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ABSTRACT BOOK

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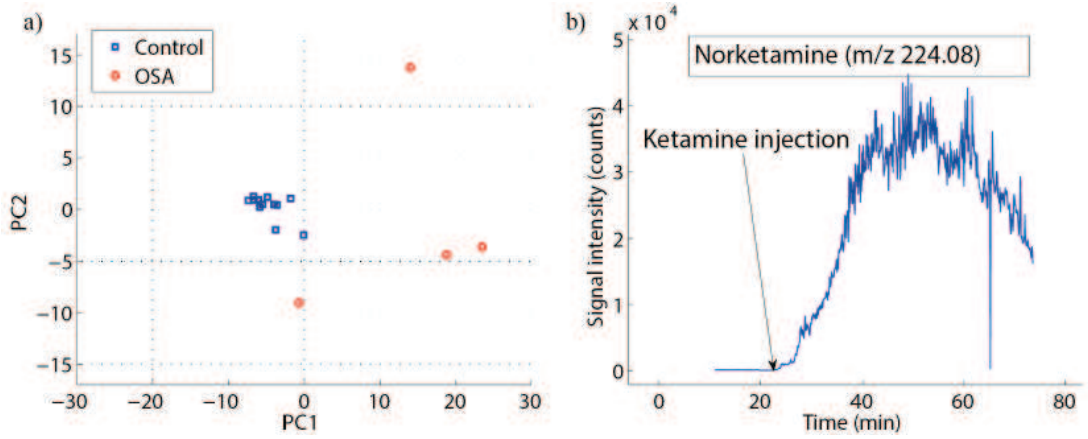
SFSM
Société Française de Spectrométrie de Masse



Conclusions
We conclude that the real-time mass spectrometric analysis of exhaled metabolites may contribute to address some of the most relevant clinical pharmacological problems, which are currently investigated through the analysis of body fluids other than breath.

Novel aspect
In vivo monitoring of exhaled compounds related to OSA and ketamine

WOS24-04 PTR-TOF-MS characterization of roasted coffees (*C. arabica*) from different geographic origins

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Introduction
The taste and aroma of high quality coffee can vary considerably among samples from the same species and variety grown in different regions. In addition to the fact that geographic origin is embedded in coffee quality, marking of origin for product differentiation is highly demanded for traceability, authentication, and marketability purposes. In this study, we developed a mass spectrometry based set-up for the high-throughput characterisation of food samples. The aromatic profiles of six roasted C. arabica coffees (Brazil, Ethiopia, Guatemala, Costa Rica, Colombia, India) were analysed by Proton-Transfer-Reaction-Time of Flight-Mass Spectrometry (PTR-ToF-MS) to characterise aromatic profiles of coffee powders and brews.

Methods
Commercially available medium roasted C. arabica coffees were used for the experiment. Coffee brewing was performed by steam pressure coffee extraction in a stove-top coffee maker known as "moka" in Italy. The headspace measurements of coffee powder and brews were performed by a commercial PTR-ToF-MS 8000 instrument connected to a multipurpose autosampler. The proton transfer reaction was controlled by drift voltage (550 V), drift temperature (110°C), drift pressure (2.30 mbar) and E/N=140 Td. Multivariate data analysis techniques were applied in order to visualize data and classify the coffees according to origin.

Results
The results showed that the volatile compositions of coffees were highly influenced by the geographic origin of the coffee beans. Significant differences were found among volatile concentrations of coffee powders and brews. Tentative identification of mass peaks aided characterisation of aroma fractions. Principal component analysis allowed separation of coffees according to origin both for powder and brew. Some mass peaks were increased in the brew whereas decreased maybe be due to the lower solubility of aroma compounds in the brew or degradation of them by hot water.

Conclusions
Six C. arabica from different geographical origins were successfully classified by their volatile profiles in powder and brew. PTR-ToF-MS spectra of the coffees contained almost five hundred mass peaks and the high mass resolution allowed the tentative identification of diverse volatile compounds useful for aroma fingerprints and origin discrimination.

Novel Aspect
PTR-ToF-MS has been used for the first time for the rapid classification of the origin of ground roasted coffee powder and brew.

WOS24-05 Evolved gas analysis by single photon ionization–mass spectrometry: a tool to distinguish different types of coffee

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Introduction
In this study, the applicability of thermogravimetry (TG) coupled to single photon ionization time-of-flight mass spectrometry (TG-SPI-TOFMS) for evolved gas analysis (EGA) of coffee was demonstrated. Coffee is a chemically well-known complex food product of large scientific and commercial interest.