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Prediction of coffee sensory quality through MS-e-nose as analytical decision maker for routine controls: possibilities and limitations.

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Text

Aroma is a primary hedonic aspect of a good coffee playing a fundamental role in coffee choice [1] and is a meaningful signature of the products [1-5]. The cup tasting is the most important criteria to define the coffee quality, nevertheless it requires trained and aligned panel, and it can seldom be implemented at-line for an immediate feedback. This study aims to apply diagnostic mass spectral fingerprints to develop an instrumental prediction model exploitable as an analytical decision maker for routine controls as a complement to define coffee sensory quality in cup. This method in combination with sensometrics, can be implemented in an automatic Total Analysis System (TAS) to provide a high throughput solution for coffee quality control.

Coffee samples were sensorially evaluated and analyzed by HS-SPME-MS and the resulting data elaborated with multivariate analysis. The panelscores were submitted to ANOVA and to a paired t-test between each expert. PLS-DA applied to the reprocessed MS spectral fingerprints enabled to select 36 (m/z) on 315 fragments suitable to correlate with high and low scores within a sensory attribute. The regression models was built with a training set of 146 objects and an external test set of 30. The leave-p-out cross-validation (20) method was used to select the number of components (fragments). Acid, bitter and woody notes were the most reliable. The mean error in the sensory scores prediction on test set with these data was within the fixed limit of ± 1 .

The results show that the HS-SPME-MS fingerprints in combination with chemometrics is a promising approach to be used as a TAS system for a high throughput solution to define the coffee sensory quality in cup. This approach offers a reliable sensory scores prediction if, and only if, applied with a robust mathematical model derived from a high number of representative samples and an accurate alignment in the lexicon to rate the samples.

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