



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

Research and Innovation Centre

Fondazione Edmund Mach

Via Mach, 1

38010 San Michele All'Adige (TN) Italy

phone +39 0461615427

fax +39 0461650872

www.fmach.it

ISBN 9788878430600



ISBN 9788878430600

**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.



SCIENTIFIC COMMITTEE

Franco Biasioli - Chair	Fondazione Edmund Mach, Italy
Jonathan Beauchamp	Fraunhofer Inst. Process Engineering and Packaging IVV, Germany
Pat Silcock	University of Otago, New Zealand
Giuliana Bianco	University of Basilicata, Italy
Emanuela Gregori	Istituto Superiore di Sanità, Italy
Paola Montoro	University of Salerno, Italy
Donatella Caruso	University of Milano, Italy
Riccardo Flamini	Crea-VE, Conegliano, Italy
Gianluca Giorgi	University of Siena, Italy
Fulvio Magni	University of Milano Bicocca, Italy
Luciano Navarini	Illycaffè, Trieste, Italy

ORGANIZING COMMITTEE

Emanuela Betta	Fondazione Edmund Mach, Italy
Franco Biasioli	Fondazione Edmund Mach, Italy
Andrea Dell'Olio	Fondazione Edmund Mach, Italy
Iuliia Khomenko	Fondazione Edmund Mach, Italy
Martina Moretton	Fondazione Edmund Mach, Italy
Michele Pedrotti	Fondazione Edmund Mach, Italy
Flaminia Vincenti	Sapienza University of Roma, Italy
Maria Assunta Acquavia - Secretary	University of Basilicata, Italy

TABLE OF CONTENTS

FOREWORD	1
CONFERENCE PROGRAM	3
LIST OF CONTRIBUTIONS	11
ABSTRACTS	17
LIST OF AUTHORS	187

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>
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&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

- | | |
|-------------|--|
| 14.00-14.15 | Terry Bates - <i>Cornell University</i>
<i>Rapid headspace solid-phase microextraction with sheets with direct analysis in real time mass spectrometry (SPMESH-DART-MS) of derivatized volatile phenols in grape juices and wines</i> |
| 14.15-14.30 | Matteo Tonezzer - <i>University of Cagliari</i>
<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>
<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>
<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

16.15-16.45	Pat Silcock - <i>University of Otago</i> <i>The use of DIMS to understand microbially induced flavour changes</i>
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

Session 7 | Food Spoilage and Off-Flavour

Chairs: Catreinus de Jong & Brian Farneti

9.30-10.00	Patrik Španěl - <i>J. Heyrovský Institute of Physical Chemistry</i> <i>Progress in Selected Ion Flow Tube Mass Spectrometry, SIFT-MS, analyses of food flavour, freshness and spoilage</i>
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>

11.05-11.45 Coffee break and Poster Session

Session 8 | Floral, Biogenics and Phenotyping

Chairs: Rupert Holzinger & Vittorio Capozzi

11.45-12.05	Štefan Matejčík - <i>Comenius University</i> <i>Ion mobility spectrometry detection of plant hormones</i>
12.05-12.25	Brian Farneti - <i>Fondazione Edmund Mach</i> <i>DI-MS as high performing VOC phenotyping tool to support the horticultural production chain management</i>
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>

13.30 Farewell buffet

LIST OF CONTRIBUTIONS

Plenary Lecture		Pag
PL.01	DI-MS – A game changer for flavour research? <i>Andy Taylor</i>	17
Keynote Speakers		
K.01	The long and winding road: a flavoursome tale of PTR-MS <i>Jonathan Beauchamp</i>	20
K.02	Twenty years of Direct Injection Mass Spectrometry (DIMS) for aroma research in Dijon <i>Jean-Luc Le Quéré</i>	22
K.03	The use of DIMS to understand microbially induced flavour changes <i>Patrick Silcock</i>	24
K.04	Progress in Selected Ion Flow Tube Mass Spectrometry, SIFT-MS, analyses of food flavour, freshness and spoilage <i>Patrik Španěl</i>	25
Invited Speakers		
I.01	What is Flavour and how can DIMS help untangle the puzzle? <i>Graham T. Eyres</i>	27
I.02	Signaling volatile compounds in the human gut microbiota: new avenues offered by direct analytical methods <i>Rubert Josep, Dell'Olio Andrea, Fogliano Vincenzo, Khomenko Iuliia, Betta Emanuela, Capozzi Vittorio, Biasioli Franco</i>	28
I.03	Real-Time Trace Analysis of Breath Volatiles using Proton Transfer Reaction Mass Spectrometry: implications for <i>in-vivo</i> flavour release measurements <i>Chris A. Mayhew</i>	30
I.04	Direct injection mass spectrometry and gas sensors: a teacher-pupil relationship <i>Rosamaria Capuano, Alexandro Catini, Corrado Di Natale</i>	32
I.05	Exploring new <i>in vivo</i> and <i>in vitro</i> methods to get insight and improve the flavour release of plant-based food products during oral processing <i>Catrienus de Jong, Rene de Wijk, Valentina Acierno, Rita Boerrigter-Eenling</i>	34
I.06	<i>In vivo</i> aroma release and perception of composite foods using nose space PTR–ToF–MS analysis with Temporal-Check-All-That-Apply <i>Karina Gonzalez-Estanol, Iuliia Khomenko, Danny Clicerì, Franco Biasioli, Markus Stieger</i>	35
I.07	Development of Fast-GC PTR-MS Method for Coffee VOCs Analysis <i>Samo Smrke, Oliver Lipp, Nicolas Wernli, Chahan Yeretziyan</i>	36
I.08	What happens when food goes into oil during deep frying? Monitoring the first minutes of frying using PTR-MS.	38

	<i>Rohmah Nur Fathimah, Muhammad Saad Arshad, Tomasz Majchrzak</i>	
I.09	DIMS techniques and the study on microbial VOCs in food: flavour attributes, fermentation monitoring and emerging trends <i>Mariagiovanna Fragasso, Antonia Corvino, Martina Moretton, Iuliia Khomenko, Vittorio Capozzi</i>	41
I.10	Automatic pre-treatment and multiblock analysis of flavor release and sensory temporal data simultaneously collected <i>in vivo</i> <i>Caroline Peltier, Michel Visalli, H�el�ene Labour�e, Cantin H�elard, Isabelle Andriot, Sylvie Cordelle, Jean-Luc Le Qu�er�e, Pascal Schlich</i>	44
I.11	Modelling the kinetics of flavour formation & release as a function of ingredients addition in real food systems <i>Ana Rita Monforte, Sara Martins</i>	46
I.12	Volatile fingerprints of food thanks to the untargeted use of SIFT-MS raw data <i>Mickael Le Behec, Marine Reyrolle, Val�erie Desauziers, Thierry Pigot, Gilles Bareille, Sylvain Berail, Ekaterina Epova, Julien Barre, Lydia Gautier, Val�erie Chesneau</i>	47
I.13	Using SI traceable gas standards to improve the accuracy of untargeted PTR-MS measurements <i>Rupert Holzinger, Dusan Materic, Sebastien Dusanter, Sergi Moreno, David Worton</i>	50
I.14	Ion mobility spectrometry detection of plant hormones <i>Vahideh Ilbeigi, Younes Valdbeigi, Ladislav Moravsk�y, �tefan Matej�cik</i>	53
I.15	DI-MS as high performing VOC phenotyping tool to support the horticultural production chain management <i>Brian Farneti</i>	56

Sponsored talk

S.01	Advantages of Next-Gen PTR-TOF instruments for food and flavour sciences <i>A. Mauracher, R.Gutmann, S. Feill, A. Jordan, J. Herbig, M. M�uller, T. Reinecke, P. Sulzer</i>	58
S.02	Improved compound identification in direct VOC analysis using an EI&CI-TOFMS <i>Luca Cappellin, Marleen Vetter, Christina Hinterleitner, Steffen Br�akling, Sonja Klee</i>	60
S.03	Application of SIFT-MS to Chemical and Sensory Screening of Packaging Materials <i>Vaughan Langford, Mark Perkins</i>	63
S.04	Characterization of Isoflavones and Its Metabolites in Foods by Direct Probe Ionization Mass Spectrometer (DPiMS) with High Resolution Detection <i>Paolo Redegalli</i>	64
S.05	GC-IMS instruments and their use in Food and Flavour Analysis <i>Hansruedi Gygax, Thomas Wortelmann</i>	67

S.06	Comparative analysis of VOC purification techniques in complex cooking Emission: adsorption, photocatalysis and combined systems. <i>Daniele Zatta, Mattia Segata, Franco Biasioli, Ottaviano Allegretti, Roberto Verucchi, Francesco Chiavarini, Luca Cappellin</i>	69
------	---	----

Orals

O.01	Direct analysis of sex-wellness products using a field deployable MS equipped with a Direct Sampling Atmospheric Pressure (DSAP) source <i>Enrico Davoli, Alice Passoni, Claudio Medana, Enrica Mecarelli, Victor Laiko, Vladimir M. Doroshenko</i>	72
O.02	Characterization of plant-based milks by combining sensory analysis with headspace and nose-space direct injection mass spectrometry <i>Michele Pedrotti, Puneet Mishra, Christian Wintermeyer, Lars Grohmann, Annika Volle, Sylvia Barnekow, Theo Verkleij</i>	74
O.03	<i>In vivo</i> analysis of nose-space concentration by direct injection mass spectrometry to study the effect of chewing rate on aroma release during food consumption <i>Karina Gonzalez-Estanol, Michele Pedrotti, Monica Fontova-Cerda, Iuliia Khomenko, Franco Biasioli, Markus Stieger</i>	76
O.04	Understanding the relationship between lipids, capsaicin and aroma release in confectionery <i>Laura Hill, Lewis Jones, Katrin Pechinger, Ni Yang</i>	78
O.05	Milk matters: Unraveling retronasal aroma release and perception of coffee by combining <i>in vivo</i> nosespace analytics with dynamic sensory methods <i>Nina Cleve, Karina Gonzalez-Estanol, Iuliia Khomenko, Luca Cappellin, Jonathan Beauchamp, Franco Biasioli</i>	81
O.06	Influence of product quantity, cooking parameter and flow tube pressure on the measurement with Sift-MS in a cooking oven <i>Grégory Schmauch, Eugen Engelmann</i>	85
O.07	Rapid headspace solid-phase microextraction with sheets with direct analysis in real time mass spectrometry (SPMESH-DART-MS) of derivatized volatile phenols in grape juices and wines <i>Terry L. Bates, Gavin Sacks</i>	87
O.08	PTR-MS as a tool to understand and improve the performance of electronic noses <i>Matteo Tonezzer</i>	89
O.09	Application of PTR-ToF-MS to monitor development of flavour in sourdough. <i>Andrea Warburton, Graham Eyres, Pat Silcock</i>	90
O.10	Easy and fast detection of abnormal olive brine fermentation – A showcase of SPOTDETECT <i>Eirini Pegiou, Maxence Paillart, Yannick Weesepeol</i>	93
O.11	Mining datasets from untargeted direct analytical methods: a data analyst point of view <i>Pietro Franceschi</i>	96

O.12	Monitoring autoxidation of vegetable oils by Proton Transfer Reaction Mass Spectrometry <i>Antonella L. Grosso, Ksenia Morozova, Giovanna Ferrentino, Matteo Scampicchio</i>	97
O.13	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>Pedro Martínez Noguera, Sylvester Holt, Raju Podduturi, Wender L.P. Bredie, Jonathan Beauchamp, Mikael A. Petersen</i>	100
O.14	Supporting sustainable energy production by PTR-MS: a review on the work accomplished on biofuel production from food waste to SOFC systems <i>Davide Papurello, Silvia Silvestri</i>	103
O.15	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>Alberto Roncone, Purna K. Khatri, Mauro Paolini, Roberto Larcher, Luca Ziller, Dana Alina Magdas, Olivian Marincas, Luana Bontempo</i>	111
O.16	Contribution of volatile organic compounds to multifloral honey flavor <i>Eugenio Aprea, Danny Clicer, Emanuela Betta, Flavia Gasperi</i>	113

Posters

P.01	Effect of different carbon sources on fermentation volatile organic compounds (VOCs) profile by <i>Levilactobacillus brevis</i> WLP672 using proton transfer reaction-time of flight-mass spectrometry (PTR-ToF-MS) <i>Sarathadevi Rajendran, Iuliia Khomenko, Patrick Silcock, Emanuela Betta, Franco Biasioli, Phil Bremer</i>	116
P.02	“Mild” Extra Virgin Olive Oil: evolution of the volatile profile during storage <i>Benedetta Fanesi, Deborah Pacetti, Erica Moret, Paolo Lucci, Lanfranco Conte, Mauro Amelio</i>	119
P.03	PTR-ToF-MS as a high sensitivity sensor for online monitoring of lacto-fermentation in plant-based beverages <i>Antonia Corvino, Maria Mazzucotelli, Iuliia Khomenko, Vittorio Capozzi</i>	122
P.04	Sensor Array for alcoholic bevarages discrimination <i>Lai Van Duy, Rosamaria Capuano, Alexandro Catini, Nguyen Van Duy, Nguyen Duc Hoa, Matteo Tonezzer, Corrado Di Natale</i>	126
P.05	Human Volatilomics with GC/IMS <i>Rosamaria Capuano, Alexandro Catini, Corrado Di Natale</i>	129
P.06	Volatile compounds of natural vanilla-extract and stable isotope ratio analysis of carbon and hydrogen of vanillin and ethyl vanillin: Validation of a GC-IRMS analytical method <i>Long Chen, Purna K. Khatri, Mauro Paolini, Roberto Larcher, Luca Ziller, Luana Bontempo</i>	131

P.07	Characterization of fresh and oxidized coriander seed oil volatilome by using PTR-MS <i>Antonella L. Grosso, Katerina Sasinova, Giovanna Ferrentino, Matteo Scampicchio</i>	134
P.08	Automated untargeted peak detection for GC-IMS data <i>Maria Mazzucotelli, Pietro Franceschi</i>	137
P.09	Application of conventional and rapid analytical strategies for hazelnut volatilome characterization <i>Maria Mazzucotelli, Pietro Franceschi, Iuliia Khomenko, Brian Farneti, Emanuela Betta, Elena Gabetti, Luca Falchero, Andrea Cavallero, Eugenio Aprea</i>	139
P.10	Preliminary screening of elderly gut microbiota metabolites of pea protein enrich-bread <i>Martina Moretton, Monica Anese, Edoardo Capuano, Nicoletta Pellegrini</i>	142
P.11	Tailoring dietary intervention based on PTR-ToF-MS rapid pre-clinical screening <i>Andrea Dell'Olio, Josep Rubert, Vincenzo Fogliano, Vittorio Capozzi, Iuliia Khomenko, Martina Moretton, Franco Biasioli</i>	145
P.12	Characterization of key aroma compounds during black garlic production: GC-MS analyses and SIFT-MS quantification <i>Kseniya Dryahina, Emre Turan, Nikola Sixtova, Gülşah Özcan Sinir, Atilla Şimşek, Patrik Španěl</i>	147
P.13	PTR-ToF-MS VOC's profiling and monitoring of Red Delicious and Granny Smith apples <i>Alessia Panarese, Iulia Khomenko, Brian Farneti, Franco Biasioli, Angelo Zanella</i>	150
P.14	PTR-MS applications inside the SISTERS project – Preventing food loss and waste of fresh vegetables by monitoring quality decay through VOCs emissions <i>Pedrotti Michele, Emanuela Betta, Khomenko Iuliia</i>	153
P.15	PTR-Tof-MS analyses as a high-throughput volatilome phenotyping technique in a Genome Wide Association study of an almond germplasm collection <i>Leonardo Luca*, Brian Farneti, Iulia Khomenko, Mario Di Guardo, Stefano La Malfa, Alessandra Gentile, Franco Biasioli, Gaetano Distefano</i>	156
P.16	Volatile organic compounds: a potential marker for early detection of kiwifruit Storage Breakdown Disorder (SBD) <i>Andrea Strano, Brian Farneti, Iulia Khomenko, Emanuela Betta, Franco Biasioli, Francesco Spinelli</i>	157
P.17	Evaluation of flavour release and perception from sugar-free chewing gum using APCI-MS and temporal sensory profiling <i>Jing Feng, Gary Gray, Rebecca Ford, Ni Yang</i>	161
P.18	Emission of volatile organic compounds from wild mushrooms and coffee using proton transfer reaction mass spectrometry <i>T. Wróblewski, A. Kamińska, A. Włodarkiewicz, D. Ushakou, G. Karwasz</i>	164
P.19	Direct-Mass Spectrometry in wine analysis <i>Annarita Panighel, Mirko De Rosso</i>	167

P.20	High-throughput automatic cooking, analysis, and data mining of food matrices by PTR-ToF-MS <i>Iuliia Khomenko</i>	169
P.21	Influence of the model cheese composition on the aroma content, release and perception <i>I. Andriot, C. Septier, C. Peltier, P. Barbet, R. Palme, C. Arnould, S. Buchin, C. Salles</i>	171
P.22	Dynamic production of standards gases with liquid & online monitoring with VOCUS CI TOF at ppb level <i>L. Damont, L. Cossard, T. Bruderer</i>	173
P.23	Relevance of VOCs in microbial cross-over: the potential of DIMS in assisting new product development <i>Mariagiovanna Fragasso, Hülya Cunedioğlu, Antonia Corvino, Ester Presutto, Andrea Dell'Olio, Giuseppe Spano, Vittorio Capozzi</i>	176
P.24	Real time MS nose space monitoring allows to get insights into biological and behavioral factors affecting the inter-individual variability on flavor release <i>Leonardo Menghi, Iuliia Khomenko, Michele Pedrotti, Danny Clicerì, Eugenio Aprea, Isabella Endrizzi, Franco Biasioli, Flavia Gasperi</i>	178
P.25	Stable isotope ratio analysis for the authentication of organic wheat, pasta and bakery products <i>Zoe Giannioti, Alberto Roncone, Michele Suman, Luana Bontempo</i>	181
P.26	Venezuelan stingless bee <i>Tetragonisca angustula</i> (Latreille, 1811) pot-pollen and cerumen pollen pot Volatile Organic Compound VOC profiles by HS-SPME/GC-MS <i>Emanuela Betta, Ricardo R Contreras, Enrique Moreno, Silvia RM Pedro, Iuliia Khomenko, Patricia Vit</i>	183

P.20 High-throughput automatic cooking, analysis, and data mining of food matrices by PTR-ToF-MS

Iuliia Khomenko*

Edmund Mach Foundation, via E. Mach, 1, San Michele all'Adige (TN)

*iuliia.khomenko@fmach.it

Summary: In this study, proton-transfer-reaction time-of-flight mass spectrometry (PTR-ToF-MS) equipped with a multipurpose head-space automated sampler (autosampler) was successfully applied for investigation of VOC profiles of food samples (beef, fish, and cauliflower) first raw and then cooked in automated way inside the autosampler. This methodology is of relevance both for process optimization in the agroindustry and for the better selection of raw materials.

Keywords: direct injection, volatile organic compounds, meat, fish, cauliflower

1 Introduction

Cooking is a very important process which makes many food products like meat, fish, or some vegetables not only safer but also more pleasant for the consumers. Aroma is a very important factor which changes during this process due to different chemical and physical reactions which happen inside food products. Direct injection mass spectrometry coupled with an automated multipurpose sampler (autosampler) gives the opportunity to monitor the quick processes of large amount of raw and cooked samples in a short period of time. Moreover the sequence programming permits to perform cooking of the samples on board of autosampler's trays which gives the opportunity to heat samples in a precise way and immediately analyze the aroma profile of just cooked samples.

2 Experimental

Three different food matrices were analysed for this study: i) beef meat of different individuals of Piedmontese cattle breed, ii) fresh wild and reared gilthead sea bream (*Sparus aurata*) in two different locations and three time points of fishing, and iii) cauliflower. PTR-ToF-MS (PTR-ToF-MS 8000, Ionicon, Austria) was coupled with an autosampler (MPS MultiPurposeSampler, Gerstel, Germany). The samples were prepared in a 20 mL vials in triplicated with the weight 3 g (i, ii), and 1 g (iii) and immediately stored at -80°C. In the case of cauliflower the antioxidant mixture was added on top of the powder grinded in liquid nitrogen. Samples were stored at 4°C prior the analysis then every vial was incubated at 25°C and measured as a raw sample. Then each sample was cooked at 70°C for 25 min into trays of the autosampler and then cooled down to 25°C before being measured. Data processing of PTR-ToF-MS spectra consisted of external calibration, peak extraction and selection [1] followed by descriptive statistics and multivariate analysis.

3 Results

According to Principal Component Analysis performed separately of each dataset the effect of cooking was observed in three cases. The concentration of VOCs increased after the thermal treatment. In the case of beef samples some higher alcohols, aldehydes and ketones were higher in cooked samples rather than in raw ones. The aroma profile of cooked fish was as well more intense than the raw one. From the PCA score plot of raw fish samples, a clear separation between fish types

was observed. According to the PCA score plot of cooked fish the differences between raw and reared fish remained but the differences between two farming systems became less evident. The reared fish from Adriatic Sea was richer in monoterpene compounds from essential oils [2] and aromatic compounds which are usually associated with the metabolism of carotenoids or thermal degradation of sugars and amino acids [2]. For these compounds a negligible effect of cooking was observed. In the case of cauliflower the trend of increasing VOCs during the thermal treatment was observed as well especially for Sulphur containing compounds like hydrogen sulfide, methanitol, and dimethyl sulfide.

4 Conclusions

In this study, PTR-ToF-MS coupled to an autosampler was successfully applied for a high-throughput and non-invasive screening of aroma profile of raw and cooked food of different origin. The coupling of direct injection mass spectrometry and a multipurpose autosampler which allows for sample handling, cooking and VOCs analysis offers new opportunity for an efficient evaluation of raw materials and of the cooking process which is of paramount important for agroindustry.

References

- [1] L. Cappellin, F. Biasioli A. Fabris, E. Schuhfried, C. Soukoulis, TD. Mark, F. Gasperi, Improved mass accuracy in PTR-TOF-MS: Another step towards better compound identification in PTR-MS, *Int J Mass spectrum*, 290(1), 60-63, (2010)
- [2] N. Alexi, E. Fountoulaki, K. Grigorakis Quality of reared gilthead sea bream (*Sparus aurata*) during ice storage, as affected by dietary fish oil substitution; an instrumental and sensory designation approach, *Aquaculture Research*, 48, 3817–3828 (2017)