# Prediction of coffee sensory quality in cup as analytical decision maker for routine controls.

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## Introduction:

Aroma is a primary hedonic aspect of a good coffee playing a fundamental role in the coffee choice [1] and can be considered as a signature of the products [2-6]. The cup tasting is nowadays the most important criteria to define the coffee quality, nevertheless it implies long time in terms of panel training and alignment, it often cannot be implemented at-line for an immediate feedback and a critical objective evaluation. The aim of this work is to use diagnostic mass spectral fingerprints in developing an instrumental prediction model that can be exploited as an analytical decision maker for routine controls as a complement to define coffee sensory quality in cup. These methods, in combination with sensometrics, can be completely implemented in an automatic TAS technology (Total Analysis System) to provide a high throughput solution for coffee quality control.

## Methods:

Coffee samples were sensorially evaluated through monadic profiling and analyzed by HS-SPME-MS and the resulting data elaborated with multivariate analysis. HS-SPME is a reliable high-concentration-capacity technique easy to automate, that can directly be online coupled with mass spectrometry. Non-separative MS methods, better known as mass spectrometry-based electronic nose or MS-nose, provide a representative, diagnostic, and generalized mass spectrometric fingerprint of coffee aroma, analyzed directly without preliminary chromatographic separation, in which ion acts as a "sensor" whose intensity derives from the contribution of each compound producing that fragment.

## Results:

*Instrumental data treatment*: HS-SPME-MS pattern is significant although the intensity of each ion (m/z) results from the contribution of all components presenting that fragment in their ionization pattern. In this case, the role of multivariate analysis to "extract" significant information from the MS profile is fundamental. PLS-DA applied to the reprocessed MS spectral fingerprints enabled to select 36 (m/z) on 315 suitable to describe high and low scores within a sensory attribute. *Sensory data treatment:* All scores of the five experts were submitted to A 1-way ANOVA and to a paired t-test between each expert. *Regression model:* the regression models was built with a training set of 146 objects and an external test set of 30. The method leave-p-out cross-validation (20) was used to select the number of components in the models Partial Least Square regression (PLS).

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. Spicy, fruity and flowery notes show a good fitting between chemical and sensory evaluation. However, all models showed a low predictive ability because of both a) the high noise due to an unbalanced pool of samples, and b) the difficulties linked to a too general lexicon used to define the notes.

## Conclusions:

The results show that the HS-SPME-MS fingerprints in combination with sensometrics 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, a robust mathematical model derived from a high number of representative samples and an accurate alignment in the lexicon to rate the samples.

## References

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