



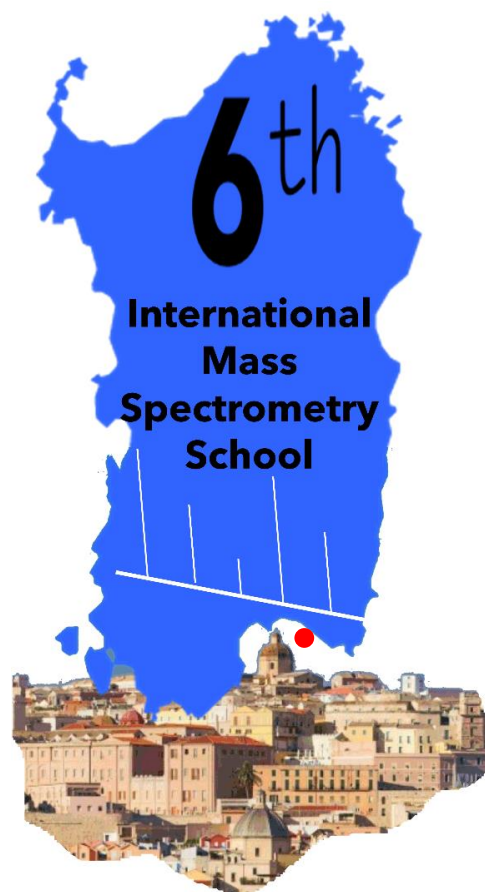
6th International Mass Spectrometry School

Fundamentals, advances, instrumentation, and applications



Cagliari, Sardinia (Italy)

September 17-22, 2023



<https://www.spettrometriadimassa.it/imss2023>



<https://www.spettrometriadi massa.it/imss2023>

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WELCOME FROM THE CHAIR AND THE SCIENTIFIC AND ORGANIZING COMMITTEES OF THE 6th IMSS

On behalf of the Division of Mass Spectrometry (DSM) of the Italian Chemical Society, we would like to welcome you to the 6th International Mass Spectrometry School (IMSS) 2023 in Cagliari, Sardinia, Italy.

The International Mass Spectrometry Foundation started this educational activity, aimed to enforce, promote and diffuse the culture of mass spectrometry, in 2013 with the first edition of this school held in Siena (Italy).

After ten years, moving in Europe and out of Europe (Siena (Italy), Natal (Brazil), Dubrovnik (Croatia), Sitges (Spain) and Belfast (Ireland)) the school comes back to Italy in the town of Cagliari, in the magnificent island of Sardinia to celebrate its 10th anniversary.

Many students attended the various editions of IMSS and each completely fulfilled its aims: give a good education, establish and favorite students-tutors and students-students interactions, high level tutors, informal and friendly atmosphere, great social events.

We think that also IMSS 2023 will be a useful occasion to enjoy science, learn or refresh principles and main applications of mass spectrometry with a look at the future, networking among participants and with tutors, enjoy ideas, suggestions by students, taste delicious food, experience the real local life in Cagliari, a very nice and lovely town in South Sardinia!

The city has a heritage of great importance, it's a green, small, clean and safe city with a Mediterranean climate. The international airport, very close to downtown, connects Cagliari to many towns in Europe.

We do wish IMSS 2023 will be an important experience for young scientists, not only from a scientific and cultural standpoint, but also for relationships, networking, talks, social events in the special atmosphere of Cagliari and Sardinia.

With the support of everybody, we do hope that IMSS 2023 will be a successful, amazing and unforgettable school!!



Gianluca Giorgi (IMSS 2023 chair) and
the IMSS 2023 scientific and organizing committees

WELCOME FROM THE IMSF PRESIDENT

It gives me great pleasure to invite you to join us at the 6th International Mass Spectrometry School in Cagliari, Sardinia for the 17-22 September 2023. Returning to Italy for the 10th anniversary of this flagship IMSF activity offers a unique opportunity to advance your MS knowledge.

Education is at the heart of the professional development the IMSF aims to stimulate. Come to Cagliari to learn from and connect with mass spectrometrists across the globe.

The exciting program of lectures and workshops covers the breadth of mass spectrometry, from fundamentals to applications. Interlaced with collaborative problem solving sessions and outstanding networking opportunities for all delegates, students and tutors alike it is one of the highlights of the 2023 mass spectrometry calendar



Ron M.A. Heeren (IMSF President)

IMSF EXECUTIVE COMMITTEE, IMSF NATIONAL AFFILIATES

Executive Committee

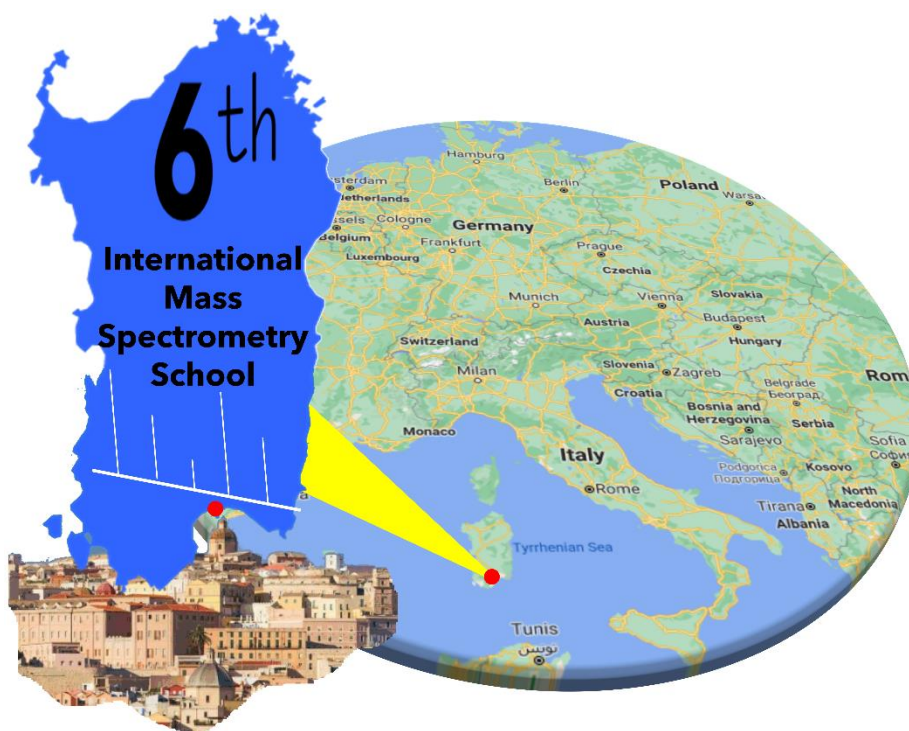
✓ Ron M. A. Heeren	President	The Netherlands
✓ Stephen Blanksby	Vice President	Australia
✓ John Langley	Past President	UK
✓ Maarten Altelaar	Treasurer	The Netherlands
✓ Martina Marchetti-Deschmann	Secretary	Austria
✓ Diego Cobice	Educational Officer	Ireland
✓ Gavin Reid	Vice-President (Conference) Chair IMSC 2024	Australia
✓ Gianluca Giorgi	Vice-President (Education) Chair IMSS 2023	Italy
✓ Julia Chamot-Rooke	Region A Repres. (Europe/Africa)	France
✓ Yu Xia	Region B Repres. (Asia/Oceania)	China
✓ Vicki Wysocki	Region C Repres. (North America)	USA
✓ Rosa Erra-Balsells	Region D Representative (Central and South America)	Argentina

National Affiliates

✓ Argentina – Rosa Erra Balsells	✓ Korea – Byungjoo Kim
✓ Australia/New Zealand – Tara Pukala	✓ Malaysia - Low Teck Yew
✓ Austria – Günter Allmaier	✓ The Netherlands – Anouk Rijs
✓ Belgium – Jeff Rozenski	✓ Norway – Leon Reubsæf
✓ Brazil – Marcos Eberlin	✓ Peoples Rep. of China – Yuanjiang Pan
✓ Canada – Derek Wilson	✓ Poland – Katarzyna Pawlak
✓ Czech Republic – Jan Preisler	✓ Portugal – Maria Helena Florencio
✓ Denmark – Steen Pontoppidan	✓ Romania – Zaharie Moldovan
✓ Finland – Olli Laine	✓ Russia – Albert Lebedev
✓ France – Isabelle Fournier	✓ Singapore – Lin Qingsong
✓ Germany – Thorsten Benter	✓ Slovenia – Helena Prosen
✓ Greece – Despina Tsipi	✓ South Africa – Egmont Rohwer
✓ Hong Kong – Andy Siu	✓ Spain – Estaban Abad
✓ Hungary – Karoly Vekey	✓ Sweden – Jonas Bergquist
✓ India – Rajesh Kumar Vatsa	✓ Switzerland – Yury Tsybin
✓ Ireland – Mike Kinsella	✓ Taiwan – Yi-Sheng Wang
✓ Israel – Yariv Brotman	✓ United Kingdom – Neil Oldham
✓ Italy – Gianluca Giorgi	✓ United States of America – Julia Laskin
✓ Japan – Michisato Toyoda	✓ Ukraine – Marina Kosevich

INTERNATIONAL MASS SPECTROMETRY SCHOOLS

<i>1st IMSS – Siena, Italy</i>	<i>2013</i>
<i>2nd IMSS – Natal, Brazil</i>	<i>2015</i>
<i>3rd IMSS – Dubrovnik, Croatia</i>	<i>2017</i>
<i>4th IMSS – Sitges, Spain</i>	<i>2019</i>
<i>5th IMSS – Belfast, Ireland</i>	<i>2022</i>



6th IMSS SCIENTIFIC COMMITTEE



Gianluca Giorgi
Univ. of Siena



Cecilia Bergamini
ARPAE, Bologna



Giuliana Bianco
Univ. of Basilicata



Donatella Caruso
Univ. of Milano



Riccardo Flamini
CREA-VE, Conegliano



Roberta Galarini
IZSUM, Perugia



Fulvio Magni
Univ. of Milano Bicocca



Luciano Navarini
Illycaffè, Trieste

6th IMSS ORGANIZING COMMITTEE



Michela Begala
Univ. of Cagliari



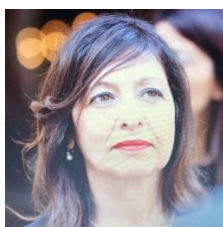
Pierluigi Caboni
Univ. of Cagliari



Luigi Atzori
Univ. of Cagliari



Tiziana Cabras
Univ. of Cagliari



Giovanna Lucia Delogu
Univ. of Cagliari



Giorgia Sarais
Univ. of Cagliari



Carlo Tuberoso
Univ. of Cagliari



Pietro Urgeghe
Univ. of Sassari

6th IMSS TUTORS

Carlos Afonso	Université de Rouen	France
Giuliana Bianco	Univ. of Basilicata	Italy
Pierluigi Caboni	University of Cagliari	Italy
Diego Cobice	Ulster University	Ireland
Chiara Cordero	Univ. of Torino	Italy
Valérie Gabelica	Université de Bordeaux	France
Pascal Gerbaux	University of Mons	Belgium
Gianluca Giorgi	University of Siena	Italy
Ron M. A. Heeren	Maastricht University	The Netherlands
Giancarlo la Marca	University of Florence	Italy
John Langley	University of Southampton	UK
Martina Marchetti-Deschmann	Technischen Universität Wien	Austria
Giuseppe Paglia	University of Milano Bicocca	Italy
Michele Suman	Barilla, Parma	Italy
Vicki Wysocki	Ohio State University	USA



ECTS CREDITS



The 6th IMSS will give ECTS credits to students who passed the examination test.

According to the Italian rules, 1 ECTS credit = 25 working hours, a participant could be eligible for 1.5 ECTS credits.

The ECTS credits will be reported in the final Certificate of Attendance with the Exam outcome together with the actual number of the working hours, so to facilitate conversions in different countries.

NICO NIBBERING TRAVEL AWARDS



The International Mass Spectrometry Foundation established the Nico Nibbering Travel Awards to support students participation in the 6th IMSS.

Prof. Nibbering was a passionate advocate for young scientists and supported the education and

career-development of mass spectrometrists from many countries around the world through his mentorship and the delivery of education and workshop programs.

The Nico Nibbering Student Travel Awards serve to honor his many contributions to international mass spectrometry and build on his legacy of supporting young scientists in this field.

BEST ORAL AWARDS



to be assigned to two young researchers under 35 years of age presenting an oral communication.

Each award consists of a certificate and an expenses contribution.

BEST POSTER AWARD



to be assigned to a young researcher under 35 years of age presenting a poster communication.

The award consists of a certificate and a 2024 online subscription to JMS.

BEST MS SOLVER AWARD



to be assigned to the Best MS Solver.
The award consists of a certificate and a gift.

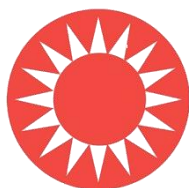
PATRONAGES



Università degli Studi di Cagliari



con il patrocinio
uniss
UNIVERSITÀ DEGLI STUDI DI SASSARI



**SARDIGNA CHIRCAS
SARDEGNA RICERCHE**



ISTITUTO
ZOOFILATTICO
SPERIMENTALE
DELLA SARDEGNA
"G. Pegreffi"



INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

MEDIA PARTNERS



SPONSORS



GENERAL INFORMATION

The IMSS 2023 is held in Cagliari, the most important city of Sardinia located in its Southern part.

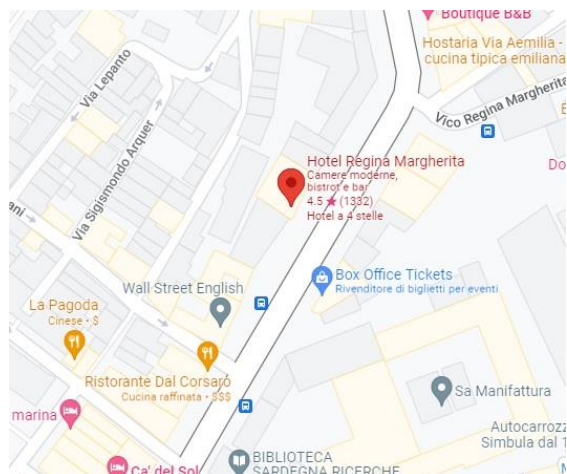
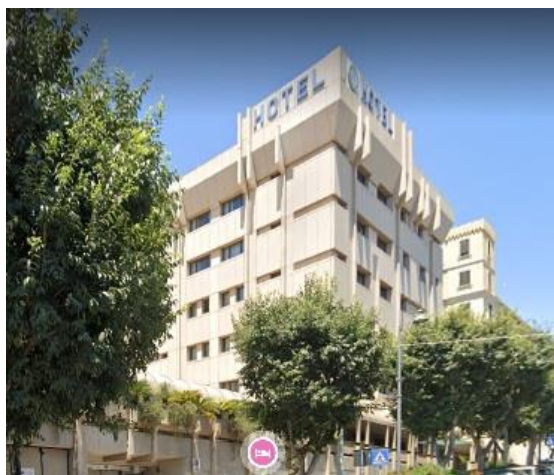
The city has a soul consisting of a millenary history, culture, nature, beach tourism, charmed by the views of Castello, the ramparts and the Roman remains, the Sardinian sea, as well as by the dynamism of a surprisingly lively city.

School venue

The IMSS 2023 venue is

Hotel Regina Margherita ****

viale Regina Margherita 44, Cagliari



VISIT SARDINIA



Discover Sardinia, its landscapes, amazing beaches, delicious food & wines

SARDEGNATurismo

<https://www.sardegnaturismo.it/en>

SOCIAL EVENTS

SUNDAY Sept. 17

h. 8:30 p.m.

Welcome cocktail at TERRAPIENO CLUB HOUSE

Viale Regina Elena 14, Cagliari

MONDAY Sept. 18

h. 6:00 p.m.

Urban trekking in Cagliari: discover the beautiful and sneaking corners of the town.

Guided tour

TUESDAY Sept. 19

h. 7:30 p.m.

**Dinner & live music at
CAPOLINEA BEACH POETTO**

Lungomare Poetto – Cagliari

WEDNESDAY Sept. 20

h. 2:15 p.m.

All to the beach!! Enjoy the magnificence of sand and sea of the Sardinia beaches.

Travel by bus

THURSDAY Sept. 21

h. 8:00 p.m.

Social dinner at AQUILA CLUB

Calata dei Trinitari – Cagliari



PROGRAM

Sunday, September 17

17:30	Registration	
18:15	Opening session	
18:45	Mass spectrometry. Where is it from? Where it is and where is it going?	J. Langley
20:00	<i>End of session</i>	
20:30	<i>Welcome cocktail</i>	

Monday, September 18

Ionization techniques: volatile molecules

8:30	Mass spectrometry: an introduction	J. Langley
9:30	Ionization of volatile molecules: electron ionization (EI), chemical ionization (CI). Fragmentation processes, energetics (Part 1)	G. Giorgi
10:15	<i>Coffee break & poster session</i>	
11:00	Ionization of volatile molecules: electron ionization (EI), chemical ionization (CI). Fragmentation processes, energetics (Part 2)	G. Giorgi
12:00	Study of complex mixtures of volatile molecules: GC, fast GC, GC×GC	C. Cordero
13:15	<i>Buffet lunch</i>	

Ionization techniques: polar molecules

14:30	Soft ionization techniques: ESI, DESI, APCI. Ambient mass spectrometry. Mechanisms of ion production	C. Afonso
16:00	<i>Coffee break & poster session</i>	
16:30	Study of complex mixtures of polar molecules: HPLC, UHPLC, LC x LC	J. Langley
18:00	<i>End of session</i>	
18:00	<i>Urban trekking</i> in Cagliari: discover the beautiful and sneaking corners of the town Guided tour	

Tuesday, September 19

MALDI. Analyzers (I)

8:30	Matrix-assisted laser desorption ionization, MALDI-2. Mechanisms of ion production	R.M.A. Heeren
9:30	Analyzers (I). Ion separation in space: beam instruments: sectors, quadrupole, time-of-flight	M. Marchetti-Deschmann
10:30	<i>Coffee break & poster session</i>	

Analyzers (II). High resolution, accurate mass measurements

11:00	Analyzers (II). Ion separation in time: ion traps, FT-ICR, Orbitrap	C. Afonso
12:00	High resolution mass spectrometry, accurate mass measurements. Examples and applications	G. Bianco
13:00	<i>Buffet lunch</i>	

Tandem mass spectrometry

14:30	Tandem Mass Spectrometry (MS/MS) and MS ⁿ : ion activation	P. Gerbaux
16:30	<i>Coffee break & poster session</i>	
17:15	Tandem Mass Spectrometry (MS/MS) and MS ⁿ : ion dissociation	P. Gerbaux
18:30	<i>End of session</i>	
19:30	<i>Poetto beach: dinner and live music!</i>	

Wednesday, September 20***Fragmentation/decomposition reactions. Artificial intelligence in MS. Proteomics***

8:30	Examples of fragmentation/decomposition reactions	D. Cobice
10:00	<i>Coffee break & poster session</i>	
10:30	Artificial intelligence in MS	C. Cordero
11:45	Bottom-up, top-down, and complex-down proteomics	V. Wysocki
13:00	<i>Buffet lunch</i>	
14:15	<i>All to the beach!</i> Travel by bus Enjoy the magnificence of sand and sea of the Sardinia beaches	
19:00	<i>Go back to Cagliari</i>	



Thursday, September 21

MS Imaging, ion mobility

8:30	Imaging mass spectrometry	R.M.A. Heeren
9:45	Ion mobility	V. Gabelica
11:00	<i>Coffee break & poster session</i>	

Do it by yourself !

11:30	Exercises on MS, HRMS and MS/MS interpretation, mechanisms,	D. Cobice, V. Gabelica, G. Giorgi
Award for the best MS solver!		
13:00	<i>Buffet lunch</i>	

Short orals. Workshop. Problem solving. MS in lipidomics & metabolomics

14:20 Short orals by students:

OR1	P1	Decoding the key aroma compounds of cocoa using mass spectrometry <i>Amandine André, Elodie Gillich, Lisa Ullrich, Irene Chetschik</i> ZHAW Zürich University of Applied Sciences, School of Life Sciences and Facility Management, ILGI Institute of Food and Beverage Innovation, Research Group Food Chemistry, Wädenswil, Switzerland
OR2	P10	MALDI 1 & 2 MS imaging of lipid double-bond positional isomers using off-line ozonolysis <i>D. Bezdeková,¹ J. Preisler,¹ M. Hendrych,² K. Dreisewerd,³ A. Bednařík¹</i> ¹ Chemistry Department, Faculty of Natural Sciences, Masaryk University, Czech Republic ² First Pathological Department, St. Anne's University Hospital Brno, Czech Republic ³ Institute of Hygiene and Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Germany
OR3	P13	The quest for the unambiguous identification of β-naphthol and triarylcarbonium colorants by MeV-SIMS - Procedures for mass calibration & data evaluation <i>Teodora Raicu,¹ Matea Krmpotić,² Zdravko Siketić,² Iva Bogdanović-Radović,² Dubravka Jembrih-Simbürger¹</i> ¹ Institute for Natural Sciences and Technology in the Arts (INTK), Academy of Fine Arts Vienna, Vienna, Austria ² Ruđer Bošković Institute, Zagreb, Croatia
OR4	P15	Structural characterization of mobility-selected ions: combining TIMS with IR ion spectroscopy on an FT-ICR MS platform <i>Lara van Tetering, Kas Houthuijs, Jelle Schuurman, Jonathan Martens, Giel Berden, Jos Oomens</i> FELIX Laboratory, Institute for Molecules and Materials, Radboud University, Nijmegen, Netherlands

OR5 P26 Leveraging LC-TIMS-QTOFMS for addressing analytical challenges in chemical exposome studies

Konstantina S. Diamanti,¹ Dimitrios E. Damalas,¹ Georgios O. Gkotsis,¹ Eleni I. Panagopoulou,¹ Maria-Christina Nika,¹ Carsten Baessmann,² Bob Galvin,² Nikolaos S. Thomaidis¹

¹ Laboratory of Analytical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, Athens, Greece

² Bruker Daltonics GmbH & Co. KG, Bremen, Germany

OR6 P28 Saliva peptidome profiling in glioblastoma multiforme brain tumour by HPLC-MS top-down platform

Alexandra Muntiu,¹ Diana Valeria Rossetti,² Federica Vincenzoni,^{1,3} Irene Messana,² Massimo Castagnola,⁴ Giuseppe La Rocca,^{3,5} Alessandro Olivi,^{3,5} Andrea Urbani,^{1,3} Giovanni Sabatino,^{3,5} Claudia Desiderio²

¹ Dipartimento di Scienze Biotechnologiche di Base, Cliniche Intensivologiche e Perioperatorie, Università Cattolica del Sacro Cuore, Rome, Italy

² Istituto di Scienze e Tecnologie Chimiche "Giulio Natta", Consiglio Nazionale delle Ricerche, Rome, Italy

³ Fondazione Policlinico Universitario A. Gemelli IRCCS, Università Cattolica del Sacro Cuore, Rome, Italy

⁴ Centro Europeo di Ricerca sul Cervello-IRCCS Fondaz. Santa Lucia, Rome, Italy

⁵ Institute of Neurosurgery, Fondazione Policlinico Universitario A. Gemelli IRCCS, Catholic University, Rome, Italy

OR7 P32 Metabolomics applied to discover prognostic markers in human heart transplantation

E.C. Montatixe Fonseca,¹ M.C. Mimmi,³ A. Corazza,⁴ M. Belliato,² C. Pellegrini,¹ S. Pelenghi¹

¹ Cardiac Surgery Unit 1, IRCCS San Matteo Hospital Foundation, Pavia, Italy

² Anesthesiology and Intensive Care Unit 2, IRCCS San Matteo Hospital Foundation, Pavia, Italy

³ Department of Molecular Medicine, University of Pavia, Italy

⁴ Department of Medical Area, University of Udine, Italy

OR8 P45 A mass spectrometry-based multi-omics approach to explore the mechanisms of drug resistance in methicillin-resistant *Staphylococcus aureus*

Pedro C. Rosado,¹ M. Matilde Marques,^{1,2} Gonçalo C. Justino¹

¹ Centro de Química Estrutural - Institute of Molecular Sciences, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal

² Departamento de Engenharia Química, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal

OR9 P51 MS fingerprinting of cyclic modified peptides and proteins with chloromethyl acryl reagents

Maria J. S. A. Silva,^{1,3} Lujuan Xu,^{1,2} Pedro M. P. Gois,³ Seah Ling Kuan,^{1,2} Tanja Weil^{1,2}

¹ Max-Planck Institute for Polymer Research, Mainz, Germany

² Institute of Inorganic Chemistry I, Ulm University, Ulm, Germany

³ Research Institute for Medicines (iMed.Ulisboa), Faculty of Pharmacy, Universidade de Lisboa, Lisbon, Portugal

OR10 P53 A spatial multi-omics investigation into spinal cord remodeling in mouse mutant strains with altered myelin basic protein abundance

Rachel Pryce,¹ Hooman Bagheri,² Alan C. Peterson,² Pierre Chaurand¹

¹ Department of Chemistry, Université de Montréal, Montreal, Quebec, Canada

² Department of Neurology and Neurosurgery, McGill University, Montreal, Quebec, Canada

16:00	Workshop with Companies	
16:40	Problem solving	
17:30	<i>Coffee break & poster session</i>	
18:00	MS in lipidomics & metabolomics	P. Caboni
19:30	Awards for the best orals!	
19:40	<i>End of session</i>	
20:30	<i>Social dinner</i>	



Friday, September 22***Quantitation; biomedical applications; data analysis; MS in food***

8:30	Quantitation by MS and MSn	M. Marchetti-Deschmann
9:30	Biomedical applications of MS: newborn screening	G. la Marca
10:30	Data analysis	G. Paglia
11:30	<i>Coffee break & poster session</i>	
12:00	Food authentication and traceability	M. Suman
13:00	<i>Award for the best poster!</i>	
13:10	ECTS test	
13:30	<i>Arrivederci!</i>	



LESSONS DOWNLOAD

**J. Langley****J. Langley_1****G. Giorgi****C. Cordero****C. Afonso****J. Langley_2****R.M.A. Heeren****M. Marchetti****C. Afonso****G. Bianco****P. Gerbaux****D. Cobice****C. Cordero****V. Wysocki****R.M.A. Heeren****V. Gabelica****Exercises****P. Caboni****M. Marchetti****G. La Marca****G. Paglia****M. Suman**

POSTER SESSIONS

Poster P1-P28 **set up:** MONDAY 8:00-8:30 a.m. **Removal:** TUESDAY 6:30 p.m.

Poster P29-P55 **set up:** WEDNESDAY 8:00-8:30 a.m. **Removal:** FRIDAY 1:00 p.m.

POSTER COMMUNICATIONS

P1 Decoding the key aroma compounds of cocoa using mass spectrometry

Amandine André, Elodie Gillich, Lisa Ullrich, Irene Chetschik

ZHAW Zürich University of Applied Sciences, School of Life Sciences and Facility Management, ILGI Institute of Food and Beverage Innovation, Research Group Food Chemistry, 8820 Wädenswil, Switzerland

P2 Antioxidant compounds produced by Maillard reaction between glucose and glycine: HRMS identification

Sara Bolchini,¹ Ksenia Morozova,¹ Lucrezia Angeli,¹ Tiny van Boekel,² Matteo Scampicchio¹

¹ Faculty of Agricultural, Environmental and Food Science, Free University of Bozen-Bolzano, Piazza Università 1, 39100 Bolzano, Italy

² Food Quality & Design, Wageningen University & Research, P.O. Box 17, 6700 AA Wageningen, The Netherlands

P3 Method development for the determination of aflatoxin M1, aflatoxicol and sterigmatocystin in sheep, goat and buffalo cheeses in LC-MS/MS

Stefano Sdogati,¹ Ivan Pecorelli,¹ Roberto Condoleo,² Guglielmo Militello,² Ilaria Di Marco Pisciotano,³ Sara Lambiase,³ Carmela Rossini,³ Stefania Massafra,⁴ Elena Torres,⁴ Maurizio Cossu,⁵ Giovanni Lo Cascio,⁶ Antonio Macaluso,⁶ Licia Pantano,⁶ Bruno Neri,² Pasquale Gallo,³ Marilena Gili,⁴ Andrea Sanna,⁵ Antonio Vella,⁶ Carlo Boselli²

¹ Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche, Via G. Salvemini, 1 - 06126 Perugia

² Istituto Zooprofilattico Sperimentale del Lazio e della Toscana, Via Appia Nuova, 1411 - 00178 Roma

³ Istituto Zooprofilattico Sperimentale del Mezzogiorno, Via Salute, 2 - 80055 Portici (Napoli)

⁴ Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle d'Aosta, Via Bologna, 148 - 10154 Torino

⁵ Istituto Zooprofilattico Sperimentale della Sardegna, Via Duca degli Abruzzi, 8 - 07100 Sassari

⁶ Istituto Zooprofilattico Sperimentale della Sicilia, Via Gino Marinuzzi, 3 - 90129 Palermo

P4 Characterization of the volatile compounds in two monovarietal wines from different worldwide origins using HS-SPME- GCxGC-ToF/MS

Aakriti Darna,^{1,2} Simone Poggessi,^{1,2} Edoardo Longo,^{1,2} Emanuele Boselli^{1,2}

¹ Oenolab, NOI Techpark Alto Adige/Südtirol, Via A. Volta 13B, 39100 Bolzano, Italy

² Free University of Bozen-Bolzano, Faculty of Agricultural, Environmental, and Food Sciences, Piazza Università 1, 39100 Bolzano, Italy

P5 Structural elucidation of agrochemical derivatives using infrared ion spectroscopy

T. van Wieringen,¹ M. J.A. Vink,¹ G. Berden,¹ J. Oomens,¹ S.J. Perry,² A. Chantzis,² J. Martens¹

¹ FELIX Laboratory, Radboud University, The Netherlands

² Syngenta AG, Bracknell, United Kingdom

- P6 Inductively Coupled Plasma Mass Spectrometry in food analysis. Trace and toxic elements for food authentication and valorisation**
A. Mara, I. Langasco, M.I. Pilo, N. Spano, G. Sanna
Department of Chemical, Physical, Mathematical and Natural Sciences, University of Sassari, Italy
- P7 Use of mass spectrometry to characterise the unique polyphenolic profile of PIWI wines**
Gavin Duley,^{1,2} Adriana Teresa Ceci,^{1,2} Edoardo Longo,^{1,2} Emanuele Boselli^{1,2}
¹ Oenolab, NOI TechPark Alto Adige/Südtirol, Via A. Volta 13B, 39100 Bolzano, Italy
² Faculty of Agricultural, Environmental and Food Sciences, Free University of Bozen-Bolzano, Piazza Università 5, 39100 Bolzano, Italy
- P8 Determination of tropane alkaloids in food matrices using LC-UHPLC-MS/MS**
Larissa Caminhas, Susanne Rath
University of Campinas (UNICAMP) - Brazil
- P9 Gas chromatography-mass spectrometry method for the quantitative determination of ethylene and diethylene glycols contamination in cough syrups**
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- P10 MALDI 1 & 2 MS imaging of lipid double-bond positional isomers using off-line ozonolysis**
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- P11 Investigating the potential of novel polymer-based MALDI matrices for the detection of compounds of low molecular weight by leveraging MALDI-HRMS analytical workflows**
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- P12 Effective temperature of porous silicon substrates in LDI-MS in function of etching parameters**
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- P13 The quest for the unambiguous identification of β -naphthol and triarylcarbonium colorants by MeV-SIMS - Procedures for mass calibration & data evaluation**
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- P14 Preferred protonation site of aromatic amines: elucidation via IR ion spectroscopy**
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- P15 Structural characterization of mobility-selected ions: combining TIMS with IR ion spectroscopy on an FT-ICR MS platform**
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- P16 Mass spectrometry and photochemical study of photoisomerization and thermal back-isomerization of heteroaryl azobenzenes anchored on peptoids for the chemical storage of solar energy**
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- P17 21-T FT-ICR MS: chemical and structural characterization of complex peat-burning particulate matter**
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- P18 Contaminants of emerging concern in drinking water: integrated chemical and bioanalytical tools**
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- P19 Detection of pesticides using Multi-Scheme Chemical Ionization (MION) Inlet and Orbitrap mass spectrometer with a filter desorbing unit**
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- P20 Structural characterisation of glyphosate and AMPA metal complexes using ion mobility-mass spectrometry**
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P21 Unveiling the chemical universe of PFAS in biota using a combined targeted and untargeted workflow, utilizing LC – VIP HESI(-) – tims – QToF MS

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P22 Analysis of transformation products of an emerging contaminant by HPLC-MSⁿ

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P23 The assessment of sample preparation conditions for the analysis of per and polyfluorinated alkyl substances (PFASs)

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P24 Evaluation for the performance of Energized Dispersive Guided Extraction system for high-throughput lipidomics studies in marine environmental matrices

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P25 Lipidomic profiling intertidal mudflat microphytobenthic biofilms

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P26 Leveraging LC-TIMS-QTOFMS for addressing analytical challenges in chemical exposome studies

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P27 A bottom-up approach to characterize the proteome of natural rubbers employed in tyres production

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P28 Saliva peptidome profiling in glioblastoma multiforme brain tumour by HPLC-MS top-down platform

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P29 Porphyrin derivatives as quadruplexes ligands: spectrometry and spectroscopy studies

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P30 Optimization of an LC-MS/MS method for the targeted analysis of brain microdialysis samples using derivatization with dimethylaminophenacyl bromide

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P31 May post-translational succination be involved in cardiac arrhythmia? A joint study between (ion mobility) mass spectrometry and molecular dynamics

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P32 Metabolomics applied to discover prognostic markers in human heart transplantation

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P33 Sterolomic profiling of human CSF and plasma to reveal altered cholesterol metabolism in Parkinson's diseases

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P34 Metabolomic profiling in differential diagnosis for Parkinson's disease and atypical parkinsonisms

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- P35 Gas chromatography-mass spectrometry reveals the metabolic signature of different phenotypes of cystic fibrosis**
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- P36 Novel approach to investigate highly complex pharmaceuticals utilizing ultrahigh-resolution mass spectrometry**
Ole Tiemann,^{1,2} Lukas Schwalb,^{1,3} Christopher P. Rüger,^{1,2,4} Martha L. Chacón-Patiño,^{4,5} Thomas Gröger,³ Ralf Zimmermann^{1,2,3}
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- P37 The role of the mass spectrometry in the discovery of new potential anticancer drugs**
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- P38 Mass-directed preparative purification of Semaglutide batches**
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- P39 Investigation of the potential biotransformation of different pharmaceuticals in zebrafish embryos (*Danio rerio*), utilizing LC-QTOFMS and LC-TIMS-QTOFMS**
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- P40 Antiretroviral molecules: investigating the break-down pathways**
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- P41 Metabolism of nine synthetic opioid in zebrafish larvae using liquid chromatography mass spectrometry**
Sara Pesavento, Matilde Murari, Franco Tagliaro, Federica Bortolotti, Rossella Gottardo
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- P42 Nitrating activity of the hemin-A β ₁₆ complex: modifications on the peptide itself**
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- P43 Chemical analysis and investigation of pharmacological activities of a birch bark extract from *Betula papyrifera***
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- P44 Proximity-dependent Biotin Identification (BioID): a tool for screening protein- protein interactions in living cells**
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- P45 A mass spectrometry-based multi-omics approach to explore the mechanisms of drug resistance in methicillin-resistant *Staphylococcus aureus***
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- P46 Evaluation of the best HDX-MS workflow for the analysis of Meningococcal PorB in native state**
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- P47 Mass spectrometry's role in the study of correlation between oxidative stress, OSAS and obesity**
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- P48 Laser settings' optimization for single cell MALDI-TOF MS imaging of human CD19+ lymphocytes**
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- P49 BeatBox and iST for streamlined FFPE tissue processing: A xylene-free, robust, and high-throughput sample preparation for proteomic analysis**
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- P50 Improved detection of tryptic peptides from tissue sections using Desorption electrospray ionisation mass spectrometry imaging (DESI-MSI)**
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- P51 MS fingerprinting of cyclic modified peptides and proteins with chloromethyl acryl reagents**
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P52 Derivatization-targeted analysis of amino compounds: from neutral loss scan to dynamic multiple reaction monitoring mode

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P53 A spatial multi-omics investigation into spinal cord remodeling in mouse mutant strains with altered myelin basic protein abundance

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P54 Finding the molecules transported by SLCs: machine learning supported targeted metabolomics

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P55 Exploring the cellular actions of chelerythrine employing an untargeted mass spectrometry proteomics approach

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P56 Determination of peptide peak purity by molecular feature extraction using accurate mass LC-MS

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