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Hyphenation of PTR-ToF-MS and newly developed software tools provides a new effective tool for coffee nose-space analysis

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Proton-transfer-reaction mass spectrometry has successfully been applied to the real-time characterization of 154aneli release during the consumption of food and/or beverages, also referred to as nose-space [1]. The coupling of Time-of-Flight (ToF) mass analyzers appears to be best suited to nose-space analysis extending the analytical capabilities of PTR-MS. The output of PTR-ToF-MS consists of hundreds of mass peaks for each cycle of analysis at a throughput of one spectrum per second or higher. The thorough exploitation of these large arrays of data represents a challenge of major importance to the experimenter.

PTR-ToF-MS was applied with the aim to study differences in the experience of coffee tasting by means of nose-space analysis. The coffee prepared from a commercial Arabica blend (Illycaffè Moka, medium roasting) was consumed by five 154anelists. Four replicates were performed for each taster. The tasting protocol was based upon the swallowing of a single small aliquot (7.5 ml) of coffee, served at controlled temperature (65 °C), followed by breathing for 3 minutes. Overall, the nose-space session generated about 4,000 mass spectra, which were extracted and analyzed.

This demanding task was greatly simplified by the employment of an in-house developed software package that operates in MATLAB environment, and allows for the easy handling of PTR-ToF-MS spectra. The general strategy underlying this analysis is described elsewhere [2]. More recently, a novel software tool called *"ToF-o-NOSE"* was expressly developed for application to nose-space analysis and integrated within the pre-existing package.

Starting from the data extracted from a nose-space session *ToF-o-NOSE* allows for:

- Immediate display of the profiles obtained for a given compound and rapid comparison between profiles generated by different compounds and/or tasters

- Direct extraction of profile parameters, such as area under the curve, maximum, mean, median *etc.* The extracted data are displayed within a worksheet format and can be easily further exploited.

PTR-ToF-MS analysis allowed for the extraction of 228 mass peaks and corresponding release profiles. For each profile up to six different parameters could be extracted. A data matrix (20 rows = tasters*replicates; 1368 columns =mass peaks*parameters) was hence generated and data were evaluated by means of principal component analysis (PCA). This allowed to graphically assess the discrimination of the five tasters. Starting from the initial data, visual inspection of profiles and statistical analysis allowed to pinpoint a subset of parameters that were the most influential on the discrimination. These corresponded to 19 mass peaks, tentatively assigned to 17 different compounds. The compounds were, for the most part, known as components of the volatile profile of coffee [3].

Our results showed that the integration of high-performance instrumental techniques with powerful data processing tools allows for more rapid and effective data exploitation in the field of nose-space analysis. In perspective, the interaction with sensory analysis could provide further insight into the physiological basis of consumer sensitivity and preference.