



INTERNATIONAL SCHOOL on MASS SPECTROMETRY

2nd Course

Ion mobility mass spectrometry

*Fundamentals, Advances, and
Applications*

EMFCSC, Erice (Italy)

September 9-14, 2024

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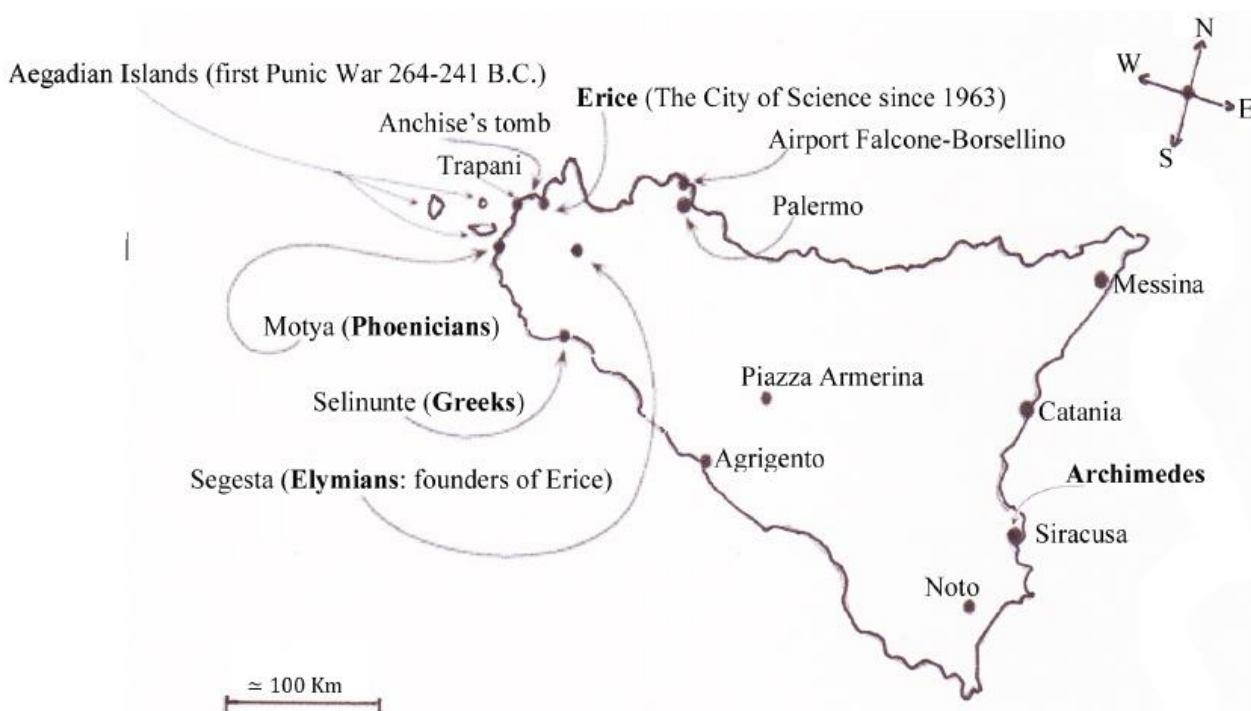
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*TO PAY A PERMANENT TRIBUTE TO ARCHIMEDES AND GALILEO GALILEI, FOUNDERS OF MODERN SCIENCE
AND TO ENRICO FERMI, THE "ITALIAN NAVIGATOR", FATHER OF THE WEAK FORCES*

«ETTORE MAJORANA» FOUNDATION AND CENTRE FOR SCIENTIFIC CULTURE

A. ZICHICHI – PRESIDENT



INTERNATIONAL SCHOOL on MASS SPECTROMETRY

1st Course

25 – 30 September 2022

2nd Course

9 – 14 September 2024

3rd Course

9 – 14 September 2026

4th Course

9 – 14 September 2028

DIRECTORS

School director

Prof. Gianluca Giorgi

University of Siena
Dept. of Biotechnology, Chemistry and Pharmacy
via Aldo Moro
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2nd Course director

Prof. David E. Clemmer

Indiana University
Bloomington (USA)
e-mail: clemmer@indiana.edu

TUTORS

Ane Arrizabalaga-Larrañaga – Wageningen Univ. and Research (The Netherlands)

Erin Baker – University of North Carolina (USA)

Perdita Barran – University of Manchester (UK)

Christopher D. Chouinard – Clemson University (USA)

David E. Clemmer – Indiana University (USA)

Hannah Florance – Agilent (UK)

Valérie Gabelica – University of Geneva (Switzerland)

Gianluca Giorgi – University of Siena (Italy)

John McLean – Vanderbilt University (USA)

Brandon Ruotolo – University of Michigan (USA)

Michal Sharon – Weizmann Institute (Israel)

Alexandre Shvartsburg – Wichita State University (USA)

Jakub Ujma – Waters, Wilmslow (UK)

Stephen Valentine – University of West Virginia (USA)

Alina Zamfir – University of Arad (Romania)



BEST ORAL AWARD



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

The award consists of a certificate and a € 100 gift card.

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 € 100 gift card.

BEST SOLVER AWARDS



Two awards to be assigned to the the best solvers of exercises at the school.

Each award consists of a certificate and a sum of € 500.

SPONSORS



MEDIA PARTNERS



PATRONAGES



TOPICS

- ✓ Ion Mobility Mass Spectrometry: fundamentals & instrumentation
- ✓ Collision cross section (CCS)
- ✓ CCS calculations for structural analysis
- ✓ Higher-order structural analysis: IMS-SID-MS, IMS-IMS-MS, IMS-CIU-MS, and FT-IMS-MS
- ✓ Mixtures and discovery: proteomics, glycomics, lipidomics, & metabolomics
- ✓ Data Analysis
- ✓ Computational Strategies: Molecular modeling, machine learning and artificial intelligence
- ✓ Structure and stability in solution: using gas-phase ions to characterize solution structures
- ✓ Commercial instrumentation
- ✓ Applications in different fields: food, drug, etc.
- ✓ Innovation in instrumentation and methodologies

SCHOOL PROGRAM

Monday, September 9th

12:00 ÷ 5:00 p.m.	Shuttle transfer from the airports in Trapani and Palermo
6:00 p.m.	Registration
6:30 p.m.	Welcome address. Presentation of the school
7:00 p.m.	Opening lecture: Mass spectrometry: state of the art and beyond Gianluca Giorgi (University of Siena, Italy), David E. Clemmer (Indiana University, USA)
8:00 p.m.	Welcome party



Tuesday, September 10th

Introduction to ion mobility: fundamentals, experimental cross sections, molecular simulations, and cross section calculations for structural analysis

Perdita Barran (Univ. of Manchester, UK), **Valérie Gabelica** (Univ. of Geneva, Switzerland)

8:30 a.m. Ion mobility mass spectrometry: background, introduction, and fundamentals of the measurements (types of mobility analyzers, timescales, resolving power)

10:15 a.m. Coffee break & poster session

11:00 a.m. Obtaining CCS values from ion mobility measurements, the role of gas, temperature, instrument and molecular ion. Introduction to computational approaches to generate CCS values from input structures, and how we (carefully) compare values from experiment and theory

12:45 p.m. End of session

1:00 p.m. Lunch

Instrumentation: Drift tube-, T-wave-, trapping-, and Field Asymmetric Waveform IMS (FAIMS)

Jakub Ujma (Waters, Wilmslow, UK), **Alexandre Shvartsburg** (Wichita State Univ., USA)

3:00 p.m. Drift-tube and traveling-wave based IMS-MS instrumentation and methods

4:30 p.m. Coffee break & poster session

5:30 p.m. Trapping IMS & FAIMS

7:00 p.m. End of session

8:00 p.m. Dinner

Wednesday, September 11th

**Mixtures and discovery:
Proteomics, glycomics, metabolomics, lipidomics, & exposomics**

Erin Baker (Univ. N. Carolina, USA), **Alina D. Zamfir** (Univ. of Arad, Romania)

8:30 a.m. Multidimensional IMS-MS Separations for complex mixture analysis:
advantages and challenges

9:00 a.m. Proteomic and glycomic analyses

10:15 a.m. Coffee break & poster session

11:00 a.m. Metabolomic, lipidomic & exposomic analyses

12:00 p.m. Database building, searching, and exercises

12:45 p.m. End of session

1:00 p.m. Lunch

**Computational and experimental strategies for large datasets: fundamental
considerations and advanced techniques**

John McLean (Vanderbilt Univ., USA), **Stephen Valentine** (Univ. of West Virginia, USA)

3:00 p.m. Fundamental considerations for CCS prediction, contemporary computational
tools, and addition of orthogonal measurements

4:45 p.m. Coffee break & poster session

5:30 p.m. Applications incorporating additional data dimensions: reaction chemistries,
spatial measurements, large-scale data interrogation

7:15 p.m. End of session

7:30 p.m. Dinner

9:30 p.m. Problem solving/Troubleshooting. Questions ... and drinks

Thursday, September 12th

**Higher-order structural analysis: IMS-SID-MS, IMS-IMS-MS, IMS-CIU-MS,
and FT-IMS-MS**

Brandon Ruotolo (Univ. of Michigan, USA)

8:30 a.m. Fundamental principles and equipment: ion activation combined with ion mobility methods

10:15 a.m. Coffee break & poster session

11:00 a.m. Case studies: ion activation techniques combined with ion mobility in action

12:45 p.m. End of session

1:00 p.m. Lunch

Excursion and gala dinner. Have fun!!

2:30 p.m. Excursion to Marsala and Selinunte: guided tour

8:30 p.m. Gala dinner

11:00 p.m. Go back to Erice



Friday, September 13th
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**Structure and stability in solution:
using gas-phase ions to characterize solution structures**

Michal Sharon (Weizmann Inst., Israel), **David E. Clemmer** (Indiana Univ., USA)

8:30 a.m. Using gas-phase ions to follow complex structural transitions in solution

10:15 a.m. Coffee break & poster session

11:00 a.m. Characterizing the physical properties of molecules in solution by IMS-MS: understanding reactivity and stability

12:45 p.m. End of session

1:00 p.m. Lunch

Short orals, applications, exercises

3:00 p.m. Short orals by students

OR1 P1 **Improving selectivity to quantify biotherapeutics in complex matrices. Differential mobility separation to avoid immunocapture interferences**

Francesco Molinaro, Ilse De Salve

Merck KgaA, RBM S.p.a. Colletterto Giacosa (TO), Italy

OR2 P3 **Effects of polyethylene nanoparticles (PE-NPs) on lettuce leaves: insights from Ion Mobility Mass Spectrometry-based lipidomics approach**

Pier Paolo Becchi, Leilei Zhang, Luigi Lucini

Department for Sustainable Food Process, Università Cattolica del Sacro Cuore, Via Emilia Parmense 84, 29122 Piacenza, Italy

OR3 P8 **Capturing the oligomerization dynamics of ALS-related Cu/Zn superoxide dismutase with temperature-controlled nESI and cyclic IMS**

Despoina Svingou, Julian Alexander Harrison, Renato Zenobi

Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 3, 8093 Zurich, Switzerland

OR4 P12 **Using mass spectrometry methods to aid the development of novel photo-enzymes: ion mobility and collision-induced unfolding for the characterisation of *de novo* designed α -helical barrels**

Ana Bath Alén,¹ Liuwei Meng,¹ Harry Spacey,² Junfeng Ma,² Katarzyna Ozga,³ Jason Kalapothakis,¹ Dek Wolfson,³ Nigel Scrutton,² Perdita Barran¹

¹ Michael Barber Centre for Collaborative Mass Spectrometry, Manchester Institute of Biotechnology, University of Manchester, 131 Princess Street, Manchester, M1 7DN, United Kingdom

² Future Biomanufacturing Research Hub, Manchester Institute of Biotechnology, University of Manchester, 131 Princess Street, Manchester, M1 7DN, United Kingdom

³ School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, United Kingdom

OR5 P14 Utilizing trapped ion mobility separation for enhanced lipid coverage in RP-UHPLC/MS analysis of biological samples

Veronika Šubrtová, Robert Jirásko, Michal Holčapek

University of Pardubice, Faculty of Chemical Technology, Department of Analytical Chemistry, Studentská 573, 532 10 Pardubice, Czech Republic

OR6 P20 Frauds in truffle species: detection of marker compounds using SPME-GC-MS and LC-ESI-IM-QTOF-MS

Pedro Gabriel Martínez Aznar,¹ Pedro Marco,¹ Markus Fischer,² Marina Creydt,² Eva Tejedor-Calvo^{1,3}

¹ Department of Plant Science, Agrifood Research and Technology Centre of Aragón (CITA), Zaragoza, Spain

² Hamburg School of Food Science - Institute of Food Chemistry, University of Hamburg, Germany

³ Department of Analytical Chemistry, Laboratory for Flavor Analysis and Enology (LAAE), Faculty of Sciences, Universidad Zaragoza, Zaragoza E-50009, Spain

OR7 P21 Digestibility and immunogenic peptide profile of pastas produced from evolutionary populations of wheat vs. traditional wheat varieties

Alejandra Muñoz-González,¹ Laura Gazza,² Silvia Folloni,³ Salvatore Ceccarelli,⁴ Gianni Galaverna,¹ Barbara Prandi,¹ Tullia Tedeschi¹

¹ Department of Food and Drug, University of Parma, Parco Area delle Scienze, 27/A, 43124 Parma, Italy

² Council for Agricultural Research and Economics, Research Centre for Engineering and Agro-Food Processing, Rome, Italy

³ Openfields, 43052 Parma, Italy

⁴ Consultant to the University of Parma, 43124 Parma, Italy

OR8 P23 An overview of internal energy in mass spectrometry sources, a key factor impacting ion mobility measurement results

Emilie Bertrand, Valérie Gabelica

School of Pharmaceutical Sciences, University of Geneva, Switzerland

OR9 P28 Characterization of the oligomeric structure of bird hemoglobin by mass spectrometry under native conditions

Turkan Nabyeva,¹ Léa Letissier,¹ Maily Kervella,² Stéphane Hourdez,³ Christine Schaeffer,¹ François Criscuolo,² Fabrice Bertile,¹ Sarah Cianferani,¹ Oscar Hernandez-Alba¹

¹ BioOrganic Mass Spectrometry Laboratory (LSMBO), University of Strasbourg, IPHC UMR 7178, CNRS, France

² Ecology, Physiology and Ethology Department (DEPE), University of Strasbourg, IPHC UMR 7178, CNRS, France

³ Benthic Ecogeochemistry Laboratory (LECOB), University of Sorbonne, UMR 8222, CNRS, France

OR10 P31 Novel strategies for the characterization of the early-stages of aggregate formation of α -synuclein using ion mobility mass spectrometry

Andrea Istrati,^{1,2} Raya Sadighi,^{1,2} Melissa Bärenfänger,^{1,2} Anouk M. Rijs^{1,2}

¹ Division of Bioanalytical Chemistry (MS-Laserlab), Department of Chemistry and Pharmaceutical Sciences, AIMMS Amsterdam Institute of Molecular and Life Sciences, Vrije Universiteit Amsterdam, 1081 HV Amsterdam, The Netherlands

² Centre for Analytical Sciences Amsterdam, 1098XH Amsterdam, The Netherlands

4:40 p.m.	Coffee break
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5:10 p.m.	Leveraging ion mobility in complex sample analysis: an in-depth exploration of techniques and applications Hannah Florance (Agilent, UK)
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5:30 p.m.	Exercises
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7:00 p.m.	Award for the best short oral! Award for the best poster! Award for the best IMMS solver!
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7:10 p.m.	End of session
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8:00 p.m.	Dinner
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9:15 p.m.	Students of the IntSMS 2024 leave their memorable mark!
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Saturday, September 14th
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Food and drug applications

Ane Arrizabalaga-Larrañaga (Wageningen, The Netherlands), **Christopher D. Chouinard** (Clemson University, USA)

8:30 a.m.	Ion mobility mass spectrometry for food analysis
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10:00 a.m.	Coffee break
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10:30 a.m.	Ion mobility mass spectrometry for drug analysis
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12:00 p.m.	Meeting students-tutors
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12:30 p.m.	Concluding remarks and Arrivederci!
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1:00 p.m.	Shuttle bus to the airports in Trapani and Palermo
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POSTER SESSIONS

Tuesday Sept. 10th: 10:15 a.m., 4:30 p.m.

Wednesday Sept. 11th: 10:15 a.m., 4:45 p.m.

Thursday Sept. 12th: 10:15 a.m.

Friday Sept. 13th: 10:15 a.m.

POSTER COMMUNICATIONS

- P1** **Improving selectivity to quantify biotherapeutics in complex matrices. Differential mobility separation to avoid immunocapture interferences**
Francesco Molinaro, Ilse De Salve
Merck KgaA, RBM S.p.a. Colletterto Giacosa (TO), Italy
- P2** **Increasing outer membrane complexity: the case of the lipopolysaccharide lipid A from marine *Cellulophaga pacifica***
Stefania De Chiara,¹ Emanuela Andretta,¹ Chiara Pagliuca,² Roberta Cirella,¹ Elena Scaglione,² Martina Di Rosario,² Maxim S. Kokoulin,³ Olga I. Nedashkovskaya,³ Alba Silipo,¹ Paola Salvatore,^{2,4,5} Antonio Molinaro,¹ Flaviana Di Lorenzo¹
¹ Department of Chemical Sciences, University of Naples Federico II, via Cinthia, 4, 80126 Naples, Italy
² Department of Molecular Medicine and Medical Biotechnologies, University of Naples Federico II, Via S. Pansini, 5, 80131 Naples, Italy
³ Far Eastern Branch, G.B. Elyakov Pacific Institute of Bioorganic Chemistry, Russian Academy of Sciences, 159/2, Prospect 100 Let Vladivostoku, 690022 Vladivostok, Russia
⁴ CEINGE-Biotechnologie Avanzate Franco Salvatore, Via G. Salvatore, 436, 80131 Naples, Italy
⁵ Task Force on Microbiome Studies University of Naples Federico II, 80100 Naples, Italy
- P3** **Effects of polyethylene nanoparticles (PE-NPs) on lettuce leaves: insights from Ion Mobility Mass Spectrometry-based lipidomics approach**
Pier Paolo Becchi, Leilei Zhang, Luigi Lucini
Department for Sustainable Food Process, Università Cattolica del Sacro Cuore, Via Emilia Parmense 84, 29122 Piacenza, Italy
- P4** **Residues of florfenicol and metabolite identification in tilapia (*Oreochromis niloticus*) tissues following oral administration and post-treatment period in tropical water temperatures**
Anna Paula R. Queiroga,¹ Gabriela F.P. Souza,¹ Jonas Augusto R. Paschoal,² Airton Gonçalves Salles Jr,¹ Michael Schlöter,³ Fabiana Pilarski,⁴ André Tadeu Gotardo,⁵ Silvana Lima Gorniak,⁵ Susanne Rath¹
¹ Institute of Chemistry, University of Campinas, Campinas, SP, Brazil
² Department of Biomolecular Sciences, University of São Paulo, Ribeirão Preto, SP, Brazil
³ Helmholtz Zentrum München, Comparative Microbiome Analysis Research Unit, Neuherberg, Germany
⁴ Aquaculture Center, São Paulo State University, Jaboticabal, SP, Brazil
⁵ Faculty of veterinary medicine and zootechnics, University of São Paulo, São Paulo, SP, Brazil

P5 Gas-phase IR spectroscopy of ion-mobility-separated biomolecules

Jan Horlebein,^{1,2} Jerome Riedel,^{1,2} Gergo Peter Szekeres,^{1,2} Maike Lettow,^{1,2} Eike Mucha,^{1,2} Gerard Meijer,¹ Kevin Pagel,^{1,2} Gert von Helden¹

¹ Fritz-Haber-Institute der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

² Institut für Chemie und Biochemie, Freie Universität Berlin, Altensteinstraße 23A, 14195 Berlin, Germany

P6 Evaluation and safety assessment of *N*-nitrosamine contamination in Brazilian cosmetic thermal waters: market analysis and method development

Maria Fernanda Araujo Vieira Matos, Gabriela Freitas Pereira de Souza, Susanne Rath

University of Campinas (UNICAMP), Brazil

P7 Development of innovative analytical strategies for the identification of New Psychoactive Substances

Ilenia Bracaglia,^{1,2} Martina Croce,^{1,2} Gaia Di Francesco,¹ Francesco Bartolini,¹ Gianmarco Pezzuti,¹ Sara Gamberoni,¹ Camilla Montesano,¹ Antonietta Lombardozi,³ Serena Detti,³ Sabino Napolitano,³ Manuel Sergi¹

¹ Department of Chemistry, University La Sapienza, 00185 Rome, Italy

² Department of Public Health and Infectious Disease, Sapienza University of Rome, 00185 Rome, Italy

³ Department of Public Security, Central Anticrime Directorate of Italian National Police, Forensic Science Police Service (DAC-SPS), Rome, Italy

P8 Capturing the oligomerization dynamics of ALS-related Cu/Zn superoxide dismutase with temperature-controlled nESI and cyclic IMS

Despoina Svingou, Julian Alexander Harrison, Renato Zenobi

Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 3, 8093 Zurich, Switzerland

P9 Drug-cyclodextrin inclusion complexes analysed by HR MS

Marijana Pocrnić, David Klarić, Nives Galić

Faculty of Science, University of Zagreb, Zagreb, Croatia

P10 Expanding the bioanalytical toolkit to investigate the metalation of biomolecules

Tshering Zangmo, Joanna Szpunar, Luisa Ronga

Université de Pau et des Pays de l'Adour, E2S UPPA, CNRS, Institute of Analytical and Physical Chemistry for the Environment and Materials (IPREM-UMR 5254), 64053 Pau, France

P11 Single-cell MALDI TOF MS Imaging of human granulocytes

Maja Lukić,^{1,2} Mia Suknović,² Ivana Marković,^{1,2} Željko Debeljak^{1,2}

¹ Clinical Institute of Laboratory Diagnostics, University Hospital Centre Osijek, Osijek, Croatia

² Faculty of Medicine Osijek, JJ Strossmayer University of Osijek, Osijek, Croatia

P12 Using mass spectrometry methods to aid the development of novel photoenzymes: ion mobility and collision-induced unfolding for the characterisation of *de novo* designed α -helical barrels

Ana Bath Alén,¹ Liuwei Meng,¹ Harry Spacey,² Junfeng Ma,² Katarzyna Ozga,³ Jason Kalapothakis,¹ Dek Wolfson,³ Nigel Scrutton,² Perdita Barran¹

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² Future Biomanufacturing Research Hub, Manchester Institute of Biotechnology, University of Manchester, 131 Princess Street, Manchester, M1 7DN, United Kingdom

³ School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, United Kingdom

- P13 Metabolomic profiling and comparative analysis of mouse retina and retinal organoids using GC-MS and LC-MS**
Pragati Gupta,¹ Claudia Wiesner,¹ Zohreh Hosseinzadeh²
¹ Leipzig University, Germany
² Radboud University Medical Center, Netherland
- P14 Utilizing trapped ion mobility separation for enhanced lipid coverage in RP-UHPLC/MS analysis of biological samples**
Veronika Šubrtová, Robert Jirásko, Michal Holčapek
 University of Pardubice, Faculty of Chemical Technology, Department of Analytical Chemistry, Studentská 573, 532 10 Pardubice, Czech Republic
- P15 Photoactive ion mobility-mass spectrometry reveals the conformational changes of fatty acid photodecarboxylase**
Liuwei Meng,¹ Jason Kalapothakis,¹ Ana Bath Alen,¹ Junfeng Ma,² Harry Spacey,² Nigel Scrutton,² Perdita Barran¹
¹ Michael Barber Centre for Collaborative Mass Spectrometry, Manchester Institute of Biotechnology, Department of Chemistry, The University of Manchester, 131 Princess Street, Manchester, M1 7DN, United Kingdom
² Manchester Institute of Biotechnology, Department of Chemistry and Future Biomanufacturing Research Hub (FBRH), The University of Manchester, 131 Princess Street, Manchester, M1 7DN, United Kingdom
- P16 Innovative liquid chromatographic-mass spectrometric technologies to purify and identify biologically active antibody-drug conjugates**
Margherita Marino,¹ Paolo Rovero,¹ Walter Mier,² Hendrik Rusche,³ Michael Chorev,⁴ Anna Maria Papini¹
¹ Interdepartmental Research Unit of Peptide & Protein Chemistry & Biology, Departments of Chemistry "Ugo Schiff" and NeuroFarba, University of Florence, 50019-Sesto F.no, Italy
² University Hospital of Heidelberg, 69120 Heidelberg, Germany
³ Fischer Analytics GmbH, Saarlandstrasse 377, 55411-Bingen, Germany
⁴ Mellitus, LLC. CIC Boston (USA), Professor Emeritus at the Hebrew University of Jerusalem, Israel
- P17 MICROBoost: Discovery of transglycosylating β -galactosidases for the enzymatic synthesis of prebiotic galacto-oligosaccharides (GOS)**
Lucia Cocorullo,^{1,2} Maxime Gavage,² Adrien Boes,³ Patrice Filée,³ Nathalie Gillard,² Moreno Galleni¹
¹ Center for Protein Engineering (CIP), Biological Macromolecules, InBioS, University of Liège, 4000 Liège, Belgium
² Analytical Laboratory, CER Groupe, 6900 Marloie, Belgium
³ Laboratory of Immunobiology, CER Groupe, 6900 Aye, Belgium
- P18 Untargeted metabolomic analysis of Parmigiano Reggiano PDO using a Region of Interest-Multivariate Curve Resolution approach**
Samuele Pellacani,¹ Sara Michelini,² Valentina Pizzamiglio,² Lorenzo Strani,¹ Marina Cocchi,¹ Caterina Durante¹
¹ Dept. Chemical and Geological Sciences, Università di Modena e Reggio Emilia, via Campi 103, 41125 Modena, Italy
² Consorzio del Formaggio Parmigiano Reggiano, via Kennedy 18, 42124, Reggio Emilia, Italy
- P19 Using ion mobility mass spectrometry imaging for the *in-situ* characterisation of plant hormones**
Chao Zhang,¹ Dominika Kaczorová,¹ Asta Žukauskaitė,² Tetiana Kalachova,³ Ivan Petřík,¹ Ivo Chamrád,¹ Jitka Šíroká,¹ Karel Doležal,^{1,2} Ondřej Novák¹
¹ Laboratory of Growth Regulators, Institute of Experimental Botany of the Czech Academy of Sciences & Faculty of Science, Palacký University Olomouc, Šlechtitelů 27, CZ-78371 Olomouc, Czech Republic

- ² Department of Chemical Biology, Faculty of Science, Palacký University Olomouc, Šlechtitelů 27, CZ-78371 Olomouc, Czech Republic
³ Institute of Experimental Botany of the Academy of Sciences of the Czech Republic, Rozvojová 313, 165 02 Prague 6, Czech Republic

P20 Frauds in truffle species: detection of marker compounds using SPME-GC-MS and LC-ESI-IM-QTOF-MS

Pedro Gabriel Martínez Aznar,¹ Pedro Marco,¹ Markus Fischer,² Marina Creydt,² Eva Tejedor-Calvo^{1,3}

¹ Department of Plant Science, Agrifood Research and Technology Centre of Aragón (CITA), Zaragoza, Spain

² Hamburg School of Food Science - Institute of Food Chemistry, University of Hamburg, Germany

³ Department of Analytical Chemistry, Laboratory for Flavor Analysis and Enology (LAAE), Faculty of Sciences, Universidad Zaragoza, Zaragoza E-50009, Spain

P21 Digestibility and immunogenic peptide profile of pastas produced from evolutionary populations of wheat vs. traditional wheat varieties

Alejandra Muñoz-González,¹ Laura Gazza,² Silvia Folloni,³ Salvatore Ceccarelli,⁴ Gianni Galaverna,¹ Barbara Prandi,¹ Tullia Tedeschi¹

¹ Department of Food and Drug, University of Parma, Parco Area delle Scienze, 27/A, 43124 Parma, Italy

² Council for Agricultural Research and Economics, Research Centre for Engineering and Agro-Food Processing, Rome, Italy

³ Openfields, 43052 Parma, Italy

⁴ Consultant to the University of Parma, 43124 Parma, Italy

P22 Resolving the structural complexity of antibody-epitope interaction in *Neisseria gonorrhoeae* strains: Insights into antibody recognition

Alessandro A. Masi,¹ Marta Tiemblo-Martin,¹ Antonio Molinaro,¹ Sanjay Ram,² Peter T. Beernink,³ Alba Silipo¹

¹ University of Naples Federico II, Via Cintia, Naples, Italy

² Department of Infectious Diseases and Immunology, University of Massachusetts Chan Medical School, Worcester, Massachusetts 01605, United States

³ Department of Pediatrics, University of California, San Francisco, Oakland, California 94609, United States

P23 An overview of internal energy in mass spectrometry sources, a key factor impacting ion mobility measurement results

Emilie Bertrand, Valérie Gabelica

School of Pharmaceutical Sciences, University of Geneva, Switzerland

P24 Insight on Lugana flavor with a new LC-MS method for detection of polyfunctional thiols

Giorgio Zanon,¹ Luca Giglini Tassotti,² Urska Vrhovsek,¹ Silvia Carlin¹

¹ Centre Research and Innovation, Edmund Mach Foundation, 38098 San Michele all'Adige (TN), Italy

² Center Agriculture Food Environment (C3A), University of Trento, 38098 San Michele all'Adige (TN), Italy

P25 A multi-platform non-targeted metabolomics procedure for the analysis of serum samples and its application to glaucoma disease

Jorge García,^{1,2} Jorge Rodríguez,² Héctor González-Iglesias,² Andrés Fernández-Vega Cueto,³ Pablo Rodríguez,¹ José Ignacio García Alonso¹

¹ Departamento de Química Física y Analítica, Facultad de Química, Universidad de Oviedo, Av. Julián Clavería, 8, 33006, Oviedo, Spain

² Instituto de Productos Lácteos de Asturias, Consejo Superior de Investigaciones Científicas (IPLA-CSIC), Paseo Río Linares, 33300, Villaviciosa, Spain

³ Instituto Oftalmológico Fernández-Vega, Av. Dres. Fernández-Vega, 34, 33012, Oviedo, Spain

- P26 An optimized DIA-MS workflow for HCP quantification in bioreactors to assess relationship in between processing conditions and critical quality attributes**
Janik D. Seidel,¹ Mark R. Condina,^{1,2} Manuela Klingler-Hoffmann,¹ Clifford Young,¹ Leigh Donnellan,¹ Craig Kyngdon,³ Peter Hoffmann¹
¹ Clinical and Health Sciences, University of South Australia, Adelaide, Australia
² Mass Dynamics, Melbourne, Australia
³ Bioanalytical Sciences, CSL Innovation Pty Ltd., Melbourne, Australia
- P27 Bioactive molecules identification in POCTEFA area plant extracts and thermal spring waters for skin enhancement microbiome in biosourced cosmetic**
Valentine Chevillon, Zeina Bourhane
IPREM – UMR5254, Université de Pau et des Pays de l'Adour, CNRS, France
- P28 Characterization of the oligomeric structure of bird hemoglobin by mass spectrometry under native conditions**
Turkan Nabyeva,¹ Léa Letissier,¹ Maïly Kervella,² Stéphane Hourdez,³ Christine Schaeffer,¹ François Criscuolo,² Fabrice Bertile,¹ Sarah Cianferani,¹ Oscar Hernandez-Alba¹
¹ BioOrganic Mass Spectrometry Laboratory (LSMBO), University of Strasbourg, IPHC UMR 7178, CNRS, France
² Ecology, Physiology and Ethology Department (DEPE), University of Strasbourg, IPHC UMR 7178, CNRS, France
³ Benthic Ecogeochemistry Laboratory (LECOB), University of Sorbonne, UMR 8222, CNRS, France
- P29 PTR-MS in food science and technology: established approaches and new avenues**
Iuliia Khomenko,^{1,2} Michele Pedrotti,¹ Martina Moretton,^{1,2} Maria Mazzucotelli,^{1,3} Antonia Corvino,^{1,3} Andea Dell'Olio,^{1,4,5} Camila Cossettin Teixeira,^{1,3} Franco Biasoli^{1,2}
¹ Fondazione Edmund Mach, Edmund Mach str 1, San Michele all'Adige (TN), Italy
² ONFoods-Research and innovation network on food and nutrition Sustainability, Safety and Security-Working ON Foods, Parma 43121, Italy
³ Center for Agriculture Food Environment C3A, University of Trento, San Michele All'Adige, Trento, Italy
⁴ Food Quality and Design, Wageningen University and Research, Wageningen, The Netherlands
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- P30 Probing the conformational diversity of Huntingtin with IM-MS – and how a GFP tag confuses things!**
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- P31 Novel strategies for the characterization of the early-stages of aggregate formation of α -synuclein using ion mobility mass spectrometry**
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- P32 Impurity profile characterization of recombinant peptide samples by LC-QTOF-ESI**
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P33 Use of Ion Mobility-Mass Spectrometry to aid the mechanistic understanding of [4Fe-4S] cluster assembly on the scaffold protein NUBP1

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