BOOK OF ABSTRACTS

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Jana Pulkrabová, Monika Tomaniová, Stefan van Leeuwen, Michele Suman, Michel Nielen and Jana Hajšlová

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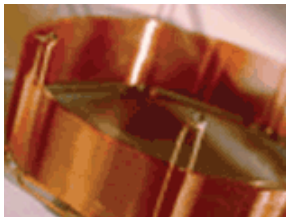

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L78
INNOVATIONS AND CHALLENGES IN QUANTITATIVE VOLATILOMICS: THE ROLE OF FID/MS CHROMATOGRAM FUSION IN ENHANCING PATTERN RECOGNITION

Andrea Caratti*[1], **Angelica Fina**[2], **Fulvia Trapani**[2], **Carlo Bicchi**[2], **Stephen E. Reichenbach**[3], **Qingping Tao**[4], **Daniel Geschwender**[4], **Chiara Cordero**[1]

[1] *Department of Drug Science and Technology, University of Turin, Italy*
[2] *University of Turin, Italy*
[3] *University of Nebraska, United States of America*
[4] *GC Image LLC, United States of America*
**Corresponding author - E-mail: andrea.caratti@unito.it*

Volatilomics is an emerging discipline aimed at characterizing volatile metabolites in various samples. Recently, two-dimensional gas chromatography (GC×GC) with parallel flame ionization detector (FID) and mass spectrometry (MS) has gained attention for combining compound identification (via MS) with accurate quantification (via FID). Typically, FID and MS traces are processed separately. This study focuses on merging MS and FID chromatograms to improve pattern recognition during template matching and enable quantitative volatilomics on a large set of features. Features matching is guided by MS spectral similarity, reducing mismatches and extracting FID responses for accurate quantification.
This approach was tested for characterizing the aromatic identity of hazelnuts, a premium confectionery ingredient. GC×GC-FID/MS traces of hazelnuts highlight molecules that differentiate cultivars, geographical origin, post-harvest treatments, bacterial/mold contamination, oxidative stability, and sensory quality [1]. This strategy aligns with the Sensomics-Based Expert System (SEBES), which act as an AI-Smelling predicting food aromas without human olfaction [2].
The dataset included raw hazelnut samples analyzed over four years of production, in which MS response variability requires normalization and internal standards correction for consistent analysis. Chromatographic misalignments over time can cause 2D peak pattern inconsistencies [3]. Data fusion, guided by MS spectral similarity, reduces false negatives by about 80% on 441 detectable features in raw hazelnuts compared to FID alone and minimizes false positives, enhancing method specificity and selectivity. Data fusion also halves processing time and facilitates metadata transfer. After pattern recognition step, FID signals are extracted for quantitation based on calibration or predicted FID response factors.
Quantitative volatilomics with parallel detector signal fusion reliably tracks aroma changes over crops and shelf-life, enabling robust marker discovery for industrial quality assessment.

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Keywords: quantitative metabolomics, comprehensive two-dimensional gas chromatography, volatilomics, MS-FID Fusion, artificial intelligence smelling