Società Chimica Italiana
Divisione di Spettrometria di Massa

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 97888784306004

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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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 - *Società Chimica Italiana-Divisione Spettrometria di Massa*
	Mario Pezzotti - *Fondazione Edmund Mach*
14.10-14.20	Why DIFFA23?
	Franco Biasioli - *Fondazione Edmund Mach*
14.20-15.05	Plenary lecture: *DI-MS – A game changer for flavour research?*
	Andy Taylor - *University of Nottingham*

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
	The long and winding road: a flavoursome tale of PTR-MS
15.35-15.55	Graham Eyres - *University of Otago*
	What is Flavour and how can DIMS help untangle the puzzle?
15.55-16.15	Andreas Mauracher - *IONICON*
	Advantages of Next-Gen PTR-ToF instruments for food and flavour sciences

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

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 - *INRAE-CSGA Dijon*
	Twenty years of Direct Injection Mass Spectrometry for aroma research in Dijon
9.30-9.50	Catrienus De Jong - *Wageningen University & Research*
	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
9.50-10.10	Markus Stieger - *Wageningen University & Research*
	In vivo aroma release and sensory perception of composite foods
10.10-10.20	Michele Pedrotti - *Wageningen University & Research*
	Characterization of plant-based milks by combining sensory analysis with headspace and nose-space direct injection mass spectrometry
10.20-10.30	Karina Gonzalez-Estanol - *Wageningen University & Research*
	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
10.30-10.40	Laura Hill - *University of Nottingham*
	Understanding the relationship between lipids, capsaicin and aroma release in confectionery

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 - *ZHAW School of Life Sciences and Facility Management* *Development of fast-GC PTR-MS method for coffee VOCs analysis*
11.30-11.45	Nina Cleve - *Fraunhofer Institute for Process Engineering and Packaging IVV* *Milk matters: Unraveling retronasal aroma release and perception of coffee by combining in vivo nosespace analytics with dynamic sensory methods*
11.45-12.05	Tomasz Majchrzak - *Gdansk University of Technology* *What happens when food goes into oil during deep frying? Monitoring the first minutes of frying using PTR-MS*
12.05-12.20	Gregory Schmauch - *Rational F&E GmbH* *Influence of product quantity, cooking parameter and flow tube pressure on the measurement with Sift-MS in a cooking oven*
12.20-12.40	Vaughan Langford - *Syft Technologies* *Application of SIFT-MS to chemical and sensory screening of packaging materials*

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 - *Cornell University* *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*
14.15-14.30	Matteo Tonezzer - *University of Cagliari* *PTR-MS as a tool to understand and improve the performance of electronic noses*
14.30-14.45	Andrea Warburton - *University of Otago* *Application of PTR-ToF-MS to monitor development of flavour in sourdough*
14.45-15.05	Paolo Redegalli - *Shimadzu Italia S.r.l.* *Characterization of isoflavones and its metabolites in foods by direct probe ionization mass spectrometer (DPiMS) with high resolution detection*
15.05-15.25	Hansruedi Gygax - *GAS Dortmund* *GC-IMS instruments and their use in food and flavour analysis*

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

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 - *J. Heyrovský Institute of Physical Chemistry*
	Progress in Selected Ion Flow Tube Mass Spectrometry, SIFT-MS, analyses of food flavour, freshness and spoilage
10.00-10.15	Antonella Grosso - *University of Bolzano*
	Monitoring autoxidation of vegetable oils by proton transfer reaction mass spectrometry
10.15-10.30	Pedro Martinez Noguera - *University of Copenhagen*
	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
10.30-10.45	Davide Papurello - *Turin Polytechnic*
	Supporting sustainable energy production by PTR-MS: a review on the work accomplished on biofuel production from food waste to SOFC systems
10.45-11.05	Rupert Holzinger - *Utrecht University*
	Using SI traceable gas standards to improve the accuracy of untargeted PTR-MS measurements

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 - *Comenius University* *Ion mobility spectrometry detection of plant hormones*
12.05-12.25	Brian Farneti - *Fondazione Edmund Mach* *DI-MS as high performing VOC phenotyping tool to support the horticultural production chain management*
12.25-12.40	Alberto Roncone - *Fondazione Edmund Mach* *Validation of gas chromatographic methods for the botanical characterization and authentication of lavender essential oil by stable isotope analysis of its organic volatile compounds*
12.40-12.55	Eugenio Aprea - *University of Trento* *Contribution of volatile organic compounds to multifloral honey flavor*
12.55-13.15	Daniele Zatta - *University of Padua* *Comparative analysis of VOC purification techniques in complex cooking emission: adsorption, photocatalysis and combined systems.*

13.15-13.30	Closing remarks Fulvio Magni - *Società Chimica Italiana-Divisione Spettrometria di Massa* Franco Biasioli - *Fondazione Edmund Mach*

13.30	Farewell buffet

LIST OF CONTRIBUTIONS

Plenary Lecture		**Pag**
PL.01	DI-MS – A game changer for flavour research? *Andy Taylor*	17

Keynote Speakers		
K.01	The long and winding road: a flavoursome tale of PTR-MS *Jonathan Beauchamp*	20
K.02	Twenty years of Direct Injection Mass Spectrometry (DIMS) for aroma research in Dijon *Jean-Luc Le Quéré*	22
K.03	The use of DIMS to understand microbially induced flavour changes *Patrick Silcock*	24
K.04	Progress in Selected Ion Flow Tube Mass Spectrometry, SIFT-MS, analyses of food flavour, freshness and spoilage *Patrik Španěl*	25

Invited Speakers		
I.01	What is Flavour and how can DIMS help untangle the puzzle? *Graham T. Eyres*	27
I.02	Signaling volatile compounds in the human gut microbiota: new avenues offered by direct analytical methods *Rubert Josep, Dell'Olio Andrea, Fogliano Vincenzo, Khomenko Iuliia, Betta Emanuela, Capozzi Vittorio, Biasioli Franco*	28
I.03	Real-Time Trace Analysis of Breath Volatiles using Proton Transfer Reaction Mass Spectrometry: implications for *in-vivo* flavour release measurements *Chris A. Mayhew*	30
I.04	Direct injection mass spectrometry and gas sensors: a teacher-pupil relationship *Rosamaria Capuano, Alexandro Catini, Corrado Di Natale*	32
I.05	Exploring new *in vivo* and *in vitro* methods to get insight and improve the flavour release of plant-based food products during oral processing *Catrienus de Jong, Rene de Wijk, Valentina Acierno, Rita Boerrigter-Eenling*	34
I.06	*In vivo* aroma release and perception of composite foods using nose space PTR–ToF–MS analysis with Temporal-Check-All-That-Apply *Karina Gonzalez-Estanol, Iuliia Khomenko, Danny Cliceri, Franco Biasioli, Markus Stieger*	35
I.07	Development of Fast-GC PTR-MS Method for Coffee VOCs Analysis *Samo Smrke, Oliver Lipp, Nicolas Wernli, Chahan Yeretzian*	36
I.08	What happens when food goes into oil during deep frying? Monitoring the first minutes of frying using PTR-MS.	38

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

Sponsored talk

S.01	Advantages of Next-Gen PTR-TOF instruments for food and flavour sciences *A. Mauracher, R.Gutmann, S. Feil1, A. Jordan, J. Herbig, M. Müller, T. Reinecke, P. Sulzer*	58
S.02	Improved compound identification in direct VOC analysis using an EI&CI-TOFMS *Luca Cappellin, Marleen Vetter, Christina Hinterleitner, Steffen Bräkling, Sonja Klee*	60
S.03	Application of SIFT-MS to Chemical and Sensory Screening of Packaging Materials *Vaughan Langford, Mark Perkins*	63
S.04	Characterization of Isoflavones and Its Metabolites in Foods by Direct Probe Ionization Mass Spectrometer (DPiMS) with High Resolution Detection *Paolo Redegalli*	64
S.05	GC-IMS instruments and their use in Food and Flavour Analysis *Hansruedi Gygax, Thomas Wortelmann*	67

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

Orals

O.01 Direct analysis of sex-wellness products using a field deployable MS equipped with a Direct Sampling Atmospheric Pressure (DSAP) source 72
Enrico Davoli, Alice Passoni, Claudio Medana, Enrica Mecarelli, Victor Laiko, Vladimir M. Doroshenko

O.02 Characterization of plant-based milks by combining sensory analysis with headspace and nose-space direct injection mass spectrometry 74
Michele Pedrotti, Puneet Mishra, Christian Wintermeyer, Lars Grohmann, Annika Volle, Sylvia Barnekow, Theo Verkleij

O.03 *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 76
Karina Gonzalez-Estanol, Michele Pedrotti, Monica Fontova-Cerda, Iuliia Khomenko, Franco Biasioli, Markus Stieger

O.04 Understanding the relationship between lipids, capsaicin and aroma release in confectionery 78
Laura Hill, Lewis Jones, Katrin Pechinger, Ni Yang

O.05 Milk matters: Unraveling retronasal aroma release and perception of coffee by combining *in vivo* nosespace analytics with dynamic sensory methods 81
Nina Cleve, Karina Gonzalez-Estanol, Iuliia Khomenko, Luca Cappellin, Jonathan Beauchamp, Franco Biasioli

O.06 Influence of product quantity, cooking parameter and flow tube pressure on the measurement with Sift-MS in a cooking oven 85
Grégory Schmauch, Eugen Engelmann

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 87
Terry L. Bates, Gavin Sacks

O.08 PTR-MS as a tool to understand and improve the performance of electronic noses 89
Matteo Tonezzer

O.09 Application of PTR-ToF-MS to monitor development of flavour in sourdough. 90
Andrea Warburton, Graham Eyres, Pat Silcock

O.10 Easy and fast detection of abnormal olive brine fermentation – A showcase of SPOTDETECT 93
Eirini Pegiou, Maxence Paillart, Yannick Weesepoel

O.11 Mining datasets from untargeted direct analytical methods: a data analyst point of view 96
Pietro Franceschi

O.12 Monitoring autoxidation of vegetable oils by Proton Transfer Reaction Mass Spectrometry 97
<u>Antonella L. Grosso</u>, Ksenia Morozova, Giovanna Ferrentino, Matteo Scampicchio

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. 100
<u>Pedro Martínez Noguera</u>, Sylvester Holt, Raju Podduturi, Wender L.P. Bredie, Jonathan Beauchamp, Mikael A. Petersen

O.14 Supporting sustainable energy production by PTR-MS: a review on the work accomplished on biofuel production from food waste to SOFC systems 103
<u>Davide Papurello</u>, Silvia Silvestri

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 111
<u>Alberto Roncone</u>, Purna K. Khatri, Mauro Paolini, Roberto Larcher, Luca Ziller, Dana Alina Magdas, Olivian Marincas, Luana Bontempo

O.16 Contribution of volatile organic compounds to multifloral honey flavor 113
<u>Eugenio Aprea</u>, Danny Cliceri, Emanuela Betta, Flavia Gasperi

Posters

P.01 Effect of different carbon sources on fermentation volatile organic compounds (VOCs) profile by *Levilactobacillus brevis* WLP672 using proton transfer reaction-time of flight-mass spectrometry (PTR-ToF-MS) 116
<u>Sarathadevi Rajendran</u>, Iuliia Khomenko, Patrick Silcock, Emanuela Betta, Franco Biasioli, Phil Bremer

P.02 “Mild” Extra Virgin Olive Oil: evolution of the volatile profile during storage 119
<u>Benedetta Fanesi</u>, Deborah Pacetti, Erica Moret, Paolo Lucci, Lanfranco Conte, Mauro Amelio

P.03 PTR-ToF-MS as a high sensitivity sensor for online monitoring of lacto-fermentation in plant-based beverages 122
<u>Antonia Corvino</u>, Maria Mazzucotelli, Iuliia Khomenko, Vittorio Capozzi

P.04 Sensor Array for alcoholic bevarages discrimination 126
<u>Lai Van Duy</u>, Rosamaria Capuano, Alexandro Catini, Nguyen Van Duy, Nguyen Duc Hoa, Matteo Tonezzer, Corrado Di Natale

P.05 Human Volatilomics with GC/IMS 129
Rosamaria Capuano, Alexandro Catini, <u>Corrado Di Natale</u>

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 131
<u>Long Chen</u>, Purna K. Khatri, Mauro Paolini, Roberto Larcher, Luca Ziller, Luana Bontempo

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

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

P.16 Volatile organic compounds: a potential marker for early detection of kiwifruit Storage Breakdown Disorder (SBD)

Andrea Strano[2]*, Brian Farneti[1], Iulia Khomenko[1], Emanuela Betta,[1], Franco Biasioli[1], Francesco Spinelli[2]

[1]Foundation Edmund Mach Research and Innovation Centre Genomics and Biology of Fruit Crops, San Michele all'Adige, Italy
[2]Alma Mater Studiorum Università di Bologna, Department of Agricultural and Food Sciences, Bologna, Italy

*andrea.strano3@unibo.it

Summary: In kiwifruit postharvest losses related to SBD represents a critical issue associated to ripening of kiwifruit at cold storage temperature. During this period fruit emits a blend of volatile organic compounds (VOCs), which may change due to injuries or physiological disorders. The present study aim to forecast SBD risk and its incidence during fruit maturation and characterize VOCs emission to identify possible markers for early detection for minimize losses.
Keywords: PTR-ToF-MS, physiological disorders, postharvest management.

1 Introduction

During last 20 years the commercial demand for the presence of new yellow-fleshed kiwi cultivars in worldwide market is constantly increasing. However, those new varieties are characterised by a shorter postharvest viability, compared to green-fleshed cultivars; for this reason, high qualitative product requires a fine tuning of pre- and postharvest strategies [4]. Postharvest losses are primarily related to physiological disorders, such as softening and storage breakdown (SBD) [1], associated to kiwifruit ripening at cold storage temperature and depends on several factors, such as agronomic factors, fruit maturity stage at harvest and storage conditions [3]. Generally, symptoms develop as water-soaked area of tissue that progressively occupy more of the inner pericarp and eventually move to the outer pericarp [5].
Because of damage caused by abiotic stresses, plant tissues react producing volatile organic compounds (VOCs); same happens in fruits. Recent progresses in untargeted metabolomics analysis led to the development of rapid, simple, and high-throughput techniques, such as Proton Transfer Reaction-Time-of-Flight-Mass Spectrometry (PTR-ToF-MS), which allows real-time VOCs analysis [2]. PTR-ToF-MS has been also recently exploited in many fruit species, validating the capacity of this technique to characterize the aroma profile for quality-oriented studies as well as for fruit storage disorders. The main advantages of employing PTR-ToF-MS are the low concentration detection limit (parts per trillion by volume), the rapidity of analysis, and the possibility to detect simultaneously molecules with different polarity and volatility [6][8][9][10][12].
Since SBD is a still an unknown aetiology factor, the aim of present research is to verify whether kiwifruit affected by SBD disorders produced VOCs uniquely connected with the disorder itself. The characterisation of SBD-dependent VOCs emission may lead to an early detection of symptoms and a possible solution to reduce their emission.

2 Material & Methods

Fruits were collected during 2018 to 2022 and from two different commercial orchards of Actinidia chinensis var. chinensis located in Latina Province, Italy. The two orchards have similar characteristics and agricultural management, with plants grafted in 2013-15 on 7- to 9-year-old 'Hayward' rootstocks. Fruit was harvested at 8-10 average °Brix. Fruit ripening stage was evaluated non- destructively by using a KiwiMeter a selecting fruit for uniform DAindex™ (1.2-1.0) according to Costa et al. (2015) [7].

To determine SBD incidence and time of occurrence a preliminary experiment was performed after each production season, in the years from 2018 to 2022. Fruits were randomly divided into eighteen international trays (IT) containing 25 fruits each. ITs were placed into cool storage (normal atmosphere 1.0±1°C and RH 98%) for 6 months. At monthly intervals, 3 ITs (75 fruits) were used to assess sugar content (°Brix), incidence (%) and severity of storage breakdown disorder (SBD) and firmness (kg) after 1 day and 3 days at room temperature (20°C). Two IT containing 20 fruits each were stored for 5 months, and SBD was assessed at 1 and 3 days of shelf-life. SBD symptoms were visually evaluated by two independent observers using a severity scale as follows: 3 = corking/granulation occurs as a complete ring around the outer pericarp and/or water soaking of the inner and outer pericarp occurs; 2 = granulation/corking occurs in the outer pericarp but as an incomplete ring and/or water soaking of the inner pericarp; 1 = specking/flecking appears in any area of the outer pericarp (near skin, middle or throughout); 0 = no SBD.

Before fruit quality assessment, the VOC emissions of the same forty kiwifruits were individually determined by PTR-ToF-MS at 1 and 3 days of shelf life. Direct injection VOC measurement was performed on 40 kiwifruits with a commercial PTR-ToF-MS 8000 apparatus (Ionicon Analytik GmbH, Innsbruck, Austria) according to the set-up described by Farneti et al. [8][9]. At 3 days of shelf-life, after SBD assessment, each fruit was incubated for 20 min into a 1-L glass jar at 21°C before the analysis.

For the analysis of PTR-ToF-MS spectral data, count losses due to the ion detector dead time were corrected off-line via a methodology based on Poisson statistics. To reach a good mass accuracy (up to 0.001 Th), internal calibration was performed. Noise reduction, baseline removal and peak intensity extraction were performed using modified Gaussian distributions to fit the peaks.

3 Results & Conclusions

During the 2018-2019 experiment the overall SBD incidence was 40% being 22.5% in the class with higher severity, 7.5% in the intermediate one and 10% in the lowest. Concerning quality parameters after 5 months of storage, it was not possible to assess them on fruit in SBD classes 2 and 3. No significant difference was found between non-affected and fruit in SBD 1. For healthy (SBD 0) and mildly affected (SBD 1) fruit, the average FF was 0.92±0.03 Kgf and SSC was 17.29±0.21 °Brix. Healthy and SBD-affected fruit clearly differentiated by their VOC profile. The PCA analysis of fruit VOCs profile assessed by PTR-ToF-MS allowed to discriminate healthy and infected fruit primarily by the variability of the first principal component (PC1:82.2%). The discrimination between healthy fruit and the one affected by SBD was more evident at 1 day of shelf-life, whereas the VOC profiles at 3 days were partially overlapping. This observation suggests that, with the progression of ripening, the increase of VOCs related with natural fruit aroma development partially masks the differences due to SBD. However, it is interesting to note that several compounds related to SBD significantly increased with the severity of the disorder (Figure 2) and seem to not be dependent on ripening. In fact, these compounds, in healthy fruit, did not change between 1 and 3 days of shelf-life. A putative identification of the SBD-related VOC masses is challenging without GC-MS analysis. However, some masses (34.0372, 48.053, 91.0747) may be indicative of alcohols produced by fermentative processes. Other masses (44.024 and 46.0372) are related with fruity aroma such as esters. One mass (154.998) may be attributed to a dithiocarboxylic acid compound [11].

References

[1] Alavi, M., Fullerton, C.G., Pidakala, P., and Burdon, J.N. (2021). Prediction of chilling injury risk in 'Zesy002' kiwifruit from softening early in storage. *N. Z. J. Crop Hortic. Sci.* https://doi.org/10.1080/01140671.2021.1934041.

[2] Biasioli, F., Yeretzian, C., Mark, T.D., Dewulf, J., and Van Langenhove, H. (2011). Direct-injection mass spectrometry adds the time dimension to (B)VOC analysis. *Trends Analyt. Chem. 30 (7),* 1003–1017 https://doi.org/10.1016/ j.trac.2011.04.005.

[3] Burdon, J. (2019). Kiwifruit biology: the commercial implications of fruit maturation. *Hortic. Rev. (Am. Soc. Hortic. Sci.) 46*, 385–421.

[4] Burdon, J., and Lallu, N. (2011). Kiwifruit (Actinidia spp.). In *Postharvest Biology and Technology of Tropical and Subtropical Fruit, Vol. 3*: Cocona to Mango, E.M. Yahia, ed. (Woodhead Publishing Limited), p.326–360.

[5] Burdon, J., Lallu, N., Francis, K., and Boldingh, H. (2007). The susceptibility of kiwifruit to low temperature breakdown is associated with pre-harvest temperatures and at-harvest soluble solids content. *Posthar. Biol. And Tech. 43 (3),* 283–290 https://doi.org/10.1016/j.postharvbio.2006.09.011.

[6] Busatto, N., Farneti, B., Tadiello, A., Oberkofler, V., Cellini, A., Biasioli, F., Delledonne, M., Cestaro, A., Noutsos, C., and Costa, F. (2019). Wide transcriptional investigation unravel novel insights of the on-tree maturation and postharvest ripening of 'Abate Fetel' pear fruit. *Hortic Res 6 (1),* 32 https://doi.org/10.1038/s41438-018-0115-1. PubMed

[7] Costa, G., Vidoni, S., Rocchi, L., Cellini, A., Buriani, G., Donati, I., and Spinelli, F. (2015). Innovative non-destructive device for fruit quality assessment and early disease diagnosis. *Acta Hortic. 1096,* 69–78 https://doi.org/10. 17660/ActaHortic.2015.1096.4.

[8] Farneti, B., Busatto, N., Khomenko, I., Cappellin, L., Gutierrez, S., Spinelli, F., Velasco, R., Biasioli, F., Costa, G., and Costa, F. (2015a). Untargeted metabolomics investigation of volatile compounds involved in the development of apple superficial scald by PTR-ToF-MS. *Metabolomics 11 (2),* 341–349 https://doi.org/10.1007/s11306-014-0696-0.

[9] Farneti, B., Khomenko, I., Cappellin, L., Ting, V., Romano, A., Biasioli, F., Costa, G., and Costa, F. (2015b). Comprehensive VOC profiling of an apple germplasm collection by PTR-ToF-MS. *Metabolomics 11 (4),* 838–850 https://doi.org/10.1007/s11306-014-0744-9.

[10] Neri, F., Cappellin, L., Spadoni, A., Cameldi, I., Algarra Alarcon, A., Aprea, E., Romano, A., Gasperi, F., and Biasioli, F. (2015). Role of strawberry volatile organic compounds in the development of Botrytis cinerea infection. *Plant Pathol. 64 (3),* 709–717 https://doi.org/10.1111/ppa.12287.

[11] Smith, M., and Jonathan, P. (2013). Applications of new mass spectrometric technologies for the structural characterisation of synthetic polymers. Thesis (Durham University), http://etheses.dur.ac.uk/7367/.

[12] Spadoni, A., Cappellin, L., Neri, F., Algarra Alarcon, A., Romano, A., Guidarelli, M., Gasperi, F., Biasioli, F., and Mari, M. (2015). Effect of hot water treatment on peach volatile emission and Monilinia fructicola development. *Plant Pathol. 64 (5),* 1120–1129 https://doi.org/10.1111/ppa.12353.