



Società Chimica Italiana

Divisione di Spettrometria
di Massa



XXII International Mass Spectrometry Conference

Florence (Italy) - August 26-31, 2018



ABSTRACT BOOK



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Results

PCA and OPLS-DA analysis were carried out to differentiate between the varieties Belana, Gunda, Wega and Queen Anne. Additionally, samples were distinguished according to their growing regions. The structural elucidation of biomarkers was performed considering the retention time, precise molecular mass, MS/MS fragmentation data, isotopic patterns and ion mobility spectra provided by the UPLC-IMS-QToF analysis platform.

A set of more than 60 lipid biomarkers was identified that allows a reliable discrimination of the four potato varieties on the one hand and their cultivation region on the other. Characteristic substances, predominantly tri- and diglycerides, were found to differentiate potatoes originating from Thuringia, North Rhine-Westphalia, Bavaria, Schleswig-Holstein and other German production areas.

These generic markers withstand impacts like different farming methods and multiple harvesting periods. Furthermore, the reliability of the model was tested by analyzing mixtures of varieties and geographical origins.

Conclusions

The results demonstrate that this metabolomics-based approach in conjunction with a comprehensive biomarker database has potential as a future screening tool for the investigation of labelled potato tubers regarding their variety and their German cultivation region to prevent food fraud. This tool may be used to preserve consumer interests and support regulators' efforts to keep pace with fraudsters.

Novel Aspect

This approach determines a potato's variety and its cultivation region within one analysis whereas methods like electrophoresis and isotope analysis require multiple tests.

WOr.05-3 NOESPACE ANALYSIS BY PTR-TOF-MS FOR THE EXTRA VIRGIN OLIVE OIL CHARACTERIZATION

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Keywords: *direct injection, volatile organic compounds, inter-individual differences*

Introduction

Extravirgin olive (EVO) oil aroma and taste influence consumer preferences. Volatile organic compounds (VOCs) release from food within oral cavity is a complex process. Nose-space (NS) analysis should unravel the retro-nasal olfaction processes happened during olive oil tasting. Proton Transfer Reaction-Mass Spectrometry with Time-of-Flight analyser (PTR-ToF-MS) was already successfully applied for NS analysis of apples [2], cereal bars [3], coffee [4,5].

Methods

In this study 2 Italian EVO oils were used: commercial vs home made (Lago di Garda, TN). Pure oil, oil mixed with tomato sauce, oil on bread prepared for each EVO oil were used for headspace (HS) and NS measurements by PTR-ToF-MS 8000. The samples were presented to 8 assessors in duplicate. For NS sampling a glass nose-piece with silicone rubber tube was fitted into assessors' nostrils and connected to PTR-ToF-MS. The method for HS analysis was described elsewhere [6].

Results

26 out of 319 mass peaks of NS dataset displayed signal related to olive oil, tomato or bread aroma. Peaks related to human metabolism were eliminated. The individual profiles differed in

peak intensity and duration. However it was possible to distinguish the two types of EVO oils. HS data confirmed diversity of the oils. Home-made EVO oil in all products was characterized by significantly higher concentrations of mass peak 99.081 tentatively identified (t.i.) as (E)-2-hexenal associated to a green-leaf and fruity flavor [1]. Commercial EVO oil was richer in t.i. pentanal, acetic acid, butanal, and several esters which are reported as oxidation products of olive oil [7]. The samples of olive oil on bread showed the best performance (higher signals intensities) for all panellists due to an increased release surface area, prolonged presence in mouth, increased interaction with saliva and mucosal surfaces. Adding tomato sauce to olive oil decreased the olive oil aroma release in NS and contaminated it with tomato aroma.

Conclusions

NS analysis performed by PTR-ToF-MS discriminated different EVO olive oils. HS and NS data were consistent. The next steps are the optimization of sample preparations, tasting protocol, and the improvement of PTR-ToF-MS sensitivity by applying an ion funnel.

The optimized methods will be applied to study different EVO olive oils within the project "VIOLIN" aiming to the valorisation and promotion of Italian EVO oils.

Novel Aspect

For the first time NS analysis was applied for olive oil profiling taking into consideration individual perception and the combination with different food matrices.

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WOr.05-4 **ULTRA-FAST IDENTIFICATION OF FISH SPECIES BY PAPERSPRAY COUPLED TO A BENCHTOP ORBITRAP MASS SPECTROMETER**

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Keywords: Food authenticity, PaperSpray, Orbitrap technology, Automations

Introduction

The largest seafood fraud investigation in the world to date found that 33% of seafood samples



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