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### Presentation Abstract

Session: Poster Session 3 (C)

Friday, Nov 11, 2011, 11:00 AM -12:15 PM

Presentation Title: C149 - Profiling of Berries by Comprehensive Two-Dimensional Gas Chromatography/Time-of-Flight Mass Spectrometry (GCxGC/TOF-MS)

Location: Exhibit Hall 4 , Section: Chemistry

Scientific Discipline: + 4. Chemistry -> a. Analytical Chemistry

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Abstract: Hypothesis/statement of problem - Comprehensive bidimensional gas chromatography coupled with TOF-MS is a promising analytical technique for the challenging task of fingerprint natural chemical markers of different kinds of berries. This is important information both for food quality control and for the identification of peculiar components of small fruits, such as natural organic acids, amino acids and antioxidants. Experimental methods - The juice (50 mL) was obtained upon mixing and centrifuging of about 200 g of fresh or frozen berries and was acidified with H<sub>2</sub>SO<sub>4</sub> to pH 1. A solution of heptadecanoic acid was added as an internal standard. A fraction of the dichloromethane extract of the acidified juice was dried under gentle nitrogen flow, and silylated with BSTFA containing 1% TMCS in pyridine. The TMS extract was then injected in a Pegasus 4D comprehensive two-dimensional gas chromatograph with time-of-flight detection (GCxGC/TOF MS). The column combination was as follows: the 1<sup>st</sup> column was a (5% diphenyl) Rxi-5ms 30m x 250 µm i.d. with a 0.25 µm film thickness; the 2<sup>nd</sup> column was a (50% diphenyl) Rxi-17ms 0.79m x 100 µm i.d. with a 0.1 µm f.t. The inlet temperature was 250°C; the temperature program

for the oven started from 40 °C kept for 2 min and raised to 280 °C at 20 °C/min. The final isothermal phase was maintained for 16.5 min. The temperature of the transfer line was 290 °C. The modulation time was 4 sec. Results - The juice of different kinds of fresh and frozen berries was characterized by means of GCxGC/TOF-MS. The main components found in the tridimensional chromatographic trace (1<sup>st</sup> column and 2<sup>nd</sup> column retention times plus abundance) were organic acids, aminoacids and phenolic compounds identified through their fragmentation pattern, retention times and by injecting standard solutions. The main advantages of the GCxGC/TOF MS analysis when compared to one dimension GC/MS are higher separation efficiency and the reduction of interferences due the column bleeding, which allows for the detection of a significant number of trace analytes that would otherwise be missed. Conclusion - It is possible to apply comprehensive GCxGC/TOF-MS not only for the determination of the aroma profiles of fruits and fruit products (as reported in previous literature) but also for the characterization of the non-volatile fractions of the juice which contains low molecular weight components potentially useful for health/pharmaceutical/nutraceutical applications and for food quality assurance.

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