



FONDAZIONE
EDMUND MACH



DIFFA23

DIRECT INJECTION FOOD FLAVOUR ANALYTICS

BOOK OF ABSTRACTS

Fondazione Edmund Mach

San Michele all'Adige (TN), Italy

20 - 22 September 2023

1st International Symposium on
Direct Injection Food Flavour Analytics (DIFFA)

Edited by

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**Proceedings of the DIFFA23 - 1st International Symposium on Direct Injection
Food Flavour Analytics**

Fondazione Edmund Mach – San Michele All’Adige (TN) Italy

20-22 September 2023

This book collects the conference proceedings of the 1st International Symposium on Direct Injection Food Flavour Analytics, held at the Fondazione Edmund Mach from 20th to 22nd September 2023.



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FOREWORD

Volatile organic compounds (VOCs), particularly flavour compounds, represent an invaluable noninvasive metric to follow the multi-faceted journey of food, from the farm to the fork and beyond, such as relating to the human microbiome after consumption or in addressing reduction strategies for food waste. VOCs thereby serve as a direct and swift means of measurement and notably act as a main driver of the perceived quality of food.

Mass spectrometry (MS) is an established yet increasingly pivotal tool in food and beverage characterization with a broad range of applications. When coupled with gas chromatography (GC), it stands as the predominant analytical method for exploring many aspects of food, from safety to traceability and nutritional aspects, and equally facilitates control measures in quality and process monitoring.

Recent remarkable advancements in both technology and methodology have paved the way for highly sensitive, specific, rapid, robust, and validated MS-based techniques that have become indispensable in food science and technology research and application. A subgroup of these technologies has been devised over the past two decades in the form of analytical approaches that enable the analysis of VOCs through direct injection. These methods have gained attention for their rapid, highly sensitive and high-throughput analytical capabilities.

A leading technology in this area is proton transfer reaction-mass spectrometry (PTR-MS), which has driven many innovative applications for direct flavour/food analysis. Commencing 2003, the University of Innsbruck, Austria, has organized a biennial event dedicated specifically to PTR-MS and its applications, including a focused session on food science and technology.

The **1st International Symposium on Direct Injection Food Flavour Analytics (DIFFA23)** was conceived with the backdrop of the PTR-MS conference but with a different aim, namely to embrace a broader community beyond PTR-MS uses, encompassing similar direct injection mass spectrometry (DIMS) technologies, such as atmospheric pressure chemical ionization-mass spectrometry (APCI-MS) and selected ion flow tube-mass spectrometry (SIFT-MS), with a primary emphasis on flavor compounds. It was also not exclusive to MS-based analytical techniques, but welcomed the inclusion of complementary non-MS approaches, such as solid-state sensors, fast gas chromatographic direct approaches and ion mobility spectrometry (IMS), amongst others, to ensure a wider reach and broader engagement. The meeting was established to foster scientific discussions of common interest and facilitate scientific collaborations. This book of abstract highlights the details of the event and contains the contribution summaries of both the oral and poster presentations.

The conference featured one plenary and four keynote lectures delivered by distinguished guests, as well as numerous invited and contributed talks and 25 poster presentations, with 97 attendees from different EU states, the USA, the UK, Israel and New Zealand. The event provided valuable insights into direct injection food/flavour analytics, with reviews from pioneering scientists who played key roles in developing and advancing DIMS methods in its early days, such as Andy Taylor, Patrik Španěl and Jean-Luc Le-Quéré, showcasing both historical developments and recent advancements in analytical performance and novel applications. Topics discussed included nose-space analysis of composite foods, rapid and high-throughput phenotyping, fermentation monitoring, both as an

innovative technological tool and for investigating the human microbiota, advanced data analysis and data mining tools. These are just a few examples of the themes explored during the conference.

Numerous partners contributed to the success of the event: the sponsors, whose engaging presentations and financial support sustained the quality of the meeting and ensured that the conference fees were kept to a minimum, as well as various supporting institutions and patronages. Special thanks go to the Fondazione Edmund Mach (FEM) for its scientific contributions and for hosting the conference at the Research and Innovation Centre, as well as the Division of Mass Spectrometry of the Italian Chemistry Society (DSM-SCI) for their organizational support and creation and hosting of the conference website. The invaluable support from these companies and institutions are further acknowledged through inclusion of their logos on the back cover of this book.

The conference started a fruitful exchange of results, ideas and issues amongst scientists working with direct tools to monitor VOCs in food science and technology, with broad attendance from sensory and applications scientists from academia and industry.

We would like to thank all those who, through their participation and support, made this event possible, which exceeded our most ambitious expectations.

Thank you all, and we look forward to seeing you at the next edition.

On behalf of the Scientific Committee

Franco Biasioli, Jonathan Beauchamp, Pat Silcock

CONFERENCE PROGRAM

20th September 2023

12.30-14.00 Registration and welcome buffet

Conference opening

14.00-14.10	Welcome addresses Fulvio Magni - <i>Società Chimica Italiana-Divisione Spettrometria di Massa</i> Mario Pezzotti - <i>Fondazione Edmund Mach</i>
14.10-14.20	Why DIFFA23? Franco Biasioli - <i>Fondazione Edmund Mach</i>
14.20-15.05	Plenary lecture: <i>DI-MS – A game changer for flavour research?</i> Andy Taylor - <i>University of Nottingham</i>

Session 1 | Unlocking Flavour with DIMS

Chairs: Pat Silcock & Nina Cleve

15.05-15.35	Jonathan Beauchamp - Fraunhofer Institute for Process Engineering and Packaging IVV <i>The long and winding road: a flavoursome tale of PTR-MS</i>
15.35-15.55	Graham Eyres - <i>University of Otago</i> <i>What is Flavour and how can DIMS help untangle the puzzle?</i>
15.55-16.15	Andreas Mauracher - <i>IONICON</i> <i>Advantages of Next-Gen PTR-ToF instruments for food and flavour sciences</i>

16.15-17.00 Tea break and poster session

Session 2 | DIMS in Health and Wellbeing

Chairs: Donatella Caruso & Eirini Pegiou

17.00-17.20	Josep Rupert - <i>Wageningen University & Research</i> <i>Signalling volatile compounds in the human gut microbiota: new avenues offered by direct analytical methods.</i>
17.20-17.40	Chris Mayhew - <i>University of Innsbruck</i> <i>Real-Time Trace Analysis of Breath Volatiles using Proton Transfer Reaction Mass Spectrometry: implications for in-vivo flavour release measurements</i>
17.40-18.00	Enrico Davoli - <i>Istituto Mario Negri</i> <i>Direct analysis of sex-wellness products using a field deployable MS equipped with a Direct Sampling Atmospheric Pressure (DSAP) source</i>
18.00-18.20	Corrado Di Natale - <i>University of Rome Tor Vergata</i> <i>Direct injection mass spectrometry and gas sensors: a teacher-pupil relationship</i>
18.20-18.40	Luca Cappellin - <i>University of Padua</i> <i>Improved compound identification in direct VOC analysis using an EI&CI-TOFMS</i>
19.00	Welcome cocktail - cloister of the monastery and historical cellar

21st September 2023

Session 3 | Linking DIMS Data to Sensory Perception

Chairs: Graham Eyres & Iuliia Khomenko

9.00-9.30	Jean-Luc Le-Quéré - <i>INRAE-CSGA Dijon</i> <i>Twenty years of Direct Injection Mass Spectrometry for aroma research in Dijon</i>
9.30-9.50	Catrienus De Jong - <i>Wageningen University & Research</i> <i>Exploring new in vivo and in vitro methods to integrate sensory and instrumental analysis to get insight and improve the flavour of plant-based food products during oral processing and drinking</i>
9.50-10.10	Markus Stieger - <i>Wageningen University & Research</i> <i>In vivo aroma release and sensory perception of composite foods</i>
10.10-10.20	Michele Pedrotti - <i>Wageningen University & Research</i> <i>Characterization of plant-based milks by combining sensory analysis with headspace and nose-space direct injection mass spectrometry</i>
10.20-10.30	Karina Gonzalez-Estanol - <i>Wageningen University & Research</i> <i>In vivo analysis of nose-space concentration by direct injection mass spectrometry to study the effect of chewing rate on aroma release during food consumption</i>
10.30-10.40	Laura Hill - <i>University of Nottingham</i> <i>Understanding the relationship between lipids, capsaicin and aroma release in confectionery</i>

10.40-11.10 Coffee break and poster session

Session 4 | Flavour Complexity and Cooking

Chairs: Fulvio Magni & Caroline Perltier

11.10-11.30	Samo Smrke - <i>ZHAW School of Life Sciences and Facility Management</i> <i>Development of fast-GC PTR-MS method for coffee VOCs analysis</i>
11.30-11.45	Nina Cleve - <i>Fraunhofer Institute for Process Engineering and Packaging IVV</i> <i>Milk matters: Unraveling retronasal aroma release and perception of coffee by combining in vivo nosespace analytics with dynamic sensory methods</i>
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12.05-12.20	Gregory Schmauch - <i>Rational F&E GmbH</i> <i>Influence of product quantity, cooking parameter and flow tube pressure on the measurement with Sift-MS in a cooking oven</i>
12.20-12.40	Vaughan Langford - <i>Syft Technologies</i> <i>Application of SIFT-MS to chemical and sensory screening of packaging materials</i>
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Session 5 | Latest DIMS Showcasing

Chairs: Jonathan Beauchamp & Karina Estanol-Gonzalez

- | | |
|-------------|--|
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| 14.15-14.30 | Matteo Tonezzer - <i>University of Cagliari</i>
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| 14.30-14.45 | Andrea Warburton - <i>University of Otago</i>
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| 14.45-15.05 | Paolo Redegalli - <i>Shimadzu Italia S.r.l.</i>
<i>Characterization of isoflavones and its metabolites in foods by direct probe ionization mass spectrometer (DPiMS) with high resolution detection</i> |
| 15.05-15.25 | Hansruedi Gygax - <i>GAS Dortmund</i>
<i>GC-IMS instruments and their use in food and flavour analysis</i> |

15.25-16.15 Tea break and poster session

Session 6 | Microbial, Fermentation and Modelling

Chairs: Riccardo Flamini & Michele Pedrotti

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16.45-17.05	Vittorio Capozzi - <i>Institute of Sciences of Food Production - National Research Council of Italy (CNR)</i> <i>DIMS techniques and the study on microbial VOCs in food: flavour attributes, fermentation monitoring and emerging trends</i>
17.05-17.20	Eirini Pegiou - <i>Wageningen University & Research</i> <i>Easy and fast detection of abnormal olive brine fermentation – A showcase of SPOTDETECT.</i>
17.20-17.40	Caroline Peltier - <i>INRAE</i> <i>Automatic pretreatment and multiblock analysis of flavor release and sensory temporal data simultaneously collected in vivo</i>
17.40-18.00	Ana Rita Monforte - <i>AFB INTERNATIONAL</i> <i>Modelling the kinetics of flavour formation & release as a function of ingredients addition in real food systems</i>
18.00-18.20	Pietro Franceschi - <i>Fondazione Edmund Mach</i> <i>Mining datasets from untargeted direct analytical methods: a data analyst point of view</i>
18.20-18.35	Mickael Le Behec - <i>Institute of Analytical Sciences and Physico-Chemistry for Environment and Materials (IPREM)</i> <i>Volatile fingerprints of food thanks to the untargeted use of SIFT-MS raw data</i>

20.00 Social dinner - cloister of the Museo Etnografico Trentino

22nd September 2023

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Chairs: Catreinus de Jong & Brian Farneti

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10.00-10.15	Antonella Grosso - <i>University of Bolzano</i> <i>Monitoring autoxidation of vegetable oils by proton transfer reaction mass spectrometry</i>
10.15-10.30	Pedro Martinez Noguera - <i>University of Copenhagen</i> <i>Using PTR-ToF-MS to quantify microbial off-flavors geosmin and 2-methylisoborneol in water. Method development, performance assessment and comparison with established GC-MS methods</i>
10.30-10.45	Davide Papurello - <i>Turin Polytechnic</i> <i>Supporting sustainable energy production by PTR-MS: a review on the work accomplished on biofuel production from food waste to SOFC systems</i>
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P.08 Automated untargeted peak detection for GC-IMS data

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Summary: GC-IMS is becoming popular in food volatilomics as a tool for untargeted fingerprinting analysis. This contribution describes an automated untargeted peak detection workflow for GC-IMS data, and its application to roasted hazelnut paste samples.

Keywords: GC-IMS, peak detection, automated, untargeted.

1 Introduction

Gas Chromatography (GC) coupled with Ion Mobility Spectrometry (IMS) is an analytical technique that has been rapidly gaining popularity in the field of food volatilomics [1]. The main advantage of GC-IMS is the detection of volatile organic compounds (VOCs) at low concentrations, enabling the use of static headspace sampling (SHS) and eliminating the need for preconcentration steps. This leads to minimal sample preparation and a relatively short analysis time, typically less than an hour. Additionally, IMS operates at atmospheric pressure and no vacuum system is needed, which leads to several benefits, including reduced bench space requirements, simplified maintenance, and low energy consumption.

The hyphenation of GC and IMS results in an orthogonal bidimensional separation of analytes. The analytical output of a GC-IMS analysis is, therefore, a tridimensional data containing: the retention times for the gas chromatographic separation, the drift times for the separation of analytes in the IMS drift tube, and the signal intensities measured by the detector. The common graphic representation of GC-IMS data is as 2D plots with the signal intensity visualized as color scale.

The most common approach for peak detection is based on the manual selection of the 2D peaks by creating a set of retention time and drift time coordinates, which are subsequently used to extract peak intensities and generate a peak table for the entire sample set. This is suitable as part of a targeted strategy when a set of analytes of interest are monitored. On the opposite, in case of untargeted fingerprinting studies this approach become time-consuming, and it is likely to be influenced by the operator's personal judgment.

A different approach is based on the application of the data analysis workflow to the entire spectral fingerprint obtained for each sample. While this approach has been successfully applied by some authors [2,3], its robustness might be affected by the spectral background when the GC separation is inefficient, and a complex volatile profile is analyzed. In this case, an automated peak detection represents a promising strategy for untargeted fingerprinting analysis.

2 Experimental

- Automated untargeted data processing

The output files of the GC-IMS instrument were imported in R, the region containing peaks was selected and data reduction by binning was applied. After this pre-processing step, peak detection

based on persistent homology was performed using the Python package findpeaks 4. The reticulate R package⁵ was used to integrate the Python code in R code. The intensities of the automatically detected peaks were extracted for each sample.

- Manual targeted data processing

To validate the automated peak detection, 30 target peaks were manually selected in the GC-IMS profile, and their signal intensities were extracted with the quantitative module of the commercial software (VOCal). Peak height was selected as the intensity measure.

3 Results

The automated data processing enabled the detection of approximately 120 peaks. For the set of target peaks, the correlation between automatically detected peak intensities (selected based on the known retention time and drift time ranges) and the peak intensities obtained from manual selection with the commercial software was verified. The results demonstrated the effectiveness and reliability of the proposed automated method.

4 Conclusions

An automated peak detection workflow for GC-IMS data was developed and evaluated by processing the GC-IMS profiles of roasted hazelnut paste samples from different geographical and botanical origins. The combination of a rapid analytical technique with an automated data processing strategy removes the bottleneck of manual peak selection and provides a promising analytical solution for food volatilomics studies.

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