



FONDAZIONE  
EDMUND MACH



# DIFFA23

DIRECT INJECTION FOOD FLAVOUR ANALYTICS

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BOOK OF ABSTRACTS

Fondazione Edmund Mach

San Michele all'Adige (TN), Italy

20 - 22 September 2023

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

*Edited by*

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**Proceedings of the DIFFA23 - 1<sup>st</sup> 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 1<sup>st</sup> International Symposium on Direct Injection Food Flavour Analytics, held at the Fondazione Edmund Mach from 20<sup>th</sup> to 22<sup>nd</sup> 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 **1<sup>st</sup> 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

20<sup>th</sup> 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 &amp; 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&amp;CI-TOFMS</i>
19.00	Welcome cocktail - cloister of the monastery and historical cellar

**21<sup>st</sup> 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 &amp; 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 &amp; Research</i> <i>In vivo aroma release and sensory perception of composite foods</i>
10.10-10.20	Michele Pedrotti - <i>Wageningen University &amp; 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 &amp; 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>
11.45-12.05	Tomasz Majchrzak - <i>Gdansk University of Technology</i> <i>What happens when food goes into oil during deep frying? Monitoring the first minutes of frying using PTR-MS</i>
12.05-12.20	Gregory Schmauch - <i>Rational F&amp;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>
12.40-14.00	Conference group photo and lunch

## 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><br><i>PTR-MS as a tool to understand and improve the performance of electronic noses</i>   |
| 14.30-14.45 | Andrea Warburton - <i>University of Otago</i><br><i>Application of PTR-ToF-MS to monitor development of flavour in sourdough</i>   |
| 14.45-15.05 | Paolo Redegalli - <i>Shimadzu Italia S.r.l.</i><br><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><br><i>GC-IMS instruments and their use in food and flavour analysis</i>  |

15.25-16.15 Tea break and poster session

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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 &amp; 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 &amp; 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



**22<sup>nd</sup> September 2023**

**Session 7 | Food Spoilage and Off-Flavour**

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>
10.45-11.05	Rupert Holzinger - <i>Utrecht University</i> <i>Using SI traceable gas standards to improve the accuracy of untargeted PTR-MS measurements</i>

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Chairs: Rupert Holzinger & Vittorio Capozzi

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12.25-12.40	Alberto Roncone - <i>Fondazione Edmund Mach</i> <i>Validation of gas chromatographic methods for the botanical characterization and authentication of lavender essential oil by stable isotope analysis of its organic volatile compounds</i>
12.40-12.55	Eugenio Aprea - <i>University of Trento</i> <i>Contribution of volatile organic compounds to multifloral honey flavor</i>
12.55-13.15	Daniele Zatta - <i>University of Padua</i> <i>Comparative analysis of VOC purification techniques in complex cooking emission: adsorption, photocatalysis and combined systems.</i>
13.15-13.30	Closing remarks Fulvio Magni - <i>Società Chimica Italiana-Divisione Spettrometria di Massa</i> Franco Biasioli - <i>Fondazione Edmund Mach</i>

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## **I.09 DIMS techniques and the study on microbial VOCs in food: flavour attributes, fermentation monitoring and emerging trends**

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*Summary:* The renewed interest in fermentation as a sustainable and consumer-friendly process leads to a revamp in related R&D activities. DIMS techniques have proven to be versatile tools for monitoring VOCs during fermentation in food and beverages, offering new approaches for improving quality and safety standards and developing new products.

*Keywords:* bacteria, yeasts, PTR-ToF-MS

### **1 Introduction**

Fermentation has been used for millennia to improve the quality and safety of edible raw materials, making a pivotal contribution (for about a third, on average) to consumption, catalysing considerable economic, social and environmental interest [1–3]. Bacteria, yeasts and filamentous fungi develop in food matrices leading to the production of fermented foods and beverages with significant modulation of sensory, nutritional, functional quality, shelf life and safety [1–3]. Fermentation represents a low-energy input transformation process at the basis of an extensive part of the traditional gastronomic heritage and is of considerable interest for the development of new products [1]. The study and control of microbial resources and their development in edible matrices are of crucial importance to maximise the benefits and minimise the risks associated with the fermentation bioprocesses in foods and beverages [4]. The search for rapid monitoring systems capable of carrying out massive screening and bioprocess evaluations over time is relevant. Volatile organic compounds released by microorganisms are interesting analytical targets, and the direct-injection mass spectrometry (DIMS) techniques represent versatile and powerful tools capable of offering both a sensor-like approach and assisting real-time volatilomics studies [5–7]. Among the DIMS approaches, Proton Transfer Reaction Time of Flight Mass Spectrometry (PTR-ToF-MS) has found wide use in the evaluation of volatiles associated with fermentation processes, representing a model method in this field [5–7].

### **2 DIMS techniques and the study on microbial VOCs in food**

DIMS techniques have been widely used in the study of VOCs associated with fermented products, demonstrating interesting potential in the field [5–8]. For example, using PTR, the volatiles associated with i) the transformation of various raw materials, both of vegetable origin (i.e. bread, wine, beer) and animal origin (yoghurt, kefir, cheese), ii) the development of prokaryotic and eukaryotic microorganisms, and iii) the carrying out of alcoholic and lactic fermentations were monitored (Table 1).

**Table 1.** Studies of VOCs monitoring in fermented products using PTR application.

Fermented product	Application
Cocoa beans	Evaluation of VOCs associated with fermented cocoa beans from different geographic origins [9]
Bread	Study of VOCs associated with the use of different starter cultures ( <i>Saccharomyces cerevisiae</i> ) during bread manufacturing [10]
	Evaluation of VOCs associated with the inoculation of different starter cultures in combination with the use of diverse flours (breadmaking) [11]
	Study of VOCs associated with the use of different flavouring starter cultures ( <i>Saccharomyces cerevisiae</i> ) for bread production [12]
	Assessment of VOCs associated with different baked and toasted gluten-free breads obtained inoculating yeast starter culture [13]
	Study of VOCs associated with the oven during the baking and toasting of gluten-free bread doughs obtained inoculating yeast starter culture [14]
Yoghurt	Evaluation of VOCs associated with the inoculation of different starter cultures (lactic acid bacteria, LAB) during yoghurt manufacturing [15]
Kefir	Assessment of VOCs associated with kefir and kefir-like cereal-based beverages using water and milk kefir grains and inoculating a specific LAB strain [16]
Cheese	Study of VOCs associated with cheeses obtained with lactic fermentation: assessing the effects of dairy system and individual animal factors [17]
Wine	Evaluation of VOCs associated with different wines coming from different origins and with different malolactic starter cultures (LAB) [18]
	Assessment of VOCs associated with different combinations of oenological yeasts to drive alcoholic fermentation in wines [19]
Beer	Study of VOCs associated with specific hop-yeast interactions during the brewing process [20]

The evaluations for which the DIMS have found application in the fermented food sector have been different, for example, assessment of different raw materials, study of various microbial resources, monitoring of the interaction between microbes and raw materials and interaction between microbes, and valuation of other post-fermentation treatments.

### 3 Conclusions

Compliance with several principles of green chemistry, DIMS represents analytical strategies to promote sustainable innovation in food systems, improving the quality and safety of fermented foods and beverages and optimising the development of new products that exploit microbial resources (e.g. fermentation, biocontrol, probiotics). Furthermore, the DIMS allow to evaluate a subset of metabolites in real-time, adding interesting information in the framework of multi-omics studies. The present work has been developed in the framework of the projects ‘iNEST’, ‘ONFOODS’, and ‘AGRITECH’ [Italian National Recovery and Resilience Plan (NRRP) projects financed by the European Commission’s Next Generation EU programme].

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