FIA-ESI-MS Fingerprinting method with chemometrics for the characterization of adulterated coffee samples

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Food products are very complex matrices, which makes the quality of these products an issue of great interest in our society. Considering the complexity of the food chain, the adulteration of food is increasing, causing food fraud cases.

In this field, drinks are food products that can be very easily adulterated. This work will focus on the thematic of fraud detection in coffee, one of the most popular beverages in the world. Coffee contains an elevated number of bioactive substances (phenolic acids, polyphenols and alkaloids; being especially abundant ellagic, caffeic and chlorogenic acids) that give place to its important antioxidant activity, known for its beneficial health effects.

The aim of this work was to develop an efficient non-targeted FIA-ESI-MS fingerprinting method in combination with chemometrics to achieve the characterization, classification, and authentication of coffee samples, together with possible adulterants (barley, chicory and flours) using partial least squares regression-discriminant analysis (PLS-DA) chemometric method.

Besides, Arabica and Robusta coffee samples were adulterated with barley, chicory and flour and the obtained FIA-ESI-MS data subjected to partial least squares (PLS) regression. Results demonstrated the feasibility of the proposed methodology to assess coffee authenticity and to quantify adulteration levels (down to 15%), showing good calibration and prediction errors.