and these results were compared. In addition, k-Nearest Neighbour (KNN) and Soft Independent Modelling of Class Analogy (SIMCA) were used and compared to determinate the sample class, and Partial Least Squares (PLS) and Principal Components Regression (PCR) were used to determinate the content of barley addition into the commercial coffees using the Pirouette® v. 2.02 program.

Considering the classification methods, KNN presented better efficiency than SIMCA, for both techniques, and attributed correctly 100% for the samples from an external validation group. After this, the models were applied to predict the class for coffee commercial samples.

The coffee content for the pattern and commercial samples were determined using PLS and PCR which showed similar predictions. When both methods were applied, the NMR data results showed better with relative errors 5.3 and 5.6% for PLS and PCR, respectively. For the FT-IR spectra data we found 16.8 and 17.5% for the same samples used in the NMR.

References:

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