Società Chimica Italiana
Divisione di Spettrometria
di Massa

IMSF
international mass spectrometry foundation

IMSC FLORENCE
2018

XXII International Mass Spectrometry Conference

Florence (Italy) - August 26-31, 2018

CONFERENCE PROGRAM

XXII International Mass Spectrometry Conference

AUGUST 26-31, 2018 **FLORENCE, ITALY**

www.imsc2018.it

SATURDAY, AUGUST 25th

2:00 p.m.	SHORT COURSE 1 **Fundamentals of Mass Spectrometry** *TU: Jürgen H. Gross, David Sparkman*	SHORT COURSE 2 **Foodomics & Mass Spectrometry** *TU: Michele Suman, Laurent Debrauwer, Fulvio Mattivi, Laura Righetti*	SHORT COURSE 3 **Mass Spectrometry Imaging** *TU: Marialaura Dilillo, Manuel Galli, Liam McDonnell, Andrew Smith, Martina Marchetti-Deschmann*	SHORT COURSE 4 **Expanded Newborn Screening by Tandem Mass Spectrometry** *TU: Giancarlo la Marca, Marzia Pasquali, Hugo Rocha*	SHORT COURSE 5 **SPME: Comprehensive Overview of the Technology & Applications to Analytical MS** *TU: Janusz Pawliszyn, Barbara Bojko, Nikita Looby, Tijana Vasiljevic*
4:30 p.m.	COFFEE BREAK				
5:00 p.m.	SHORT COURSE 1	SHORT COURSE 2	SHORT COURSE 3	SHORT COURSE 4	SHORT COURSE 5
6:00 p.m.	END OF SESSION				

SUNDAY, AUGUST 26TH

REGISTRATION 11:00 A.M. - 6:00 P.M.

9:00 a.m.	SHORT COURSE 1	SHORT COURSE 2	SHORT COURSE 3	SHORT COURSE 4	SHORT COURSE 5
11:00 a.m.	COFFEE BREAK				
11:30 a.m.	SHORT COURSE 1	SHORT COURSE 2	SHORT COURSE 3	SHORT COURSE 4	SHORT COURSE 5
1:00 p.m.	END SHORT COURSES				
5:00 p.m.	OPENING CEREMONY				
6:00 p.m.	**PLENARY LECTURE** **Marco Leona - The Metropolitan Museum of Art, New York (USA)** *At the intersection between chemistry and art: scientific research for the study and preservation of cultural heritage*				
7:00 p.m.	**Welcome Exhibition & Mixer**				

MONDAY, AUGUST 27th

REGISTRATION 8:00 A.M. - 7:00 P.M.

8:30 a.m.	**PLENARY LECTURE 2** **Richard Caprioli**, Vanderbilt University (USA) *Advances in MALDI imaging mass spectrometry: molecular microscopy in the new age of biology and medicine*				
9:15 a.m.	BREAK				
9:30 a.m.	**MO1 - Nucleic Acids** *KN: Mary Rodgers*	**MO2 - Clinical Proteomics** *KN: Thomas Joos*	**MO3 - Ion Spectroscopy & Photodissociation** *KN: Mark Johnson*	**MO4 - Hyphenated Techniques** *KN: Janusz Pawliszyn*	**MO5 - Volatile Molec. & Nose-Space Analysis** *KN: Jonathan Beauchamp*
11:30 a.m.	**COFFEE BREAK / POSTER SESSIONS** MPS-S01 - MPS-S10 Odd numbers (11:30 a.m.- 1:00 p.m.)				
12:30 p.m.	**LUNCH SYMPOSIA (12:30 P.M.- 1:45 P.M.)**				
		BRUKER DALTONICS	**WATERS**	**SCIEX**	**JEOL**
1:30 p.m.	**COFFEE BREAK / POSTER SESSIONS** MPS-S01 - MPS-S10 Even numbers (1:30 p.m.- 3:00 p.m.)				
3:00 p.m.	**MO6 - Clinical Chemistry** *KN: Marzia Pasquali*	**MO7 - Quantitative Proteomics** *KN: Marcus Bantscheff*	**MO8 - Chiral Discrimination** *KN: Masaaki Fujii*	**MO9 - Ambient MS, New Ionization Methods** *KN: Renato Zenobi*	**MO10 - Polymers** *KN: Chrys Wesdemiotis*
5:00 p.m.	BREAK				
5:15 p.m.		WORKSHOP M1 **Mass Spectrometry in Virology** *OR: Günter Allmaier*	WORKSHOP M2 **Police Casework-Successes & Challenges from an Academic Perspective** *OR: Simona Francese*	WORKSHOP M3 **Environmental Mass Spectrometry: from Trace Analysis to Effect Assessment** *OR: Marc Suter*	WORKSHOP M4 **Are MS-Based Methods Fit for Purpose?** *OR: Lorens P. Sibbesen*
7:00 p.m.	END OF SESSION				

TUESDAY, AUGUST 28th

REGISTRATION 8:00 A.M. - 7:00 P.M.

8:30 a.m.	**Thomson Medal Award ceremony** **PLENARY LECTURE 3 - THOMSON MEDALIST** **Albert J. R. Heck**, Netherlands Proteomics Centre, Utrecht University (The Netherlands) *Gaining weight in mass spectrometry. From analyzing electrons to intact molecular machineries*				
9:15 a.m.	BREAK				
9:30 a.m.	**TO1 - Therapeutic drug monitoring & drug discovery** *KN: Rob Vreeken*	**TO2 - Single Cell** *KN: Zhibo Yang*	**TO3 - Noncovalent Interactions** *KN: Carol Robinson*	**TO4 - HRMS: Instrum., Methods & Applications** *KN: Alan Marshall*	**TO5 - MS Imaging: Instrumentation** *KN: Ron Heeren*
11:30 a.m.	**COFFEE BREAK / POSTER SESSIONS** TPS-S01 - TPS-S10 Odd numbers (11:30 a.m.- 1:00 p.m.)				
12:30 p.m.	**LUNCH SYMPOSIA (12:30 P.M.- 1:45 P.M.)**				
		BRUKER DALTONICS	**AGILENT TECHNOLOGIES**	**SCIEX**	**THERMO FISHER SCIENTIFIC**
1:30 p.m.	**COFFEE BREAK / POSTER SESSIONS** TPS-S01 - TPS-S10 Even numbers (1:30 p.m.- 3:00 p.m.)				
3:00 p.m.	**TO6 - Post Translational Modifications** *KN: Jesper Olsen*	**TO7 - MS Analysis Of Forensic Sci. Evidence** *KN: Gérard Hopfgartner*	**TO8 - Ion activation & dissociation** *KN: Julia Laskin*	**TO9- Metal & Non-metal Clusters: Gas Phase Structures & Reactivity** *KN: Gereon Niedner-Schatteburg*	**TO10 - Astrochemistry** *KN: Christine Joblin*
5:00 p.m.	BREAK				
5:15 p.m.		WORKSHOP T1 **Careers in Mass Spectrometry** *OR: Jackie Mosely*	WORKSHOP T2 **Transforming Drug Discovery & Clinical Biomarker Bioanalysis ...** *OR: Ragu Ramanathan*	WORKSHOP T3 **Integration of Native MS With Structural Biology Methods** *OR: Michal Sharon, Frank Sobott*	
7:00 p.m.	END OF SESSION				

WEDNESDAY, AUGUST 29th

REGISTRATION 8:00 A.M. - 7:00 P.M.

8:30 a.m.	**PLENARY LECTURE 4 - CURT BRUNNÉE AWARD** **Daniel E. Austin**, Brigham Young University (USA) *Lithographically patterned electrodes for miniaturized ion trap mass spectrometers and other ion optics devices*				
9:15 a.m.	BREAK				
9:30 a.m.	**WO1 - Native MS and structural proteomics** *KN: Michal Sharon*	**WO2 - JMS Award Symposium**	**WO3 - Reaction mechanisms and elusive intermediates** *KN: Stephen Blanksby*	**WO4 - Pharmaceuticals** *KN: Walter Korfmacher*	**WO5 - Food Integrity, Authenticity & Traceability** *KN: Saskia van Ruth*
11:30 a.m.	**COFFEE BREAK / POSTER SESSIONS** WPS-S01 - WPS-S10 Odd numbers (11:30 a.m.- 1:00 p.m.)				
12:30 p.m.	**LUNCH SYMPOSIA (12:30 P.M.- 1:45 P.M.)**				
		PERKINELMER	**AGILENT TECHNOLOGIES**	**BIOGNOSYS**	**THERMO FISHER SCIENTIFIC**
1:30 p.m.	**COFFEE BREAK / POSTER SESSIONS** WPS-S01 - WPS-S10 Even numbers (1:30 p.m.- 3:00 p.m.)				
3:00 p.m.	**WO6 - MS Tools In Doping & Toxicology** *KN: Tiia Kuuranne*	**WO7- MS Imaging: Applications** *KN: Liam McDonnell*	**WO8 - Gas Phase Ion Chem. & Thermochem.** *KN: Scott McLuckey*	**WO9 - FTMS and innovative methods for (bio) analyses** *KN: Joseph Loo*	**WO10 - Food Additives & Contaminants** *KN: Michel W.F. Nielen*
5:00 p.m.	BREAK				
5:15 p.m.		WORKSHOP W1 **MS-Based Techniques for the Characterization of Nano- materials in Food, ...** *OR: Francesco Cubadda, Stefan Weigel*	WORKSHOP W2 **Mass Spectrometry in Microbiology** *OR: Vladimír Havlíček*	WORKSHOP W3 **Advances in Protein Structure Analysis with Mass Spectrometry** *OR: Kevin Downard*	WORKSHOP W4 **The EU_FT-ICR_MS Network** *OR: Carlos Cordeiro, Christian Rolando*
7:00 p.m.	END OF SESSION				

THURSDAY, AUGUST 30th

REGISTRATION 8:00 A.M. - 5:00 P.M.

8:30 a.m.	**PLENARY LECTURE 5 - THOMSON MEDALIST** **John R. Yates**, The Scripps Research Institute, La Jolla (USA) *Driving Innovation - From a Protein Sequence to a Proteome*				
9:15 a.m.	BREAK				
9:30 a.m.	**ThO1 - Glycomics, Saccharides & Glycoconjugates** *KN: Isabelle Compagnon*	**ThO2 - Probing Protein Structure & Dynamics** *KN: Thomas J. D. Jørgensen*	**ThO3 - Natural Substances & Their Complexes** *KN: Pierre-Marie Allard*	**ThO4 - Environmental MS** *KN: Susan Richardson*	**ThO5 - Safe & Valuable Food** *KN: Laurent Debrauwer*
11:30 a.m.	**COFFEE BREAK / POSTER SESSIONS** ThPS-S01 - ThPS-S13 Odd numbers (11:30 a.m.- 1:00 p.m.)				
12:30 p.m.	**LUNCH SYMPOSIA (12:30 P.M.- 1:45 P.M.)**				
		WATERS	**AGILENT TECHNOLOGIES**	**SHIMADZU**	**THERMO FISHER SCIENTIFIC**
1:30 p.m.	**COFFEE BREAK / POSTER SESSIONS** ThPS-S01 - ThPS-S13 Even numbers (1:30 p.m.- 3:00 p.m.)				
3:00 p.m.	**ThO6 - Lipidomics** *KN: Michael Wakelam*	**ThO7 - Developments & Applications In Ion Mobility MS** *KN: David Clemmer*	**ThO8 - Petroleomics, Hydrocarbons & Biofuels** *KN: Ryan Rodgers*	**ThO9 - Materials & Nano Materials** *KN: Norbert Jakubowski*	**ThO10 - Novel Food; Nanoparticles In Food & Beverage; Future Applications** *KN: Ruud Peters*
5:00 p.m.	END OF SESSION				
8:00 p.m.	**CONFERENCE DINNER**				

FRIDAY, AUGUST 31st

REGISTRATION 8:00 A.M. - 1:00 P.M.

8:30 a.m.	**PLENARY LECTURE 6** **Helmut Schwarz**, Technische Universität Berlin, Berlin (Germany) *Mass Spectrometry and Theoretical Chemistry in Service of Catalysis Research: A Ménage-à-Trois at Its Best*				
9:15 a.m.	BREAK				
9:30 a.m.	**FO1 Metabolomics** *KN: Augustin Scalbert*	**FO2 - Informatics tools & data analysis** *KN: Marc-Andre Delsuc*	**FO3 - Cultural Heritage & Archaeology** *KN Caroline Tokarski*	**FO4 - Atomic MS: Metallomics & IRMS** *KN: Gary M. Hieftje*	**FO5 - Nutraceutics Directions** *KN: Riadh Ksouri*
11:30 a.m.	BREAK				
11:45 a.m.	**PRESENTATION OF IMSC 2020**				
12:15 p.m.	*Arrivederci & farewell drinks*				

Fundamental Mass Spectrometry	Instrumentation and Methods	Food & Beverage	Organic and Inorganic MS: Challenges & Applications	Life Sciences

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WELCOME FROM THE CHAIR AND THE SCIENTIFIC COMMITTEE OF THE 22ND IMSC

On behalf of the Division of Mass Spectrometry (DSM) of the Italian Chemical Society, we would like to welcome you to the 22nd International Mass Spectrometry Conference 2018 in Florence.

IMSC is not new in Florence. In fact, its seventh edition was hosted in this town in 1976, many years ago. During the decades mass spectrometry has developed a lot in Italy in many fields with top level scientists.
After 42 years, the city of Florence, one of the most beautiful cities in the world, is ready to host the 22nd edition of IMSC which will be the occasion to celebrate the 60th anniversary of this conference.
The IMSC 2018 venue is the historic "Fortezza da Basso", a masterpiece of Renaissance military architecture, built in 1534-1537, fully restored and located downtown, a few steps away from many hotels and all the attractions (museums, theatres, monuments, etc) of the city.

As all the previous editions, IMSC 2018 will cover all aspects of mass spectrometry, from fundamentals to instrumentation and applications.
The conference is organized with short courses, oral and poster sessions, workshops, awards, commercial exhibition and a social program.

We think that IMSC 2018 will be an useful occasion to enjoy science, network and meet old friends or new colleagues, to get new ideas for your job, for establishing new collaborations, starting new projects,... in the unique charm, amazing history and culture of Florence!

The city does not need a lot of presentation: it is an open sky museum with a unique historical heritage, a green, small, clean and safe city with a Mediterranean climate. Florence can be easily reached from all over Europe, through the city airport or those in Pisa and Bologna.

Florence has a University, founded in 1321, and many industries, among them the most important Italian fashion and leather goods brands which were born in Florence.
You will find very friendly and open people and, last but not least, many occasions to taste delicious and healthy food accompanied by the very famous Tuscan and Supertuscan wines!

Pre- and post-conference tours offer you the opportunity to enjoy and visit different towns and magnificent places in Tuscany and in Italy.

We do wish IMSC 2018 will be an important experience, not only from a scientific standpoint, but also for relationships, discussions, talks, social events... in the special atmosphere of Florence.
Please come and give your important contribution to make IMSC 2018 a successful, amazing and unforgettable conference!!

Gianluca Giorgi (IMSC 2018 chair)

and the Scientific Committee

Giuseppe Avellone

Gianluca Bartolucci

Giuliana Bianco

Donatella Caruso

Leopoldo Ceraulo

Francesco De Angelis

Simonetta Fornarini

Roberta Galarini

Giancarlo la Marca

Fulvio Magni

Giorgio G. Mellerio

Gloriano Moneti

Giovanni Sindona

Michele Suman

Pietro Traldi

WELCOME FROM THE PRESIDENT OF THE IMSF

Dear colleagues and friends,

The International Mass Spectrometry Foundation Board is pleased to join the IMSC 2018 Organizing Committee in inviting you to amazing and historic Florence for what promises to be a memorable scientific and cultural experience! We have the opportunity to discuss the latest developments, wide applications and future goals in our fast-paced field of mass spectrometry while enjoying one of the world's most beautiful cities and the wonderful hospitality and cuisine of Tuscany. The IMSF, the Italian Chemical Society Division of Mass Spectrometry and many of our national MS societies are offering travel grants to young investigators, so we hope to welcome a strong representation of our rising stars, as well as the enthusiastic participation of our established leaders and many active scientists. We thank all those who are responsible for the planning and execution of the conference and all the participants who will share their latest achievements and creative ideas with our diverse community.

See you in Firenze!

Catherine E. Costello
IMSF President


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INTERNATIONAL MASS SPECTROMETRY CONFERENCES

1st IMSC – London, UK	1958
2nd IMSC – Oxford, UK	1961
3rd IMSC – Paris, FR	1964
4th IMSC – Berlin, DE	1967
5th IMSC – Brussels, BE	1970
6th IMSC – Edinburgh, UK	1973
7th IMSC – Florence, IT	1976
8th IMSC – Oslo, NO	1979

9th IMSC – Vienna, AT	1982
10th IMSC – Swansea, UK	1985
11th IMSC – Bordeaux, FR	1988
12th IMSC – Amsterdam, NL	1991
13th IMSC – Budapest, HU	1994
14th IMSC – Tampere, FI	1997
15th IMSC – Barcelona, SP	2000
16th IMSC – Edinburgh, UK	2003

17th IMSC – Prague, CZ	2006
18th IMSC – Bremen, DE	2009
19th IMSC – Kyoto, JP	2012
20th IMSC – Geneva, CH	2014
21stIMSC – Toronto, CA	2016
22nd IMSC –Florence, IT	2018
23rd IMSC – Rio de Janeiro, BR	2020

IMSF EXECUTIVE COMMITTEE, IMSF NATIONAL AFFILIATES

International Mass Spectrometry Foundation (IMSF)

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- *Poland – Piotr Stefanowicz*
- *Portugal – Maria Helena Florencio*
- *Romania – Zaharie Moldovan*
- *Russia – Albert Lebedev*
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22nd IMSC SCIENTIFIC COMMITTEE

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THOMSON MEDAL AWARDS

The Thomson Medals are named after Sir J. J. Thomson who was responsible for the first mass spectrograph and its resulting data more than 100 years ago. He also predicted many features of modern mass spectrometry. Thomson discovered the electron using mass spectrometry and won the Nobel Prize in 1906 for his research.

The Medals are sponsored by the International Mass Spectrometry Foundation (IMSF) and were first awarded in 1985.

2018 Thomson Medal Winners are

***Prof. Albert J. R. Heck**, Utrecht University (The Netherlands)*

***Prof. John R. Yates**, The Scripps Research Institute, La Jolla (USA)*

The Thomson Medal Award plenary lectures will take place on Tuesday August 28 and Thursday, August 30 in Plenary room.

The previous winners are:

- **2016** M. N. Eberlin, S. McLuckey
- **2014** C. V. Robinson, R. Zenobi
- **2012** R. Aebersold, A. Makarov, F. Tureček
- **2009** C. E. Costello, C. C. Fenselau and P. Roepstorff
- **2006** J. H. Bowie, M. L. Gross and M. Karas
- **2003** R. M. Caprioli, F. Hillenkamp and V. L. Talrose
- **2000** J. B. Fenn, D. F. Hunt and A. G. Marshall
- **1997** M. T. Bowers, D. E. Games and J. F. J. Todd
- **1994** C. Brunnée, C. Djerassi and H. Schwarz
- **1991** K. Biemann, H. Matsuda and N. M. M. Nibbering
- **1985** J. H. Beynon, R. G. Cooks, K. R. Jennings, F. W. McLafferty, and A. O. C. Nier

CURT BRUNNÉE AWARD

Sponsored by Thermo Fisher Scientific for outstanding contributions to the development of instrumentation for mass spectrometry by a person under the age of 45 at the time of the award.

2018 Curt Brunnée Award is

Prof. Daniel E. Austin, *Brigham Young University (USA)*

The Curt Brunnée Award plenary lecture will take place on Wednesday August 29 in Plenary room.

The previous winners are:

- **2016** Yury Tsybin, Spectroswiss Sarl, Lausanne
- **2014** Dimitris Papanastasiou, Fasmatech, Athens
- **2012** Zheng Ouyang, Purdue University
- **2009** Alexander Makarov, Thermo Scientific
- **2006** Roman Zubarev, Uppsala University
- **2003** Michisato Toyoda, Osaka University
- **2000** Scott McLuckey, Purdue University
- **1997** Michael Guilhaus, University of New South Wales
- **1994** Gareth Brenton, Swansea

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2018 JOURNAL OF MASS SPECTROMETRY STUDENT AWARD

Presentations will be made during the JMS Award Symposium on **Wednesday August 29, 9:30-11:30 a.m.**, Room 1, Level 0.

G. P. Zeegers, R. Zenobi
ETH Zürich, Chemistry and Applied Biosciences, Zürich (Switzerland)
Anion Formation in MALDI Depends on Matrix and Target Plate Material Choice

K. Stevens, P. Mittal, A. Abell, T. Pukala Tara
University of Adelaide, Physical Sciences, Adelaide (Australia)
Combining Bio-Conjugation and Matrix-Assisted Laser Desorption Ionisation Mass Spectrometry for Biomolecule Detection and Localisation in Tissues

Daniel J. Ryan, N. Patterson, J. Moore, J. Spraggins, R. Caprioli
Vanderbilt University, Department of Chemistry, Nashville (USA)
Histology-Directed Proteomics: Combining Autofluorescence Guided Micro-Digestions with Liquid Surface Extractions

C. Lombard-Banek, R. Onjiko, S. Moody, P. Nemes
University of Maryland (USA)
Dual Microprobe CE-ESI-HRMS for the Characterization of Proteins and Metabolites in Single Embryonic Cells of Live Frog Embryos

M. da Silva Katyeny, A. O. Maldaner, F. Fabriz Sodré
Instituto de Química, Universidade de Brasília, Brasília (Brazil)
Wastewater-based Epidemiology: Use of Adulterants to Estimate Cocaine Consumption Patterns in Brasília, Brazil by LC-QToF-MS

DIVISION OF MASS SPECTROMETRY, ITALIAN CHEMICAL SOCIETY AWARD FOR YOUNG SCIENTISTS 2018

Since 2000, the Division of Mass Spectrometry of the Italian Chemical Society has established the "DSM-SCI Award for Young Scientists" for a young scientist (under 35 years) for the best publication in which mass spectrometry plays a key role.

In 2018 the winner is

Dr. Marcello Manfredi *Università degli Studi del Piemonte Orientale, Novara*

The previous winners are:

2000: David Bongiorno
2001: Antonina Gucciardi
2002: Maria Pia Vitale
2003: Sara Rinalducci
2004: Ester Marotta
2005: Ingrid Zagnoni
2006: Vera Muccilli
2007: ex-aequo Francesca Attanasio, Maria Chiara Monti
2008: Valeria Cavatorta
2009: Caterina Fraschetti
2010: Alessandra Tata
2014: Giovanni Caprioli
2015: Cristiana Labella
2016: Sara Granafei
2017: Andrew Smith

https://onlinelibrary.wiley.com

Chemistry, A European Journal Best Poster Awards to be assigned at the XXII International Mass Spectrometry Conference which will be held in Florence (Italy) on August 26-31, 2018 to a young researcher under 40 years presenting a poster communication within the following scope: **chromatography and sample preparation coupled to mass spectrometry.**

Each of the three awards includes a voucher of the value of € 250,00 for buying Wiley books and a certificate.

The winner will be announced during the conference.

http://www.ruffino.com

Ruffino Poster Award to be assigned at the XXII International Mass Spectrometry Conference which will be held in Florence (Italy) on August 26-31, 2018 to a young researcher under 35 years presenting a poster communication in one of the following sessions:

Food integrity, authenticity & traceability

Food additives & contaminants

Safe & valuable food

The award includes € 500,00 and a certificate.

The winner will be announced during the conference.

separations

http://www.mdpi.com/journal/separations

MDPI-Separations Best Poster Award be assigned at the XXII International Mass Spectrometry Conference which will be held in Florence (Italy) on August 26-31, 2018 to a young researcher under 40 years presenting a poster communication within the following scope: **chromatography and sample preparation coupled to mass spectrometry.**

The award includes € 500,00 and a certificate.

The winner will be announced during the conference.

Springer

http://www.springer.com

Springer - Analytical and Bioanalytical Chemistry Best Poster Award to be assigned at the XXII International Mass Spectrometry Conference which will be held in Florence (Italy) on August 26-31, 2018 to a young researcher under 35 years presenting a poster communication in one of the following sessions:

Mass spectrometry imaging

Mass spectrometric analysis of forensic science evidence

Therapeutic drug monitoring & drug discovery

The award includes a Springer Book voucher and a certificate.

The winner will be announced during the conference.

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an Open Access Journal by MDPI

Springer

CONTRIBUTORS

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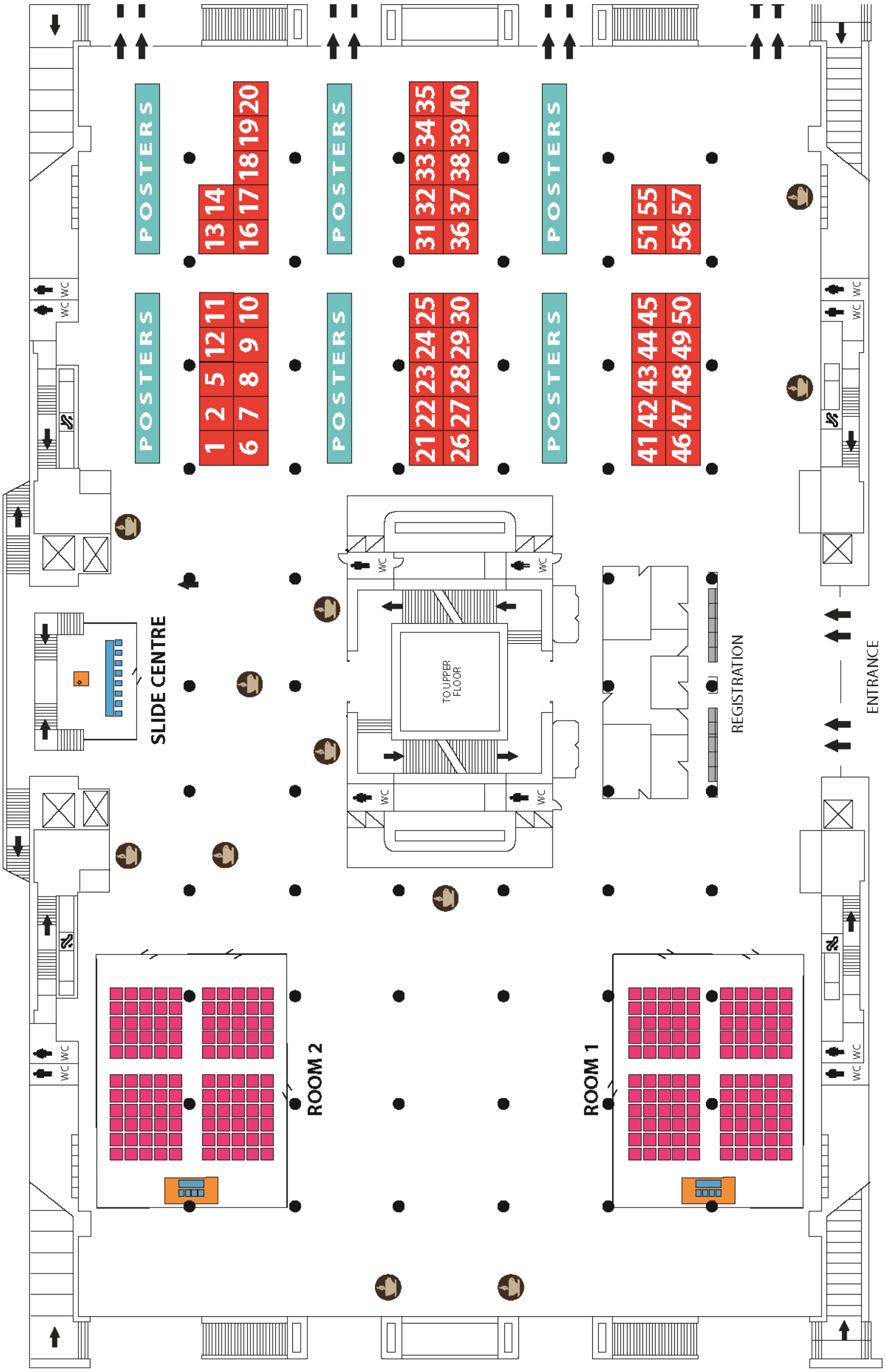

LEVEL 0

PADIGLIONE SPADOLINI - Exhibition area floor plan

EXHIBITORS

Advion

BOOTH N. 45

Advion is a leader in high performance, small footprint mass spectroscopy & synthesis solutions for life science. Using our deep scientific and engineering expertise, we develop a portfolio of purpose-built mass spectrometers, nanoelectro-spray ionization sources, and flow-chemistry synthesis systems characterized by reliability, quality, flexibility and fit for purpose design.

www.advion.com

AFFINISEP

BOOTH N. 10

Since 2004, AFFINISEP develops and manufactures a full range of solid phase for sample preparation (SPE kits) and passive samplers. AFFINIMIP®SPE based on molecularly imprinted polymers targets a full range of applications like Antibiotics, Mycotoxins, Pesticides, EDCs, Glyphosate&AMPA, Bisphenols, Clopyralid, Picloram, Zeranols, Phenolics, etc according to European and international regulations.

www.affinisep.com

Agilent

BOOTH N. 51, 56

Agilent is a global leader in life science, diagnostics and analytical laboratory technologies. Leveraging more than 50 years of expertise, we create instruments, software, services and solutions that provide trusted answers to our customers' most critical questions to increase productivity and advance the quality of life.

www.agilent.com

Avanti® POLAR LIPIDS, INC.

BOOTH N. 26

Avanti has the tools to help you succeed in Lipidomics. Our mass spec standard line includes deuterium labeled lipids available in complex standard mixtures or as individual compounds. We have been supplying lipid mass spec standards to the LipidMAPS consortium and many others for over 15 years. Our Analytical Services Division is also available to perform targeted or broad range Lipidomic analysis for a fee. Please visit our website for more information.

www.avantilipids.com

BIOGNOSYS
NEXT GENERATION PROTEOMICS

BOOTH N. 47

Biognosys provides innovative services and products for protein discovery and quantification using cutting edge mass spectrometry technology. We strive to be the company that provides the best possible solutions to support researchers in their protein analysis needs.

www.biognosys.com

Biotage®

BOOTH N. 55

Biotage is a global leader in life science technology. With a broad scope of tools for synthesis, work-up, purification, evaporation and analysis, the company provides solutions, knowledge and expertise in the areas of analytical chemistry, medicinal chemistry, and process-development. Our focus is on developing technology to speed experimental procedures.

www.biotage.com

BOOTH N. 41, 46

Bruker is a global technology leader delivering innovative, integrated analytical instrumentation for use in the Food Safety, Environmental analysis, Life Science, Pharmaceutical, Forensic and Clinical Research markets. Bruker Daltonics, a division of the Bruker Corporation, provides cutting edge mass spectrometry solutions which include MALDI-TOF, UHR-QTOF, Ion Traps, FTMS as well as LC and GC systems to solve the most demanding analytical questions presented to these markets today.
www.bruker.com

BOOTH N. 42

El-Mul is a designer and manufacturer of advanced tailor-made charged particle detection solutions. We provide detection systems to Mass Spectrometry, Electron Microscopy and Ion Beam vendors. We develop solutions from functional requirements through performance optimization and full engineering design to serial manufacturing.
www.el-mul.com

BOOTH N. 13

The European Network of Fourier-Transform Ion-Cyclotron-Resonance Mass Spectrometry Centers (EU_FT-ICR_MS, http://www.eu-fticr-ms.eu/) is an infrastructure funded by the EU Horizon 2020 program (Grant 731077). The network includes 3 companies and 11 academic centers which cover all The FT-ICR MS application fields from 8 European countries.
www.eu-fticr-ms.eu

BOOTH N. 38

Real time, in-vivo analysis of biologically relevant metabolites. Fossil Ion Technology develops and commercializes SUPER SESI, an ion source compatible with high resolution MS, that enables real-time analysis of low volatility metabolites in air. Combining its high ionization efficiency, with the best MS in the market, SUPER SESI allows in-vivo monitoring of large and biologically relevant metabolites in gas phase. Applications: breath analysis, real time analysis of vapors released by mice, plants, cell cultures
www.fossiliontech.com

BOOTH N. 37

GL Sciences is a manufacturer from Japan, specialised in Chromatography consumables and instruments for over 50 years. Inertsil, InertSustain and InertCap are our best known chromatography columns. The OPTIC is a unique Multi Mode Inlet, used with any GC brand, all over the world.
www.glsciences.eu

BOOTH N. 12

The 2020 edition of the International Mass Spectrometry Conference will be held at Rio de Janeiro, Brazil

BOOTH N. 11

The world's leading PTR-MS company, producing PTR-TOFMS real-time trace gas analyzers with a detection limit < 1 pptv for VOCs and the award-winning sampling system for aerosol & particulate matter (CHARON) as well as fast GC interfaces. We manufacture APi-TOF, CI-TOF and modular time-of-flight mass spectrometers for research & OEM.
www.ionicon.com

BOOTH N. 43

IonSense manufactures Direct Analysis in Real Time technology in the DART® open-air ionization source for use with LC/MS products from all major vendors. Present highlights are the utility of automated pipetting of low volume sample aliquots onto the QuickStrip-96™ for rapid sample analysis, and DART-TD (swab-based thermal desorber) for use in food safety, forensics & drug development applications.
www.ionsense.com

BOOTH N. 2

IONTOF is a manufacturer of innovative instruments for surface analysis with different product lines for time-of-flight secondary ion mass spectrometry (TOF-SIMS) and high-sensitivity low-energy ion scattering (LEIS).
Founded as a classical spin-off of the University of Münster, IONTOF has meanwhile become the technological leader in the field of TOF-SIMS and LEIS instrumentation.
www.iontof.com

BOOTH N. 25, 30

JEOL is global leader in instrumentation for scientific research and industrial applications, providing innovative technologies for MS, NMR and Electron Microscopy. The AccuTOF-GC x GC/MS unit is the only high-resolution MS combining GCxGC with high-resolution and a choice of EI, CI, PI, FD and FI ion sources. JEOL's multi-turn ion optics provide very high resolution for the SpiralTOF MALDI system (ultrahigh resolving power of >75.000, sub-ppm mass accuracy, and monoisotopic precursor selection. The InfiTOF high-resolution gas analysis system provides a resolving power of > 30.000 with an instrument the size of a PC.
www.jeol.com

BOOTH N. 24

KR Analytical are suppliers of ambient Ion sources including AP-MALDI and ASAP. We also provide MALDI Image preparation equipment from SunChrom, Chemyx syringe pumps and ApexGasgen nitrogen generators. Low cost AP-MALDI can be interchanged with ESI, adding MALDI capability to your LC-MS.
www.kranalytical.co.uk

BOOTH N. 48

Our strengths are the "know-how" in the instrumental chemical analysis of micropollutants, the versatility and the ability to adapt to the needs of the customers. We are the forerunners in the creation of Ready to Use Kits containing multi-component mixtures of hundreds of standard pesticides for the calibration of scientific instrumentation with high technological content (GCMSMS, GCHRMS, LCMSMS, LCHRMS, LCFTMS, etc.). We have a complete line of QuEChERS products for the extraction and the clean-up (D-SPE) and we are the first to have realized the products "Ready to Use" for the extraction "SweEt". We mainly deal with pesticides and metabolites. We produce "Ready to Use" single-component and multi-component solutions, including new blends made according to the QuPPe-AO and QuPPe-PO methods. More information at our website www.labinstruments.it

BOOTH N. 49

LECO life sciences instrumentation delivers rapid, accurate analysis. Our mass spectrometers (TOFMS) and elemental determiantors are ideal for pharmaceutical research/drug discovery, metabolomics, forensic science/toxicology, and flavor/fragrance analysis. For pharmaceutical applications, software on select instruments helps you stay compliant with the FDA regulations on the storage and management of electronic records.
www.leco-europe.com

BOOTH N. 44

MetaSci is specialized in providing high quality libraries of human metabolites and small molecule compounds for various research application. We offer the widest collection of human metabolites in our Human Metabolome Library (HML) which is comprised of ~1,000 human metabolites and metabolic intermediates. It can be used in many applications such as quantitative metabolomics, metabolic pathway analysis, food analysis, environmental analysis, instrument calibration, peak identification and quantification and analytical method development.
www.metasci.ca

BOOTH N. 1

MS Vision offers flexible and cost effective service on a wide range of mass spectrometry and LC Systems in Europe. We support all common LC MS platforms from Sciex, Thermo and Waters. Meet us at booth no 1 to find out how we can ensure maximum performance and uptime of your instruments.
www.msvision.eu

BOOTH N. 5

The NIST Mass Spectrometry Data Center is responsible for the development of evaluated reference mass spectral libraries for the identification of chemical compounds and the analysis of complex mixtures.
www.nist.gov

BOOTH N. 34

Peak Scientific produces market-leading nitrogen, hydrogen and zero air systems mainly for the fields of LC-MS (Liquid Chromatography-Mass Spectrometry) and GC (Gas Chromatography). What differentiates us is our world-class technical support and ongoing service care throughout the generator's lifespan, wherever you may be in the world.
www.peakscientific.com

BOOTH N. 16, 17, 18, 19

With 9,000 employees serving over 150 countries, PerkinElmer is a global leader committed to innovating for a healthier world. Our innovative detection, imaging, informatics and service capabilities, combined with deep market knowledge and scientific expertise, help customers gain earlier and more accurate insights to improve lives and the world around us.
www.perkinelmer.com

BOOTH N. 50

For more than 125 years, Pfeiffer Vacuum has been the world's leading provider of vacuum solutions. Our portfolio comprises a full range of hybrid and magnetically levitated turbopumps, backing pumps, measurement and analysis devices, components and vacuum chambers. Please visit
www.pfeiffer-vacuum.com for more information!

BOOTH N. 14

PharmaFluidics is a disruptive player in the field of micro-Chip chromatography for biomarker discovery and the analytical development of biopharmaceuticals. Our expertise is the lithographic design and surface treatment of silicon wafers for the development of analytical chromatography columns (ÂµPACTM) with a separation bed of highly ordered and free-standing pillars.
www.pharmafluidics.com

BOOTH N. 36

Photonis designs and manufactures state-of-the-art detectors for various types of mass spectrometry techniques including LC-MS, GC-MS, Ion Trap, MALDI-TOF, among others. We work with instrument manufacturers to customize our products to fit their exact specifications. From MCPs, to Channeltrons and Ion Guides, our products allow you to analyze every molecule.
www.photonis.com

BOOTH N. 9

The leader in quantitative ultra-fast high-throughput analysis for mass spectrometry presents the new LUXON ION SOURCE with a sample to sample speed below one second. The Luxon process can be integrated with automated liquid handling and robotic transfer arm systems to provide real highthroughput and continuous automation for your laboratory workflow. This patented ionization source offers outstanding analytical performance in pharmaceutical, bioanalytical, forensic, food and environmental industries and performs exceptionally well in other analytical fields. The Luxon Ion Source is the second-generation sample introduction and ionization source based on the LDTD® technology to provide the fastest and most robust process in mass spectrometry.
www.phytronix.com

BOOTH N. 35, 40

SCIEX's global leadership and world-class service and support in the capillary electrophoresis and liquid chromatography-mass spectrometry industry has made it a trusted partner to thousands of the scientists and lab analysts worldwide who are focused on basic research, drug discovery and development, food and environmental testing, forensics and clinical research.
www.sciex.com

BOOTH N. 6, 7, 8

Shimadzu is a worldwide leading manufacturer of analytical instrumentation. The company's equipments in mass spectrometry are used as essential tools for the quality control of consumer goods in all areas of food safety, environmental, consumer protection, healthcare... Discover our new solutions to help researchers making steps ahead at booth 6-8.
www.shimadzu.eu

BOOTH N. 57

Spectroswiss technologies boost the performance and productivity of your FTMS instruments helping to advance the most challenging applications. Our software, Peak-by-Peak, provides advanced data processing tools. Our hardware, FTMS Booster, enables high-performance data acquisition for any FTMS instrument. Our FTMS Diagnostics services help you to better use your FTMS instruments.
www.spectroswiss.ch

BOOTH N. 39

Tecan is a leading provider of laboratory instruments and solutions in biopharmaceuticals, forensics and clinical diagnostics. The Company specializes in the development, production and distribution of automated workflow solutions for the life sciences sector.
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BOOTH N. 21, 22, 23, 28, 29

Thermo Fisher Scientific is the world leader in serving science. Our mission is to enable our customers to make the world healthier, cleaner and safer. We help our customers accelerate life sciences research, solve complex analytical challenges, improve patient diagnostics and increase laboratory productivity. For more information, please visit
www.thermofisher.com

BOOTH N. 27

TOFWERK designs and delivers state-of-the-art time-of-flight (TOF) mass spectrometers (MS) for a broad range of laboratory and field applications. Our end-user product line includes the ICPTOF, Vocus PTR-TOF, IMS-TOF, and EI-TOF for GC. Additionally, our engineers and scientists collaborate with research laboratories and OEM customers to develop custom MS solutions based on our modular design platform. This platform - which includes optimized vacuum system designs, high-speed data acquisition hardware and software, data processing and visualization software, and our TOF mass analyzers - enables rapid prototyping and characterization of new instruments.
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BOOTH N. 31, 32, 33

Waters Corporation creates business advantages for laboratory-dependent organizations by delivering scientific innovation to enable customers to make significant advancements. Waters helps customers make profound discoveries, optimize laboratory operations, deliver product performance, and ensure regulatory compliance with a connected portfolio of separations and analytical science, laboratory informatics, mass spectrometry, as well as thermal analysis.
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BOOTH N. 20

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www.springer.com

www.spectroscopyeurope.com

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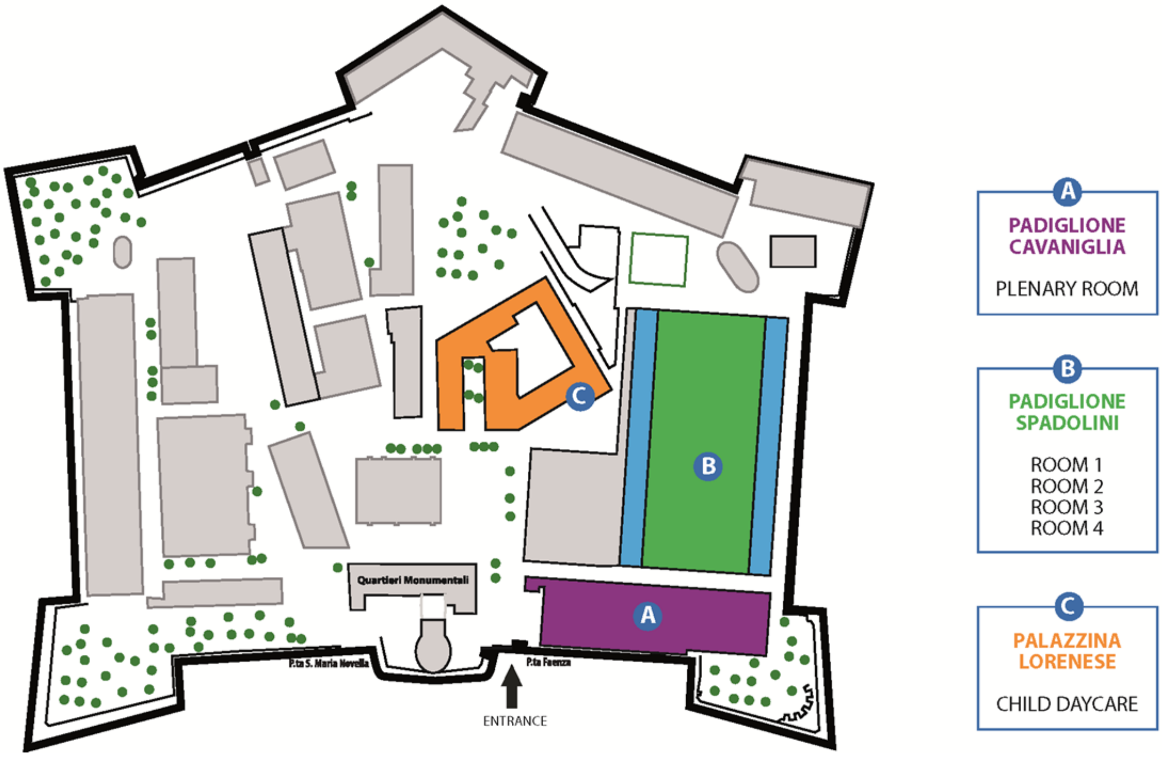
CONFERENCE VENUE AND FLOOR PLANS

Conference venue

Address:

Fortezza da Basso
Viale Filippo Strozzi, 1
50129 Firenze

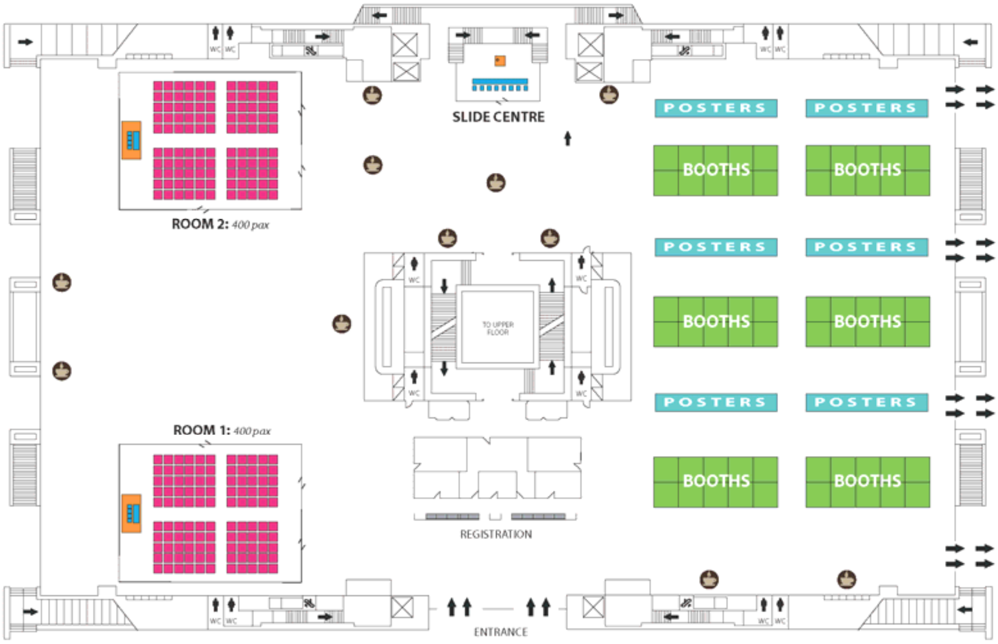
The **Fortezza da Basso** is a masterpiece of the military Renaissance architecture, commissioned by Duke **Alessandro de' Medici**, planned by Antonio da Sangallo il Giovane and built between 1534 and 1537.



LEVEL 0

PADIGLIONE CAVANIGLIA

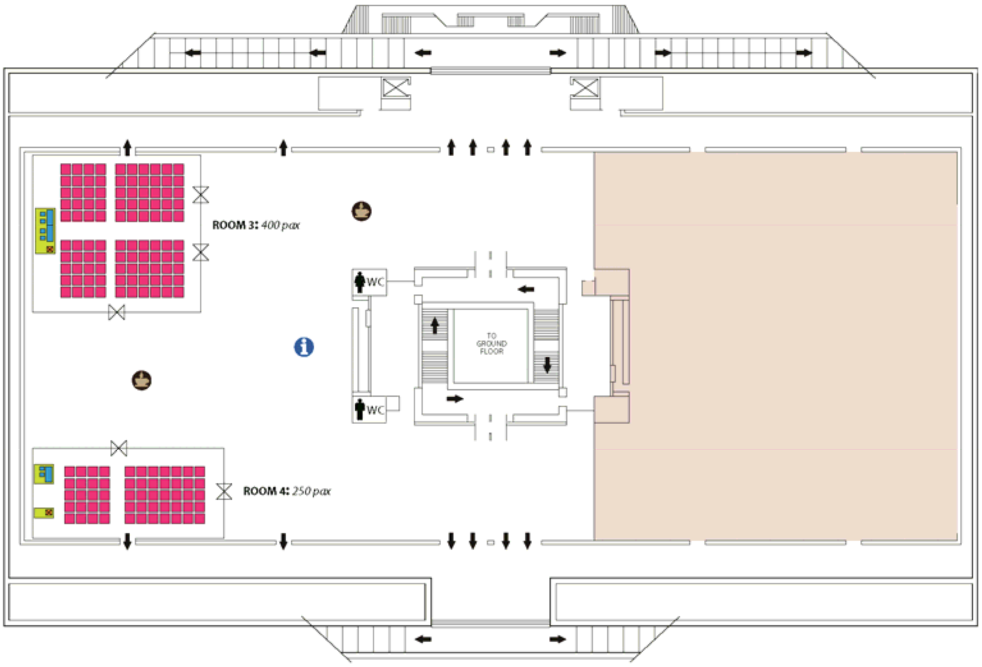
Plenary room



LEVEL 0

PADIGLIONE SPADOLINI

Rooms 1, 2
Registration
Slide center
Exhibition area



LEVEL 1

PADIGLIONE SPADOLINI

Rooms 3, 4

GENERAL INFORMATION

Reception Desk and Congress Secretariat

Located on the ground floor of Padiglione Spadolini just in front of the main entrance.

Opening hours:

- Sunday August 26th, 11:00 a.m. – 6:00 p.m.
- Monday August 27th, 8:00 a.m. – 7:00 p.m.
- Tuesday August 28th, 8:00 a.m. – 7:00 p.m.
- Wednesday 29th, 8:00 a.m. – 7:00 p.m.
- Thursday 30th, 8:00 a.m. – 5:00 p.m.
- Friday 31st, 8:00 a.m. – 1:00 p.m.

Wi-Fi

Free Wi-Fi will be provided within the Conference venue for its entire duration.

Username: IMSC2018

Password: imsc2018

Speaker Preview Room

A Speaker Preview Room is provided for all oral presentations at the ground floor of Padiglione Spadolini just behind the Registration Desk.
Presentations must be in PowerPoint format only (MAC or PC) and saved on an USB key.
All presenters should load their files at least three hours before the scheduled presentation time.
An audio, video and basic running check of the presentation will be performed.

Official Language

All sessions of the scientific program are in English. There will be no simultaneous translations offered.

Congress Card

The customized IMSC Congress Card is downloadable for free at **http://www.conventionbureau.it/tmpcardpage/en/congress-card.shtml** click on "INTERNATIONAL MASS SPECTROMETRY CONFERENCE - IMSC 2018" on the right column of the page. The Card is valid for your stay in Florence during the conference and provides special offers and discounted fees at museums, historical sites, shops, restaurants, wellness centers, golf clubs, bike rental stands, taxis and car rental agencies. The discounts will be granted simply by showing the Card! The Congress Card is not nominal and can be used by the participants as well as by anyone accompanying them. A further bonus is that it is also valid a few days prior to and after the congress date.

Child Daycare

A safe, clean environment within the congress area where your children will be taken care of and engaged in fun activities by specialized, English-speaking teachers.
The service is provided for children age 1-12.
If your child needs to take a nap, please note that a stroller is needed. However, there will be a relaxing area with mats and pillows for children to rest.
If your child needs lunch, please note that it will be served between 12 p.m. and 1 p.m. Please tick the respective timeslot box on the childcare request form.

Welcome Mixer

Sunday, August 26th 2018 h. 7:00 p.m.
At the Conference venue, exhibition area, ground floor.
Enjoy an exhibition of the quartet with opera singers followed by drinks and finger food.

Gala Dinner

Thursday, August 30th 2018 h. 8:00 p.m.

Villa Viviani, located on the hill of Settignano, a 15-minute bus ride away from Florence city center, is an historical abode: the most ancient part of the building dates back to the 13th century, when the Tanagli family built a luxurious house, giving the possibility to admire the city of Florence and its surroundings from a highpoint.

Dress code: casual   Bus transfer from the Conference venue provided.

Farewell drinks

Friday, August 31st 2018 h. 12:15 p.m.
Congress Venue, exhibition area, ground floor.

Telephone country code: 0039

Parking

There are several parking lots located to the Conference venue. Some of them are:

Parcheggio Stazione Fortezza Fiera (500 m from the conference venue)
Piazzale Caduti nei Lager - 50129 Firenze
Tel. 055 5030 2209

Parcheggio Stazione Binario 16 (300 m from the conference venue)
Piazzale Montelungo, 50129 Firenze
Tel. 055 5030 2209

Taxi

Taxi services in Florence operate 24 hours a day, 7 days a week. Taxis are "stationed" at special taxi parking stands in most of the major squares in the city, at the train station and at the airport and they can be requested by phone.
Some taxi services are:

Taxi Firenze 4242 Tel. 055 4242 / 0577 4798 Text 3346622550

4390 Taxi Firenze Tel. 055 4390

SHORT COURSES

Venue

University of Florence
Via Gino Capponi, 9
50121 Firenze

Timetable

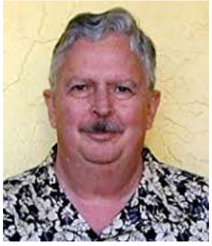
Saturday, August 25th 2:00 p.m. - 6:00 p.m.

Sunday, August 26th 9:00 a.m. -1:00 p.m.

Methodology: Lectures Language and Presentation: English, Slides

1) FUNDAMENTALS OF MASS SPECTROMETRY

Tutors:



O. David Sparkman

University of the Pacific in Stockton, California (USA)

Jürgen H. Gross

University of Heidelberg (Germany)

A two-day course on the interpretation of mass spectra of organic compounds. Starting at the introductory level, the course is intended to provide the fundamentals for an understanding of the basic principles and applications of mass spectrometry of organic molecules.

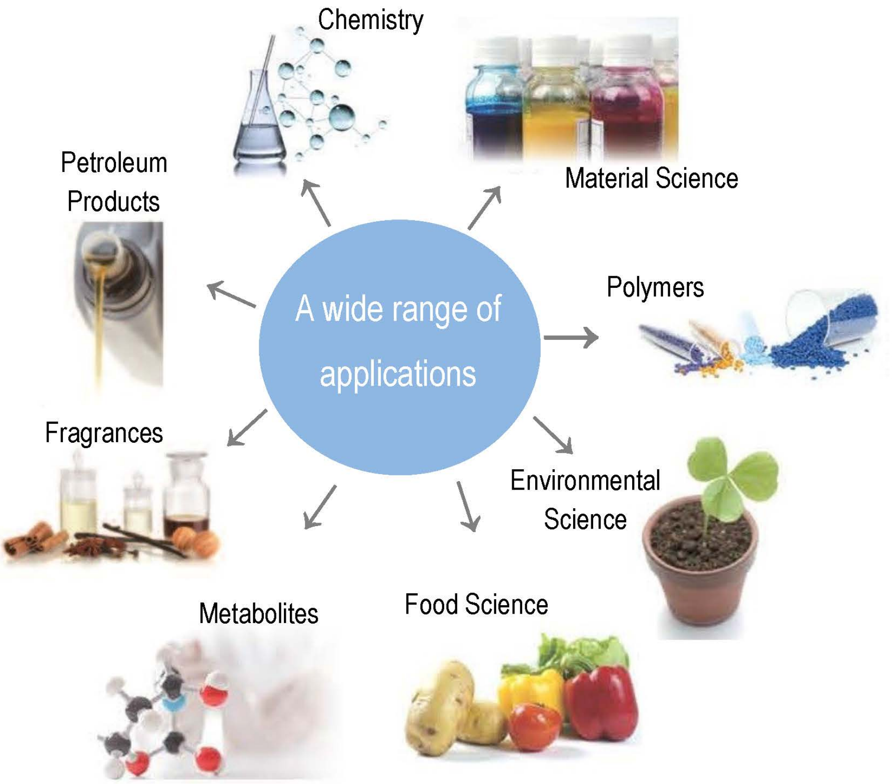
Key topics of the short course are ionization processes, the formation and interpretation of isotopic patterns, uses of high-resolution and accurate mass for molecular formula determination, and an introduction to the fragmentation pathways of odd-electron and even-electron ions. Information regarding available mass spectral databases will be provided along with how to use them with all types of organic mass spectrometry including MS/MS data.

With an emphasis on the analysis of small molecules, you will learn to systematically employ all of the above mass spectral data for compound identification and structure elucidation.

To complete the course, a compact lecture on instrumentation and its common modes of operation will be included.

Take-home exercises and solutions via web.


AccuTOF GCx-plus


A wide range of applications
Chemistry
Material Science
Polymers
Environmental Science
Food Science
Metabolites
Fragrances
Petroleum Products

2) FOODOMICS & MASS SPECTROMETRY

Tutors:

Michele Suman

Barilla G.R. F.lli SpA
Parma (Italy)

Laurent Debrauwer

INRA Toxalim
Toulouse (France)

Fulvio Mattivi

University of Trento
Trento (Italy)

Laura Righetti

University of Parma
Parma (Italy)

Metabolomics gained progressively the scene of the last decade as the combination of modern analytical techniques with chemometric pattern recognition, targeting also food science and nutrition research and giving at the same time new relevant pathways for food safety, quality and traceability.

Metabolic fingerprinting usually implies a very simple sample preparation (a generic extraction, mainly) to not a priori discriminate potential candidate compounds, otherwise a particular class of molecules (e.g. triglycerides, etc.) can be preselected by adequate sample prep and/or chromatographic separation: in this last case the term used for defining such a strategy is called profiling.

In the particular case of food metabolomics, metabolites can be present in their original form, e.g. fruit or meat, etc... or metabolome can be also influenced by the food processing technologies.

Effectively, the identification of markers usually represents the last step within metabolomics studies with the final aim of discovering metabolite pathway and significant compounds generated for instance during the food processing.

In particular, Foodomics was defined by Cifuentes et al. as "a discipline that studies the food and nutrition domains through the application and integration of advanced -omics technologies to improve consumer's well-being, health, and knowledge": a sort of holistic and comprehensive understanding of 360° food quality.

Many relevant publications on the applicability of high resolution mass spectrometry combined with ultra-high performance liquid chromatography (UHPLC-HRMS) are oriented to food metabolomics.

Recently, direct ambient MS approaches, such as DART-MS and innovative applications of ion mobility spectrometry (IMS), have been proposed as further solutions for fingerprinting-foodomics.

There is also opened a future direction for volatile fingerprinting-foodomics by the exploitation of a new generation of ion sources coupled to GC-HRMS detectors.

Topics:

- Introduction to MS, Food processing & Foodomics
- Foodomics in many different ways: genomics, proteomics, metallomics, sensomics, isotopolomics
- Metabolomics studies for food nutrition and safety
- Ambient Mass Spectrometry for Foodomics outcomes
- Food quality and traceability following the metabolomics way
- Exercise with real case studies/examples working time together among teachers & students

3) MASS SPECTROMETRY IMAGING

Tutors:

Marialaura Dilillo

Fondazione Pisana per la Scienza, Pisa (Italy)

Manuel Galli

Università Milano Bicocca, Monza (Italy)

Liam McDonnell

Fondazione Pisana per la Scienza, Pisa (Italy)

Andrew Smith

Università Milano Bicocca, Monza (Italy)

Martina Marchetti-Deschmann

University of Technology Wien (Austria)

This short course will be dedicated to the instrumentation employed in MS imaging as well as the theoretical/practical aspects of sample preparation and data analysis.

Topics:

- Introduction to MS-Imaging
- Sample preparation
- Matrix deposition
- Identification, validation and increased coverage
- Processing and interpretation of the acquired data
- Applications and latest trends in MSI

4) EXPANDED NEWBORN SCREENING BY TANDEM MASS SPECTROMETRY

Tutors:

Giancarlo la Marca

Univ. of Florence and
Meyer Children's Hospital,
Florence (Italy)

Marzia Pasquali

University of Utah,
School of Medicine
Salt Lake City (USA)

Ugo Rocha

National Institute of
Health "Ricardo Jorge"
Porto (Portugal)

Tandem mass spectrometry (MS/MS) has become a leading technology used in clinical chemistry and has shown to be particularly sensitive and specific when used in newborn screening (NBS) tests. The success of tandem mass spectrometry is due to important advances in hardware, software and clinical applications during the last 25 years. MS/MS permits a very rapid measurement of many metabolites in different biological specimens by using filter paper spots or directly on biological fluids. Its use in NBS give us the chance to identify possible treatable metabolic disorders even when asymptomatic and the benefits gained by this type of screening is now recognized worldwide.

Today the use of MS/MS for second-tier tests and confirmatory testing is promising especially in the early detection of new disorders such as some lysosomal storage disorders, ADA and PNP SCIDs, X-adrenoleucodistrophy (X-ALD), Wilson disease, guanidinoacetate methyltransferase deficiency (GAMT), and Duchenne muscular dystrophy. The new challenge for the future will be reducing the false positive rate by using second-tier tests, avoiding false negative results by using new specific biomarkers and introducing new treatable disorders in NBS programs.

Topics:

- Introduction to the expanded newborn screening
- Preanalytical phase and sample collection
- Instrumentation and methods
- Second Tier tests
- Organic acidurias, aminoacidopathies, lysosomal storage disorders, etc
- Analysis and interpretation of the results

5) SOLID-PHASE MICROEXTRACTION: COMPREHENSIVE OVERVIEW OF THE TECHNOLOGY AND APPLICATIONS

Tutors:

Janusz Pawliszyn

University of Waterloo (CDN)

Barbara Bojko

Nicolaus Copernicus University of Torun (PL)

Nikita Looby

University of Waterloo (CDN)

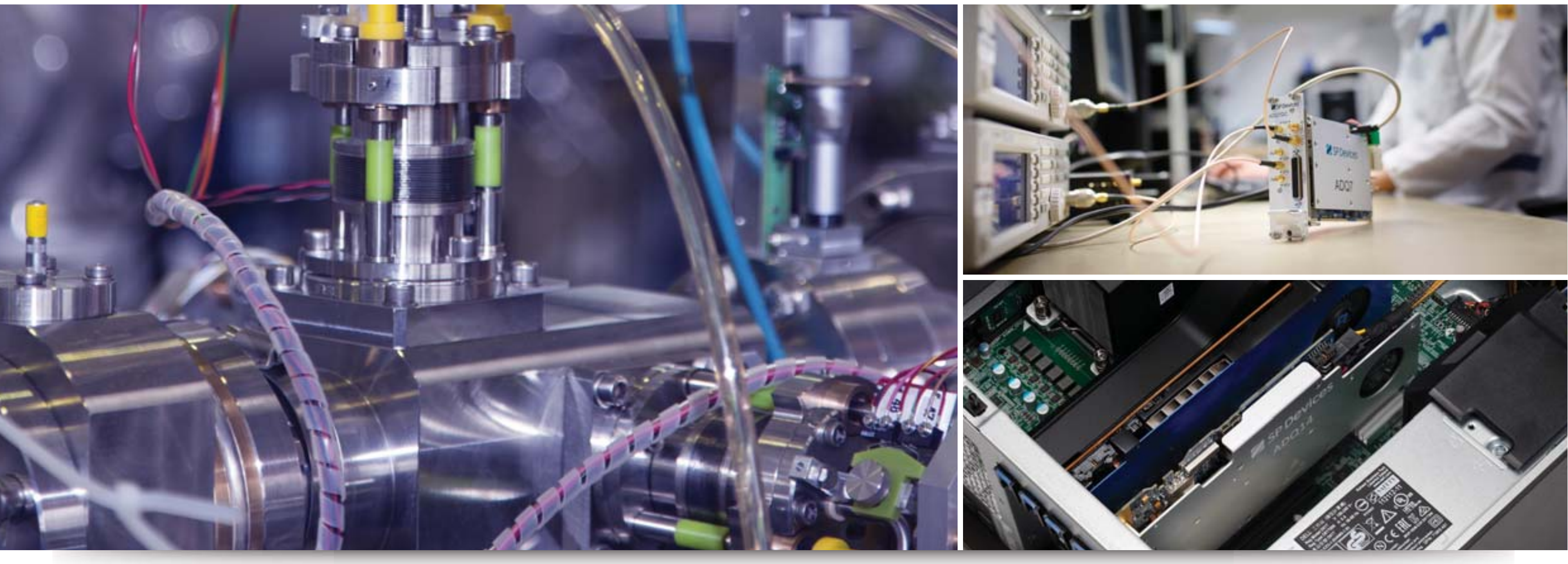
Tijana Vasiljevic

University of Waterloo (CDN)

Sample preparation is an often overlooked but extremely important aspect of any analytical method. Solid-phase microextraction (SPME) is a simple, fast, sensitive, and environmentally-friendly equilibrium/diffusion-based sample preparation technique that allows the integration of sampling and sample preparation steps, as well as direct introduction to the analytical instrument on a single device. Due to these unique features, SPME concept is considered one of the “Greatest Ideas” in analytical chemistry and during the last twenty-five years have proven to be in continuous evolution.

This course will cover both basic and advanced SPME topics with the focus on the main principles of SPME including thermodynamic and kinetic theory, calibration methods and coupling strategies of SPME to GC-MS, LC-MS and direct coupling to MS. A complete method development strategy will be described and illustrated in detail by real-life examples to facilitate quantitative determinations. A variety of SPME applications in the fields such as forensic, environmental, food and beverage, industrial hygiene and clinical analysis will be presented. The discussion will include the comparison of the performance of SPME to various established methods relevant for particular application. Recent advances in SPME will be highlighted including (1) direct coupling to mass spectrometry, (2) on-site sampling, (3) the use of SPME for ligand-receptor binding and plasma protein binding studies, (4) the use of SPME to perform in vivo sampling of freely moving animals (e.g. targeted analysis) (5) automation of SPME in 96-well plate format for applications requiring high-throughput (e.g. water/clinical analysis), (6) the use of SPME for direct tissue sampling (clinical applications), (7) in-vivo metabolomics and lipidomics using SPME, (8) brief overview of new technologies: needle trap and thin film microextraction.

The course is targeted at both new and current SPME users. The primary goal of the course is to provide the users of the technique with deeper insight into the main principles of this technique and thus increase their productivity and the quality of analytical results. This course will be of interest to analytical chemists, laboratory supervisors, scientists and industry regulators in the environmental, food and beverage, pharmaceutical, clinical, medical, cosmetic, industrial hygiene and many other fields. The unique features of high throughput, in vivo sampling, and direct coupling to MS will be of particular interest to researchers actively using other sample preparation technologies in combination with mass spectrometry.



MONDAY, August 27th, 2018 5:15 – 7:00 p.m

WKS-M1 – Mass spectrometry in virology ROOM 1 - level 0

Organizer:

Günter Allmaier

Vienna University of Technology
Vienna (Austria)

The detailed characterization starting from intact viruses (e.g. human rhinovirus), viral gene therapy platforms (e.g. lentivirus or adeno-associated virus) or vaccine (e.g. virus-like particles from human papilloma virus or modified influenza viruses) species down to functional protein complexes derived from viruses and individual proteins or lipids is gaining more and more importance due the improved instrumentation and new combinations of them. Even the interaction of antibodies or antibody fragments with viruses is of general interest in virology. More and more different virus species (e.g. Noravirus variants) are emerging and are connected to certain diseases. So they are coming into the focus of biomedical as well as biotechnological research. The same holds true for vaccine particles, virus-like particles and advanced viral gene therapy particles, all belonging to the group of bionanoparticles, due to the fact that detailed physicochemical characterization of viral nanoparticles is required by EMA, FDA and other authorities. So emerging techniques, methods and strategies based on mass spectrometry will be presented even if not fully developed and discussed.

WKS-M2 – Police casework - successes and challenges from an academic perspective ROOM 2 - level 0

Organizer:

Simona Francese

Sheffield Hallam University
Sheffield (UK)

Translational research is at the heart of every researcher that seeks to make an impact on society rather than keeping their research at the level of an academic exercise.

In order to translate academic research into a forensic tool that is operationally deployable, academics need a strong interaction with the end users (practitioners, law enforcement agencies etc..). This interaction is aimed to the development of technologies that withstand court scrutiny and meet law requirements for collection, storage and treatment of the evidence.

This interaction lasts for as long as a controlled vocabulary is also employed to enable both parts to understand issues, desirables, and solutions in a synergic approach.

This workshop covers all aspect of the challenges of such interaction and collaboration from an academic perspective. From networking, to fostering contacts, technological development, pseudo-operational trials and integration in the forensic workflow, this workshop surveys successes, failures and hopes in the application of academic research to police casework from the first step to full deployment.

WKS-M3 – Environmental Mass Spectrometry: from trace analysis to effect assessment ROOM 3 - level 1

Organizers:

Marc Suter

Eawag
Dübendorf (CH)

Jennifer Schollee

Eawag
Dübendorf (CH)

Environmental Mass Spectrometry has evolved from simple trace analysis, allowing the detection and quantification of a limited set of pollutants, to where it is now possible to monitor thousands of chemicals in a data-independent way. One major challenge in this is the annotation of unknown features found in a sample. Thanks to current highly accurate and high resolution instrumentation, experimentally determined accurate mass, isotope distribution, MS/MS spectra and physico-chemical information obtained from sample preparation and interaction with the chromatographic phase, facilitates the structural identification of unknowns. Furthermore, when chemical samples are linked to biological effects, using e.g. in vitro assays, in what is called effect-directed analysis (EDA), information is gained that allows i) focusing on samples with (adverse) environmental effects and ii) unravelling the molecular mechanisms of toxic action.
This workshop will cover strategies used and challenges encountered when trying to identify unknown compounds in environmental matrices, and applying effect-directed analysis.

Conceptual:

5:00 - 5:20 p.m. Effect-Directed Analysis: adding another dimension to toxicant identification
Marja H Lamoree, Vrije Universiteit, Amsterdam, the Netherlands

5:20 - 5:35 p.m. From target to non-target screening with HR-MS - tools to identify and prioritize contaminants in the environment
Jennifer E Schollée, Eawag, Dübendorf, Switzerland

5:35 - 5:50 p.m. Effect assessment using bioanalytical tools
Marc J-F Suter, Eawag, Dübendorf, Switzerland

Non-target:

5:50 - 6:05 p.m. Longitudinal non-target screening of the river Rhine
Michael Schlüsener, Federal Institute of Hydrology, Koblenz, Germany

6:05 - 6:20 p.m. HILIC-MS (non-)target screening, monitoring and toxicological evaluation of highly polar compounds in drinking water and sources
Annemieke Kolkman, KWR, Nieuwegein, The Netherlands

Effect-directed

6:20 - 6:35 p.m. Non-targeted and targeted analysis of emerging water disinfection byproducts of toxicological importance
Xing-Fang Li, University of Alberta, Edmonton, Canada

6:35 - 6:50 p.m. Effect-directed analysis with thin-layer chromatography for prioritization of non-target features
Stefan Weiss, Zweckverband Landeswasserversorgung, Stuttgart, Germany

WKS-M4 – Are MS-based methods fit for purpose? ROOM 4 - level 1

Organizer:

Lorens P. Sibbesen

Eurachem
Method Validation Working Group

Mass Spectrometry (MS) has developed tremendously over the years and thousands of scientists are currently finding new ways of applying and exploiting the principles for new purposes in many different fields.
The question is however, whether MS-based methods are always fit for purpose. That is, will the laboratory be able to deliver useful and reliable results to the end-user by applying methods based on this highly advanced technology?
Analytical chemistry is basically about solving a problem by identifying an appropriate method, carefully performing the method on the given samples (including sample preparation), and then issuing the result. But analytical chemistry constantly faces new challenges in terms of requests for analysis of new parameters in complex samples at lower and lower levels. Scientists keep pace with these challenges by coming up with increasingly sophisticated (and sensitive) analytical techniques. Mass spectrometry has proven to be applicable for a wide variety of analytical tasks.
The question is whether MS-based methods, useful for solving specific analytical tasks in the R&D laboratory, can also be applied in routine testing laboratories. Are these methods "fit for the purpose" and how do we demonstrate that through validation?

This workshop will give a brief introduction on:

What we mean by "Fitness for Purpose" (based on the Eurachem Guide)
MSc. Lorens P. SIBBESEN, LAB Quality Int., Denmark (chair of MVWG)

An example of validation of an MS-based method
Dr. Burcu BİNİCİ, Senior Researcher, UME/TÜBİTAK, Turkey

Challenges in validating MS-based methods
Dr. Perihan YOLCI OMEROGLU, Uludag University, Bursa, Turkey

Based on the introduction, the workshop will give participants the opportunity to discuss challenges and experiences in the field. The Eurachem "Fitness for Purpose" guide can be downloaded from www.eurachem.org

TUESDAY, August 28th, 2018 5:15 – 7:00 p.m

WKS-T1 – Careers in Mass Spectrometry ROOM 1 – level 0

Organizer:

Jackie Mosely

Durham University
Durham (UK)

Our aim is to illustrate the wide variety of career options and debate the future requirements for the "expert" user by inviting 3-4 significant mass spectrometrists from diverse scientific and internationally widespread backgrounds to provide short presentations describing their career paths.
We will also invite experts from the mass spectrometry recruitment sector to be present to discuss the many options for mass spectrometry careers, the current market demand for mass spectrometry skills and more broadly analytical sciences.

WKS-T2 – Transforming Drug Discovery and Clinical Biomarker Bioanalysis: It's Time for a Paradigm Shift from SRM to HRMS

ROOM 2 – level 0

Organizer:

Ragu Ramanathan

Pfizer Inc.
Groton (USA)

To understand the state of high resolution mass spectrometry (HRMS) for characterization and quantification of drug discovery and clinical biomarkers, a survey will be conducted before the IMSC 2018. Based on survey results, the presentation will summarize anticipated trends and will serve as an introduction to the workshop. Following the introduction, panel presentations from five Pharmaceutical industry/Academic speakers (30-45 minutes) will address the current status and future expectations of working with HRMS platforms for characterization and quantification of biomarkers. Following the panel presentations, in the remaining 30-45 minutes, the audience and the panel presenters will actively engage in scientific discussion regarding opportunities and limitations of using HRMS platforms for qualitative/quantitative biomarker applications.

WKS-T3 – Integration of native MS with structural biology methods

ROOM 3 – level 1

Organizers:

Michal Sharon

Weizmann Institute
of Science
Rehovot (Israel)

Frank Sobott

University of Leeds
Leeds (UK)

This workshop aims to provide a platform for discussion on the means by which Native MS can be integrated with other Structural Proteomics and Structural Biology Techniques. While each method has its own advantages and limitations, here we will focus on their enhanced value in combination: a whole that is more than the sum of its parts. The workshop will include up to 6 short presentations, each will be followed by an audience-driven discussion with the opportunity to ask questions to peers and a panel of experts.

WEDNESDAY, August 29th, 2018 5:15 – 7:00 p.m

WKS-W1 – MS-Based Techniques for the Characterization of Nanomaterials in Food, Biological and Other Complex Matrices

ROOM 1 – level 0

Organizers:

Francesco Cubadda

ISS-Italian Institute of Health
Rome (Italy)

Stefan Weigel

BfR-Federal Institute for Risk Assessment
Berlin (Germany)

Thorough characterization of nanomaterials is essential for establishing their physicochemical identity and for assessing their functional properties and potential toxicological hazards, which are both dependent on physicochemical characteristics. Electron microscopy is essential for imaging of nano-objects and studying their morphology. However, especially for the study of nanoparticles in food, biological and other complex matrices, the use of a multi-method approach is crucial, since at the moment no individual method alone is able to cover the whole necessary size range and all the different types of nanomaterials.

State-of-the-art mass spectrometric techniques for the analytical determination of nanoparticles in dispersion and (after proper sample preparation) in complex matrices have recently become available. Relevant examples are single particle ICP-MS and Asymmetric Flow Field Flow Fractionation (AF4) coupled with different detectors (UV, DLS, MALS) and ICP-MS. Techniques based on atomic mass spectrometric are element-specific (i.e. provide information on the chemical identity) and have the potential to measure size, size distribution, number concentration, mass concentration of particles (and in some instances concentration of the dissolved fraction, if present). Furthermore, the use of molecular mass spectrometry for the characterisation of organic nanoparticle components has been explored, e.g. MALDI-ToF-MS and ToF-SIMS.

The workshop aims to provide a platform for discussion on the prospects of MS-based techniques for the characterization of nanomaterials and the impact they may have on scientific and regulatory developments, e.g. on nanomaterials in food.

WKS-W2 – Mass spectrometry in Microbiology

ROOM 2 – level 0

Organizer:

Vladimír Havlíček

Academy of Sciences of the Czech Republic
Prague (Czech Republic)

The workshop covers many aspects of MS in microbiology, and in particular:

- Overview of ribosomal typing by MALDI-ToF;
- Dereplication of microbial compounds from mass spectrometry imaging datasets by Metaspace
- Microbial metabolomics
- Non-invasive diagnosis of aspergillosis in a rat model by molecular mass spectrometry plus CycloBranch dereplication tool
- Free talks and roundtable discussion.

WKS-W3 – Advances in Protein Structure Analysis with Mass Spectrometry ROOM 3 – level 1

Organizer: **Kevin Downard**

University of New South Wales
Sydney (Australia)

This workshop will comprise presentations from leading experts in academia and industry from across Europe and the world to address the latest advances and applications in protein structure analysis using mass spectrometry. It will comprise up to 6 short talks describing conformational charge effects, ion mobility studies, hydrogen exchange, protein footprinting and related technologies to study protein structures and interactions including protein folding, misfolding, aggregation and intrinsically disordered proteins. The benefits of using of a combination of these approaches will be highlighted together with the latest instrumentation developments. Key to the success of the workshop will be audience engagement with ample time allowed for open discussion and questions.

WKS-W4 – The EU_FT-ICR_MS network ROOM 4 – level 1

Organizers:

Carlos Cordeiro

Universidade de
Lisboa - Faculdade
de Ciências
Lisboa (Portugal)

Christian Rolando

Université de Lille,
Faculté des Sciences
et Technologies
Villeneuve d'Ascq
(France)

The aim of this workshop is to present the opportunities offered by the European Network of Fourier-Transform Ion-Cyclotron-Resonance Mass Spectrometry Centers (EU_FT-ICR_MS, http://www.eu-fticr-ms.eu/) which is an infrastructure funded by the EU Horizon 2020 program (Grant 731077). The network includes 3 companies and 11 academic centers which cover all The FT-ICR MS application fields from 8 European countries. In the workshop the main actions of the EU_FT-ICR_MS will be illustrated by the group leaders of the different centers or companies:

1. Trans National Access to provide the EU academic, SME and industrial communities' with access to world-class FT-ICR MS centers free of charge.
2. Workshops and summer school to build an EU community of end-users and FT-ICR MS scientists.
3. Development of open access to data and open source software for very high resolution data.
4. New FT-ICR MS application fields by innovative and cooperative research between European FT-ICR MS academic scientists and private companies (instrumentation and software).

LUNCH SYMPOSIA

MONDAY, August 27th, 2018 12:30 - 1:45 p.m.

BRUKER DALTONICS	Room 1 – Level 0
JEOL	Room 4 – Level 1
SCIEX	Room 3 – Level 1
WATERS	Room 2 – Level 0

TUESDAY, August 28th, 2018 12:30 - 1:45 p.m.

AGILENT TECHNOLOGIES	Room 2 – Level 0
BRUKER DALTONICS	Room 1 – Level 0
SCIEX	Room 3 – Level 1
THERMO FISHER SCIENTIFIC	Room 4 – Level 1

WEDNESDAY, August 29th, 2018 12:30 - 1:45 p.m.

AGILENT TECHNOLOGIES	Room 2 – Level 0
BIOGNOSYS	Room 3 – Level 1
PERKINELMER	Room 1 – Level 0
THERMO FISHER SCIENTIFIC	Room 4 – Level 1

THURSDAY, August 30th, 2018 12:30 - 1:45 p.m.

AGILENT TECHNOLOGIES	Room 2 – Level 0
SHIMADZU	Room 3 – Level 1
THERMO FISHER SCIENTIFIC	Room 4 – Level 1
WATERS	Room 1 – Level 0

Fundamental Mass Spectrometry	Instrumentation and Methods	Food & Beverage	Organic and inorganic MS: challenges & applications	Life sciences

SATURDAY, August 25th, 2018

2:00 ÷ 6:00 p.m.	**Short Courses** *Venue: University of Florence, Via Gino Capponi, 9 - Florence*	
	1. **Fundamentals of Mass Spectrometry**	***Room 4***
	2. **Foodomics & Mass Spectrometry**	***Room 9***
	3. **Mass Spectrometry Imaging**	***Room 5***
	4. **Expanded Newborn Screening by Tandem Mass Spectrometry**	***Room 3***
	5. **SPME: Comprehensive Overview of the Technology & Applications to Analytical MS**	***Room 7***

SUNDAY, August 26th, 2018

9:00 a.m. ÷ 1:00 p.m.	**Short Courses** *Venue: University of Florence, Via Gino Capponi, 9 – Florence*	
	1. **Fundamentals of Mass Spectrometry**	***Room 4***
	2. **Foodomics & Mass Spectrometry**	***Room 9***
	3. **Mass Spectrometry Imaging**	***Room 5***
	4. **Expanded Newborn Screening by Tandem Mass Spectrometry**	***Room 3***
	5. **SPME: Comprehensive Overview of the Technology & Applications to Analytical MS**	***Room 7***
5:00 p.m.	**IMSC 2018 Opening Ceremony** Gianluca Giorgi, Catherine Costello, Rector University of Florence **IMSC 2018 Youth Ceremony** • Nico Nibbering Travel Awards • Italian Chem. Soc., Division of Mass Spectrometry Award and fellowships	***Plenary room*** ***Level 0***
6:00 p.m.	**PL01: Plenary Lecture** **At the intersection between chemistry and art: scientific research for the study and preservation of cultural heritage** ***Marco Leona*** Department of Scientific Research, The Metropolitan Museum of Art, New York, USA	***Plenary room*** ***Level 0***
7:00 p.m.	**Welcome Exhibition & Mixer**	***Exhibition room*** ***Level 0***

MONDAY, August 27th, 2018

8:30-9:15 a.m.	**PL02: Plenary Lecture** *Chair: Ron M. A. Heeren* **Advances in MALDI imaging mass spectrometry: molecular microscopy in the new age of biology and medicine** ***Richard Caprioli*** Depts. of Biochemistry, Chemistry, Pharmacology and Medicine Vanderbilt University School of Medicine, Nashville, USA	***Plenary room*** ***Level 0***
9:15-9:30 a.m.	Break	
9:30-11:30 a.m.	**MOr.01 - Nucleic acids** *Chairs: Daniele Fabris, Giuliana Bianco*	***Plenary room*** ***Level 0***
9:30-10:10 a.m.	**Structures, energetics and reactivity of nucleic acids and their molecular building blocks via tandem MS and computations approaches** *M. T. Rodgers* Wayne State University, Detroit, USA	
10:10-10:30 a.m.	**Tandem mass spectrometric sequencing of isomeric methylnucleosides on RNA toward the understanding of epitranscriptome** *H. Nakayama, Y. Yamauchi, T. Isobe, M. Taoka* RIKEN Center for Sustainable Resource Science, Wako, Japan	
10:30-10:50 a.m.	**TEAD1: Yin and Yang of the cell regulation** *P. Novak, R. Liskova, L. Slavata, J. Cerny, K. Valis* Institute of Microbiology, Laboratory of Structural Biology, Prague, Czech Republic	
10:50-11:10 a.m.	**Hsa-miR-1587 G-quadruplex formation and dimerization induced by NH_4^+, molecular crowding environment and jatrorrhizine derivatives** *W. Tan, L. Yi, Z. Zhu, L. Zhang, J. Zhou, G. Yuan* Peking University, Chemistry, Beijing, China	
11:10-11:30 a.m.	**Biophysical characterization of aptamer-metabolite interactions using ion mobility mass spectrometry** *S. Piccolo, E. Daems, F. Sobott, V. Gabelica* INSERM, CNRS & University of Bordeaux (ARNA laboratory), IECB, Pessac, France	

9:30-11:30 a.m.	**MOr.02 - Clinical proteomics** *Chairs: Giuseppina Maccarrone, Donatella Caruso*	***Room 1*** ***Level 0***
9:30-10:10 a.m.	**Immunoassays in multiplex for biomarker discovery and validation** *T. O. Joos* University of Tubingen, Reutlingen, Germany	
10:10-10:30 a.m.	**Shedding new light on spinal cord injury** *M. Salzet, J. Quanico, M. Karnoub, C. Meriaux, Z. Laouby, F. Rodet, D. Cizkova, I. Fournier, R. Assaker* U1192 Inserm, PRISM Laboratory, University Lille, Villeneuve D'Ascq, France	
10:30-10:50 a.m.	**Multiomic plasma analysis of patients with hepatocellular carcinoma by mass spectrometry** *R. De Oliveira, R. Amaral, T. Da Silva, M. Castro, W. Fontes, C. Ricart, M. De Sousa, M. Eberlin, J. Garcia, A. Martins* University of Brasilia, Laboratory of Biochemistry and Protein Chemistry, Brasilia, Brazil	
10:50-11:10 a.m.	**Identification of proteomic and lipidomic markers in inflammatory bowel diseases by MS-based techniques and multivariate statistical analysis** *E. Robotti, M. Manfredi, E. Conte, E. Barberis, A. Buzzi, V. Caneparo, D. Cecconi, J. Brandi, E. Vanni, S. Landolfo, M. Gariglio, E. Marengo, M. De Andrea* University of Piemonte Orientale, Alessandria, Italy	

11:10-11:30 a.m.	**A novel mass spectrometry based assay for the diagnosis and typing of systemic amyloidosis** *P. Boersema, T. Huang, J. Bijzet, C. Zimmerli, O. Vitek, B. Hazenberg, P. Picotti* ETH Zurich, Institute of Molecular Systems Biology, Zurich, Switzerland

9:30-11:30 a.m.	**MOr.03 - Ion spectroscopy & Photodissociation** *Chairs: Nicolas C. Polfer, Simonetta Fornarini*	***Room 2*** ***Level 0***
9:30-10:10 a.m.	**New frontiers for cryogenic chemistry and optical spectroscopy of mass-selected ions** *M. Johnson* Yale University, Department of Chemistry, New Haven, USA	
10:10-10:30 a.m.	**Structural characterization of ETD product ions using IR ion spectroscopy** *J. Oomens, L. Kempke, J. Martens, G. Berden* Radboud University, FELIX Laboratory, Nijmegen, Netherlands	
10:30-10:50 a.m.	**Structures and photodissociation action spectroscopy of nucleic acid cation radicals** *F. Turecek* University of Washington, Department of Chemistry, Seattle, USA	
10:50-11:10 a.m.	**Photochemistry of glyoxylate embedded in sodium chloride clusters, a laboratory model for tropospheric sea-salt aerosols** *N. K. Bersenkowitsch, M. Oncak, C. van der Linde, A. Herburger, M. K. Beyer* Universität Innsbruck, Ionenphysik und Angewandte Physik, Innsbruck, Austria	
11:10-11:30 a.m.	**Photodissociation spectroscopy of *m/z*-selected functionalised protonated pyridine ions: are some predictive patterns emerging?** *M. Benajmin, M. Samuel, K. Patrick, S. Blanksby, A. Trevitt* University of Wollongong, School of Chemistry, Wollongong, Australia	

9:30-11:30 a.m.	**MOr.04 - Hyphenated techniques** *Chairs: Myeong Hee Moon, Michele Suman*	***Room 3*** ***Level 1***
9:30-10:10 a.m.	**Hyphenation of sampling/sample preparation to mass spectrometry** *J. Pawliszyn* University of Waterloo, Chemistry, Waterloo, Canada	
10:10-10:30 a.m.	**Simultaneous quantification of sixteen polyphenols in 31 legumes by using HPLC-MS/MS Dynamic-MRM triple quadrupole** *G. Caprioli, M. Ricciutelli, S. Vittori, N. F. Kamgang, G. Sagratini* University of Camerino, School of Pharmacy, Camerino, Italy	
10:30-10:50 a.m.	**On-line coupling of Surface Plasmon Resonance to ambient mass spectrometry** *H. Liu, Y. Zhang, X. Li, H. Nie, Y. Bai* Peking University, College of Chemistry and Molecular Engineering, Beijing, China	
10:50-11:10 a.m.	**Online high pressure proteolytic biosensor- mass spectrometry (PROTEX-SPRMS): a new powerful tool for protein epitope and affinity identification and antibody characterization** *L. Lupu, P. Wiegand, Y. Baschung, F. Völklein, A. Lazarev, K. Schmitz, M. Przybylski* Steinbeis Centre for Biopolymer Analysis and Biomedical Mass Spectrom., Rüsselsheim am Main, Germany	
11:10-11:30 a.m.	**Chemical profiling of the human skin surface for malaria vector control using a non-invasive solvent modified sorptive sampler with GC×GC-ToFMS and UPLC-IMS-HRMS** *M. Wooding, T. Dodgen, M. Bouwer, Y. Naudé, E. Rohwer* University of Pretoria, Department of Chemistry, Pretoria, South Africa	

9:30-11:30 a.m.	**MOr.05 - Volatile molecules & nose-space analysis** *Chairs: Egmont Rohwer, Giorgio Mellerio*	***Room 4*** ***Level 1***
9:30-10:10 a.m.	**Exploring food aroma release and perception using direct-injection mass spectrometry** *J. Beauchamp* Fraunhofer Institute for Process Engineering and Packaging IVV, Department of Sensory Analytics, Freising, Germany	
10:10-10:30 a.m.	**High-pressure photoionization time of flight mass spectrometry combined with dynamic purge-injection for rapid analysis of volatile metabolites in urine** *H. Lei, L. Hua, E. Li, H. Li* Dalian Institute of Chemical Physics, Chinese Academy of Sciences, CAS Key Laboratory of Separation Sciences for Analytical Chemistry, Dalian, China	
10:30-10:50 a.m.	**Nose-space of dark chocolates using PTR-ToF-MS and link to flavour perception through simultaneous Temporal Dominance of Sensations (TDS)** *Z. Deuscher, I. Andriot, S. Cordelle, M. Repoux, R. Boulanger, H. Labouré, P. Schlich, J. Le Quéré* INRA, Centre des Sciences du Goût et de l'Alimentation (CSGA), Dijon, France	
10:50-11:10 a.m.	**In nose-space analysis through Proton Transfer Reaction mass spectrometry: investigating variability in flavor release and perception during chewing gum consumption** *M. Pedrotti, I. Khomenko, V. Fogliano, F. Biasioli* Foundation Edmund Mach, Wageneningen University FQD, Wageningen, Netherlands	
11:10-11:30 a.m.	**Methodology for qualitative and quantitative analysis of volatile compounds from composite materials at elevated temperatures** *C. Lourenço, S. Bergin, D. Francis, S. Staines, J. Hodgkinson, C. Walton, J. Saffell, R. Tatam* Cranfield University, School of Aerospace, Transport and Manufacturing, Cranfield, United Kingdom	

11:30 a.m. - 12:30 p.m.	Coffee Break **Poster Sessions MPS-S01 – MPS-S10** *Odd numbered abstracts*	***Exhibition hall*** ***Level 0***

12:30 - 1:45 p.m.	**Lunch Symposia**

BRUKER DALTONICS	**Room 1 – Level 0**
JEOL	**Room 4 – Level 1**
SCIEX	**Room 3 – Level 1**
WATERS	**Room 2 – Level 0**

1:30 - 3:00 p.m.	Coffee Break **Poster Sessions MPS-S01 – MPS-S10** *Even numbered abstracts*	***Exhibition hall*** ***Level 0***

3:00-5:00 p.m.	**MOr.06 - Clinical chemistry** *Chairs: Hugo Rocha, Giancarlo la Marca*	***Plenary room*** ***Level 0***
3:00-3:40 p.m.	**Tandem mass spectrometry in the clinical laboratory: can standardization improve operation?** *M. Pasquali* University of Utah, School of Medicine, Salt Lake City, USA	
3:40-4:00 p.m.	**A combined micro-extraction by packed sorbent-UHPLC-ESI-MS/MS procedure for the analysis of prostanoids and isoprostanoids in dried blood spots of preterm newborns with Patent Ductus Arteriosus** *D. Biagini, S. Antoni, S. Ghimenti, T. Lomonaco, F. G. Bellagambi, A. Cuttano, R. T. Scaramuzzo, M. Ciantelli, F. Di Francesco, R. Fuoco* University of Pisa, Department of Chemistry and Indutrial Chemistry, Pisa, Italy	

4:00-4:20 p.m.	**Profiling of membrane lipids relevant to Alzheimer's disease pathogenesis** *Z. Spacil, E. Cechova, P. Telensky, S. Olkowicz, L. Opalka, K. Sheardova, R. Jancalek, J. Klanova, A. Hampl, J. Damborsky* Masaryk University, Faculty of Science, Research Centre for Toxic Compounds in the Environment, Brno, Czech Republic
4:20-4:40 p.m.	**The use of stable isotopes in the study of albumin metabolism in patients with acute lung disease** *M. Simonato, S. Gianbelluca, L. Vedovelli, M. Dalla, C. Ori, V. Carnielli, P. Cogo* Istituto di Ricerca Pediatrica "Città della Speranza", Padova, Italy
4:40-5:00 p.m.	**Mass-spectrometry approach for rapid intraoperative identification of brain tumor tissues - a way for online analysis** *S. Pekov, V. Eliferov, E. Zhvansky, A. Vorobyev, V. Shurkhay, A. Sorokin, I. Popov, A. Potapov, E. Nikolaev* Moscow Institute of Physics and Technology, Dolgoprudnyj, Russian Federation

3:00-5:00 p.m.	**MOr.07 - Quantitative proteomics** *Chairs: Michael Linscheid, Nathalie Norais*	**Room 1** **Level 0**
3:00-3:40 p.m.	**Drug effects on protein homeostasis** *M. Bantscheff* GSK, Heidelberg, Germany	
3:40-4:00 p.m.	**Measuring nascent proteomics in signaling and cellular differentiation** *A. Burlingame, N. Phillips, C. Forester* UCSF, Pharmaceutical Chemistry, San Francisco, USA	
4:00-4:20 p.m.	**A chemical probe for understanding how proteome foldedness changes under proteostasis stress** *G. Reid, D. Cox, Y. Hong, D. Hatters* University of Melbourne, School of Chemistry, Department of Biochemistry and Molecular Biology, Parkville, Australia	
4:20-4:40 p.m.	**TMT quantification in MS^2 using high field asymmetric waveform ion mobility spectrometry** *P. Sibylle, B. Eric, P. Thibault* Institute for Research in Immunology and Cancer (IRIC), Universite de Montreal, Montreal, Canada	
4:40-5:00 p.m.	**The key to big biobanks: analyzing 24 proteomes per day by micro-flow SWATH® acquisition and Spectronaut Pulsar Analysis** *J. Muntel, N. Morrice, R. Bruderer, L. Reiter* Biognosys AG, R&D, Schlieren, Switzerland	

3:00-5:00 p.m.	**MOr.08 - Chiral discrimination** *Chairs: Anne Zehnacker-Rentien, Maurizio Speranza*	***Room 2*** ***Level 0***
3:00-3:40 p.m.	**Chiral recognition in protonated molecular clusters studied by mass-coupled IR-UV double resonance spectroscopy with cold ion trap** *M. Fujii* Laboratory for Chemistry and Life Science, Institute of Innovative Research, Tokyo Institute of Technology, Tokyo, Japan	
3:40-4:00 p.m.	**A new MS-based hyphenated method for analysis of hexuronic acid epimers and sulfate patterns in glycosaminoglycan oligosaccharides by MS^n coupled to infrared ion spectroscopy** *G. Renois-Predelus, B. Schindler, L. Barnes, S. Chambert, A.-R. Allouche, I. Compagnon* Institut Lumière Matière, Université Claude Bernard Lyon 1, Lyon, France	
4:00-4:20 p.m.	**Chiral discrimination in collision-induced dissociation experiments: a theoretical approach of the cycloPhe-HisH$^+$ system** *A. Pérez-Mellor, R. Spezia* Laboratoire de Chimie Théorique, LCT, Sorbonne Université, CNRS, Paris, France	

4:20-4:40 p.m.	**Enantioselective reduction from quaternary copper D,L amino acid complexes: origin of the weak chiral effect observed with D/L aspartic and glutamic acids** *D. Lesage, S. Alves, E. Darii, J.-C. Tabet* SPI, LEMM, CEA, INRA, Université Paris Saclay, Gif-sur-Yvette, France
4:40-5:00 p.m.	**Direct enantiomer-selective mass spectrometry of multi-component chiral mixtures** *M. H. M. Janssen* MassSpecpec D BV, R&D, Enschede, Netherlands

3:00-5:00 p.m.	**MOr.09 - Ambient MS and new ionization methods** *Chairs: Jentaie Shiea, Pietro Traldi*	***Room 3*** ***Level 1***
3:00-3:40 p.m.	**Breath metabolomics using Secondary Electrospray Ionization (SESI) - high resolution mass spectrometry** *R. Zenobi* ETH Zurich, Zurich, Switzerland	
3:40-4:00 p.m.	**Direct detection of small *n*-alkanes at sub-ppbv level in breath air by photoelectron induced O_2^+ cation chemical ionization mass spectrometry at kPa pressure** *Y. Wang, L. Hua, H. Li* Dalian Institute of Chemical Physics, Chinese Academy of Sciences, CAS Key Laboratory of Separation Sciences for Analytical Chemistry, Dalian, China	
4:00-4:20 p.m.	**Direct coupling of magnetic-particle-based sample preparation strategies to mass spectrometry via microfluidic open interface** *M. Tascon, V. Singh, M. Huq, J. Pawliszyn* University of Waterloo, Chemistry, Waterloo, Canada	
4:20-4:40 p.m.	**Development of the feedback control system for the advanced tapping mode scanning probe electrospray ionization (t-SPESI)** *Y. Otsuka, B. Kamihoriuchi, A. Takeuchi, F. Iwata, T. Matsumoto* Osaka University, Department of Chemistry, Toyonaka, Japan	
4:40-5:00 p.m.	**Direct mass spectrometry analysis using in-capillary ionic liquids-based dispersive liquid-liquid microextraction and sonic-spray ionization** *Q. Ma* Chinese Academy of Inspection and Quarantine, Beijing, China	

3:00-5:00 p.m.	**MOr.10 - Polymers** *Chairs: Marek M. Kowalczuk, Leopoldo Ceraulo*	***Room 4*** ***Level 1***
3:00-3:40 p.m.	**Mass spectrometry methods for the characterization of functional materials** *C. Wesdemiotis* The University of Akron, Departments of Chemistry and Polymer Science, Akron, OH, USA	
3:40-4:00 p.m.	**Unravelling the architecture of branched polyester oligomers by combined trapped ion-mobility spectrometry – tandem mass spectrometry** *R. Voeten, P. van de Bram, J. Jordens, Y. Mengerink, R. Peters, R. Haselberg, P. Schoenmakers, G. W. Somsen* VU Amsterdam, Amsterdam, Netherlands	
4:00-4:20 p.m.	**MS/MS reading of polyurethane barcodes used as taggants in polymeric materials** *S. Poyer, S. Chimjarn, D. Karamessini, J. Lutz, L. Charles* Aix-Marseille Université, Institut de Chimie Radicalaire, Marseille, France	
4:20-4:40 p.m.	**Electrospray ionization mass spectrometry of nonpolar polyisobutylenes** *S. Kéki, L. Nagy, T. Nagy, G. Deák, Á. Kuki, M. Purgel, M. Narmandakh, B. Iván, M. Zsuga* University of Debrecen, Department of Applied Chemistry, Debrecen, Hungary	
4:40-5:00 p.m.	**Analysis of polystyrene based microplastics in the environment** *G. F. Schirinzi, M. Llorca, M. Farré, D. Barcelò* CSIC, IDAEA, Barcelona, Spain	

5:15-7:00 p.m.	**Workshops**	
	WKS-M1 - Mass spectrometry in virology	**ROOM 1 - Level 0**
	WKS-M2 - Police casework - successes and challenges from an academic perspective	**ROOM 2 - Level 0**
	WKS-M3 - Environmental Mass Spectrometry: from trace analysis to effect assessment	**ROOM 3 - Level 1**
	WKS-M4 - Are MS-based methods fit for purpose?	**ROOM 4 - Level 1**

TUESDAY, August 28th, 2018

8:30-9:15 a.m.	**Thomson Medal Award Ceremony** *Chair: Catherine E. Costello* **PL03: Plenary Lecture: THOMSON MEDALIST** **Gaining weight in mass spectrometry. From analyzing electrons to intact molecular machineries** ***Albert J. R. Heck*** Netherlands Proteomics Centre, Utrecht University, The Netherlands	***Plenary room*** ***Level 0***
9:15-9:30 a.m.	Break	
9:30-11:30 a.m.	**TOr.01 - Therapeutic drug monitoring and drug discovery** *Chairs: Gérard Hopfgartner, Fabio Garofolo*	***Plenary room*** ***Level 0***
9:30-10:10 a.m.	**Therapeutic drug monitoring and drug discovery: is it all known or are we innovative and game changing?** *R. M.A. Heeren, F. Cuyckens, R. J. Vreeken* Janssen R&D, Beerse, Belgium	
10:10-10:30 a.m.	**A highly selective and sensitive LC-MS/HRMS assay for Coporporphyrin-I and –III, emerging endogenous biomarkers of OATP, in first-in-human clinical trials** *R. Ramanathan* Pfizer, Inc, Medicine Design, Groton, USA	
10:30-10:50 a.m.	**Development of an ex vivo solid-phase microextraction calibration model towards in vivo quantitation of doxorubicin in lungs during a novel chemotherapeutic procedure** *A. Roszkowska, M. Tascon, B. Bojko, K. Gorynski, R. G. A. Gomez, N. Looby, S. P. Reck Dos, M. Cypel, J. Pawliszyn* University of Waterloo, Department of Chemistry, Waterloo, Canada	
10:50-11:10 a.m.	**Characterization of paclitaxel metabolites by UHPLC-MS/MS: biomedical application of the study in targeted drug delivery systems** *C. Sottani, E. Grignani, E. Studioso, D. Cottica* Istituti Clinici Scientifici - Maugeri, Environmental Research Center, Pavia, Italy	
11:10-11:30 a.m.	**The effects of low temperature storage on the structure of Herceptin®: to freeze, or not to freeze: that is the question** *R. Upton, K. Pacholarz, D. Firth, S. Estdale, P. Barran* Manchester Institute of Biotechnology, University of Manchester, Manchester, United Kingdom	

9:30-11:30 a.m.	**TOr.02 - Single cell** *Chairs: Peter Nemes, Giuliana Bianco*	***Room 1*** ***Level 0***
9:30-10:10 a.m.	**Single cell mass spectrometry: from qualitative to quantitative studies** *Z. Yang* University of Oklahoma, Department of Chemistry and Biochemistry, Norman, USA	
10:10-10:30 a.m.	**Analysis of single mammalian cells with SCoPE-MS with mPOP** *H. Specht, G. Harmange, D. Perlman, J. Neveu, C. Adams, N. Slavov, B. Budnik* Harvard University, FAS Division of Science, Cambridge, USA	
10:30-10:50 a.m.	**LiveCell MS methodology in the context of drug discovery** *C. Newman, A. West* The University of Nottingham, School of Pharmacy, Nottingham, United Kingdom	
10:50-11:10 a.m.	**In situ mass spectrometry unravels metabolic differences between cells of the live vertebrate embryo (Xenopus laevis)** *E. Portero, S. Moody, P. Nemes* University of Maryland, Chemistry and Biochemistry, College Park, USA	
11:10-11:30 a.m.	**A ToF-SIMS tandem MS Imaging method to probe the composition of cellular organelles** *G. L. Fisher, C. E. Chini, B. Johnson, M. M. Tamkun, M. L. Kraft* Physical Electronics, Marketing & Applications, Chanhassen, USA	

9:30-11:30 a.m.	**TOr.03 - Noncovalent interactions** *Chairs: Renato Zenobi, Francesco De Angelis*	***Room 2*** ***Level 0***
9:30-10:10 a.m.	**Membrane proteins - the lipid connection** *C. Robinson* University of Oxford, Physical and Theoretical Chemistry Laboratory, United Kingdom	
10:10-10:30 a.m.	**Aryl bis-sulfonamides bind to the active site of a homotrimeric isoprenoid biosynthesis enzyme IspF and extract the essential divalent metal cation cofactor** *K. Root, K. Barylyuk, A. Schwab, J. Thelemann, B. Illarionov, M. Fischer, F. Diederich, R. Zenobi* ETH zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland	
10:30-10:50 a.m.	**Native MS of noncovalent RNA: protein complexes** *V. Wysocki* Dept of Chemistry and Biochemistry, Ohio State University, USA	
10:50-11:10 a.m.	**Exploring the inhibition mechanisms of amyloid protofibrils using Fourier Transform Ion Cyclotron Resonance-Mass Spectrometry (FTICR-MS)** *Y. P. Y. Lam, C. K. C. Chiu, C. A. Wootton, J-I. Song, M. Li, I. Hands-Portman, M. P. Barrow, P. B. O'Connor* University of Warwick, Department of Chemistry, Coventry, United Kingdom	
11:10-11:30 a.m.	**Different means of solubilization of membrane proteins for native MS** *N. Morgner, O. Peetz* Frankfurt University, Physical Chemistry, Frankfurt, Germany	

9:30-11:30 a.m.	**TOr.04 - High resolution MS: instrumentation, methods & applications** *Chairs: Evgeny Nikolaev, Gianluca Giorgi*	***Room 3*** ***Level 1***
9:30-10:10 a.m.	**Life at the frontier: 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometry** *A. Marshall, P. M. L. Chacon, Y. E. Corilo, C. L. Hendrickson, L. He, S. F. Niles, J. C. Putman, S. M. Rowland, D. F. Smith, R. L. Ware, C. R. Weisbrod, R. P. Rodgers* Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, USA	
10:10-10:30 a.m.	**Bridging the gap between images and molecules: Parallel acquisition of FTMS mass spectrometry imaging and MS/MS data coupled with automated and high confidence lipid identifications** *S. Ellis, M. Paine, G. Eijkel, J. Pauling, P. Husen, M. Jervelund, M. Hermansson, C. Ejsing, R. M. A. Heeren* Maastricht University, The Maastricht Multimodal Molecular Imaging Institute (M4I), Maastricht, Netherlands	

10:30-10:50 a.m.	**Large-scale ring trial metabolomics study of human blood plasma using diverse FT-ICR-MS systems** *S. Forcisi, F. Moritz, B. Kanawati, J. Uhl, C. Thompson, A. Barsch, G. Kruppa, M. Easterling, T. Ring, P. Schmitt-Kopplin* Helmholtz Zentrum München, Research Unit Analytical BioGeoChemistry, Neuherberg, Germany	
10:50-11:10 a.m.	**Single cell metabolomics with LAESI-21T-FTICR-MS** *L. Pasa-Tolic, C. R. Anderton, D. Veličković, S. Stopka, L. Samarah, R. Khattar, J. Shaw, B. Agtuca, G. Stacey, A. Vertes* Pacific Northwest National Lab, Environmental Molecular Sciences Lab, Richland, USA	
11:10-11:30 a.m.	**Comprehensive high-resolution mass spectrometric evolved gas analysis in the context of petroleomics: analysis of bitumen, heavy crude oils and asphaltenes** *C. Rüger, A. Neumann, C. Grimmer, U. Käfer, M. Sklorz, T. Gröger, T. Streibel, R. Zimmermann* University of Rostock, Institute of Chemistry, Rostock, Germany	

9:30-11:30 a.m.	**TOr.05 - MS imaging: instrumentation** *Chairs: Liam McDonnell, Fulvio Magni*	***Room 4 Level 1***
9:30-10:10 a.m.	**Molecular imaging at the interface of health and disease** *R. M. A. Heeren* M4I, The Maastricht MultiModal Molecular Imaging institute, Maastricht University, Maastricht, The Netherlands	
10:10-10:30 a.m.	**Novel hyperspectral Imaging Mass Spectrometry to delineate Amyloid polymorphism** *J. Hanrieder* University of Gothenburg, Department of Neuroscience and Physiology, Gothenburg, Sweden	
10:30-10:50 a.m.	**Validation studies of phosphopeptide enrichment procedures using TiO_2-attached membrane funnel-based spray ionization for Imaging Mass Spectrometry** *Y.-L. W. Hung, C. T.-W. Dominic* The Chinese University of Hong Kong, Chemistry Department, Hong Kong, Hong Kong	
10:50-11:10 a.m.	**Infrared Laser Ablation Microsampling coupled with MALDI imaging** *K. Murray, F. Donnarumma, K. Wang, T. Solouki, M. Pettit* Louisiana State University, Department of Chemistry, Baton Rouge, USA	
11:10-11:30 a.m.	**Pulsed cold plasma for post-ionization in MALDI-MS imaging** *J. Soltwisch, U. Röhling, K. Dreisewerd* University of Münster, Institute for Hygiene, Münster, Germany	

11:30 a.m. - 12:30 p.m.	Coffee Break **Poster Sessions TPS-S01 – TPS-S10** *Odd numbered abstracts*	***Exhibition hall Level 0***

12:30 - 1:45 p.m.	**Lunch Symposia**	
	AGILENT TECHNOLOGIES	**Room 2 – Level 0**
	BRUKER DALTONICS	**Room 1 – Level 0**
	SCIEX	**Room 3 – Level 1**
	THERMO FISHER SCIENTIFIC	**Room 4 – Level 1**

1:30 - 3:00 p.m.	Coffee Break **Poster Sessions TPS-S01 – TPS-S10** *Even numbered abstracts*	***Exhibition hall Level 0***

3:00-5:00 p.m.	**TOr.06 - Post Translational Modifications** *Chairs: Joseph A. Loo, Fulvio Magni*	***Plenary room Level 0***
3:00-3:40 p.m.	**Rapid, sensitive and quantitative phosphoproteomics for large-scale cell perturbation analysis** *J. Olsen* University of Copenhagen, Faculty of Health and Medical Sciences, Denmark	
3:40-4:00 p.m.	**Comprehensive NISTmAb reference spectral libraries for reliable and robust identification of post-translational modifications in human and recombinant IgG antibodies** *Q. Dong, Y. Liang, X. Yan, S. Markey, Y. Mirokhin, D. Tchekhovskoi, T. Bukhari, S. Stein* National Institute of Standards and Technology, Bimolecular Measurement Division, Gaithersburg, USA	
4:00-4:20 p.m.	**SEAGal: the method to fish for uncommon phosphorylations** *V. Gorshkov, Y. Palarasah, K. Skjødt, F. Kjeldsen* University of Southern Denmark, Department of Biochemistry and Molecular Biology, Odense, Denmark	
4:20-4:40 p.m.	**Proteome-wide effects of singlet oxygen produced by next generation Iridium anti-cancer metallodrugs** *C. K. C. Chiu, P. Zhang, Y. P. Y. Lam, C. A.Wootton, M. P. Barrow, P. J. Sadler, P. B. O'Connor* University of Warwick, Department of Chemistry, Coventry, United Kingdom	
4:40-5:00 p.m.	**Polyamine modifications in diatom biosilica proteomes** *A. Milentyev, C. Heintze, N. Poulsen, N. Kroeger, A. Shevchenko* Max Planck Institute of Molecular Cell Biology and Genetics, Shevchenko Lab, Dresden, Germany	

3:00-5:00 p.m.	**TOr.07 - Mass spectrometric analysis of forensic science evidence** *Chairs: Simona Francese, Gloriano Moneti*	***Room 1 Level 0***
3:00-3:40 p.m.	**Extended mass spectrometry workflow for the analysis of drugs of abuse in biological fluids and tissues** *G. Hopfgartner* University of Geneva, Life Sciences Mass Spectrometry, Switzerland	
3:40-4:00 p.m.	**The death of Thomas Chatterton - an LC-MS^n investigation** *P. Gates* University of Bristol, School of Chemistry, Bristol, United Kingdom	
4:00-4:20 p.m.	**Class identification of novel psychoactive substances using mass spectral library searching with hierarchical clustering** *A. Moorthy, W. Wallace, A. Kearsley, D. Tchekhovskoi, S. Stein* National Institute of Standards and Technology, Mass Spectrometry Data Center, Gaithersburg, USA	
4:20-4:40 p.m.	**Identifying wood from protected species with DART fingerprint spectra and the software platform OMFF** *S. Martínez-Jarquín, C. Lancaster, E. Espinoza, R. Winkler* CINVESTAV, Biochemistry and Biotechnology, Irapuato, Mexico	
4:40-5:00 p.m.	**Green forensics - isotopic traceability in horticulture. Geographical origin of roses** *E. De Rijke, M. Trisna, S. Verdegaal, R. Magnússon, J. Schoorl, C. Cerli, C. De Koster* University of Amsterdam, Institute for Biodiversity and Ecosystem Dynamics, Amsterdam, Netherlands	

3:00-5:00 p.m.	**TOr.08 - Ion activation and dissociations** *Chairs: Vicki Wysocki, Gianluca Giorgi*	***Room 2 Level 0***
3:00-3:40 p.m.	**Understanding fragmentation of complex ions using Surface-Induced Dissociation experiments** *J. Laskin* Purdue University, Dept. of Chemistry, West Lafayette, USA	

3:40-4:00 p.m.	**Investigation of hemicryptophane host-guest binding energies using advanced tandem mass spectrometry** *P. Bayat, D. Gatineau, D. Lesage, V. Robert, A. Martinez, R. B. Cole* Sorbonne Université, IPCM, Paris, France
4:00-4:20 p.m.	**Tandem ToF mass spectrometry of biomolecules: from dual stage to curved field and parabolic analyzers as second stage** *E. Pittenauer, G. Allmaier* TU Wien, Institute of Chemical Technologies and Analytics, Wien, Austria
4:20-4:40 p.m.	**Specific radical-driven dissociation of hydrogen-excess and -deficient radical peptides produced by MALDI in-source decay mass spectrometry** *M. Takayama* Yokohama City University, Graduate School of Nanobioscience, Yokohama, Japan
4:40-5:00 p.m.	**Juggling fragile van der Waals complexes in an ion trap for multiplexed infrared photodissociation** *L. Tesler, M. Bell, T. Harmon, L. Bailey, N. Polfer* University of Florida, Dept. of Chemistry, Gainesville, USA

3:00-5:00 p.m.	**TOr.09 - Metal and non-metal clusters: gas phase structures and reactivity** *Chairs: Evan Williams, Pietro Traldi*	***Room 3*** ***Level 1***
3:00-3:40 p.m.	**Tandem cryo ion trap mass spectrometry for kinetics and spectroscopy of transition metal clusters** *G. Niedner-Schatteburg* FachbereichChemie and Forschungszentrum OPTIMAS, TU Kaiserslautern, Kaiserslautern, Germany	
3:40-4:00 p.m.	**UV-VIS spectroscopy and photochemistry of trapped ions using FT-ICR-MS** *C. Van der Linde, M. Oncák, N. K. Bersenkowitsch, A. Herburger, T. Taxer, M. K. Beyer* Universität Innsbruck, Institut für Ionenphysik und Angewandte Physik, Innsbruck, Austria	
4:00-4:20 p.m.	**ESI in the study of the interactions between phosphino-Cu(I) complexes and Cu(II) salts with model peptides relevant to human copper transporters (hCTR)** *F. Tisato, K. Bossak-Ahmed, M. Porchia, W. Bal, A. Bonna* ICMATE – CNR, Padova, Italy	
4:20-4:40 p.m.	**Structure and reactivity of antimonato polyoxovanates in solution and in the gas phase** *U. Warzok, L. K. Mahnke, M. Wendt, W. Bensch, C. A. Schalley* Free University Berlin, Institute for Chemistry and Biochemistry, Berlin, Germany	
4:40-5:00 p.m.	**FT-ICR MS studies of thiomolybdate clusters as model catalysts for hydrogen evolution** *A. Baloglou, M. Oncák, C. Van der Linde, M. Grutza, P. Kurz, M. K. Beyer* Universität Innsbruck, Institut für Ionenphysik und Angewandte Physik, Innsbruck, Austria	

3:00-5:00 p.m.	**TOr.10 – Astrochemistry** *Chairs: Paul Mayer, Simonetta Fornarini*	***Room 4*** ***Level 1***
3:00-3:40 p.m.	**Cosmic PAHs: formation and UV processing** *C. Joblin* University Toulouse / CNRS, Toulose, France	
3:40-4:00 p.m.	**Relaxation and fragmentation dynamics of polycyclic aromatic hydrocarbons excited by an ultrashort XUV pulse** *M. Herve, P. Castellanos, G. Karras, V. Despre, A. Marciniak, E. Constant, V. Loriot, A. Kuleff, A. Tielens, F. Lepine* Université Lyon 1, Institut Lumière Matière (ILM), Lyon, France	
4:00-4:20 p.m.	**Experimental study of high-energy ion/molecule interactions relevant to planetary atmospheres** *V. Krizova, J. Zabka, I. Zymak, M. Polasek* Charles University in Prague, Faculty of Science, Prague, Czech Republic	

4:20-4:40 p.m.	**Investigating the possibility of forming prebiotic molecules by gas phase ion-molecule reactions. Application to glycine** *R. Spezia, Y. Jeanvoine, A. Largo, W. L. Hase, J. Lemaire, D. Scuderi* CNRS, Sorbonne Université, Laboratoire de Chimie Théorique, Paris, France
4:40-5:00 p.m.	**The threshold displacement energy of Buckminsterfullerene C60 and formation of the endohedral defect Fullerene He@C59** *M. Stockett, M. Wolf, M. Gatchell, H. Schmidt, H. Zettergren, H. Cederquist* Stockholm University, Department of Physics, Stockholm, Sweden

5:15-7:00 p.m.	**Workshops**		
	WKS-T1 -	**Careers in Mass Spectrometry**	**ROOM 1 - Level 0**
	WKS-T2 -	**Transforming Drug Discovery and Clinical Biomarker Bioanalysis: It's Time for a Paradigm Shift from SRM to HRMS**	**ROOM 2 - Level 0**
	WKS-T3 -	**Integration of native MS with structural biology methods**	**ROOM 3 - Level 1**

WEDNESDAY, August 29th, 2018

8:30-9:15 a.m.	**CURT BRUNNÉE AWARD Ceremony** *Chair: Scott A. McLuckey* **PL04: Plenary Lecture** **Lithographically patterned electrodes for miniaturized ion trap mass spectrometers and other ion optics devices** ***Daniel E. Austin*** Brigham Young University, Department of Chemistry and Biochemistry and Department of Electrical and Computer Engineering, Provo, USA	***Plenary room*** ***Level 0***
9:15-9:30 a.m.	Break	
9:30-11:30 a.m.	**WOr.01 - Native MS and structural proteomics** *Chairs: Frank Sobott, Nathalie Norais*	***Plenary room*** ***Level 0***
9:30-10:10 a.m.	**Native mass spectrometry: a technique of many faces** *M. Sharon, G. Ben-Nissan, S. Vimer, J. Cveticanin* Weizmann Institute of Science, Department of Biomolecular Sciences, Rehovot, Israel	
10:10-10:30 a.m.	**Native Mass Spectrometry reveal functioning mechanism of membrane protein translocation pathway** *S. Mehmood, M. McDowell, I. Sinning, C. Robinson* University of Oxford, Department of Chemistry, Oxford, United Kingdom	
10:30-10:50 a.m.	**Charge-independent mass spectrometry of single virus capsids above 100MDa with nanomechanical resonators** *C. Masselon, S. Hentz, S. Dominguez-Medina, S. Fostner, M. Halim, M. Defoort, E. Vernhes, P. Boulanger* CEA, DRF/BIG/Large Scale Biology Laboratory, Grenoble, France	
10:50-11:10 a.m.	**A cross-linking/mass spectrometry workflow based on MS-cleavable cross-linkers and the MeroX software for mapping protein-protein interactions** *C. Iacobucci, M. Götze, A. Sinz* Martin-Luther-Universität Halle-Wittenberg, Institut für Pharmazie, Halle, Germany	

11:10-11:30 a.m.	**Can we use HDX-MS to model protein conformations?** *A. Borysik* King's College London, Chemistry, London, United Kingdom

9:30-11:30 a.m.	**WOr.02 - JMS Award Symposium** *Chairs: Richard Caprioli, John Langley*	***Room 1*** ***Level 0***
9:30-9:50 a.m.	Presentation of the JMS Award Symposium	
9:50-10:10 a.m.	**Anion formation in MALDI depends on matrix and target plate material choice** *G. P. Zeegers, R. Zenobi* ETH Zürich, Chemistry and Applied Biosciences, Zürich, Switzerland	
10:10-10:30 a.m.	**Combining bio-conjugation and matrix-assisted laser desorption ionisation mass spectrometry for biomolecule detection and localisation in tissues** *K. Stevens, P. Mittal, A. Abell, T. Pukala* University of Adelaide, Physical Sciences, Adelaide, Australia	
10:30-10:50 a.m.	**Histology-directed proteomics: combining autofluorescence guided micro-digestions with liquid surface extractions** *D. Ryan, N. Patterson, J. Moore, J. Spraggins, R. Caprioli* Vanderbilt University, Department of Chemistry, Nashville, USA	
10:50-11:10 a.m.	**Dual microprobe CE-ESI-HRMS for the characterization of proteins and metabolites in single embryonic cells of live frog embryos** *C. Lombard-Banek, R. Onjiko, S. Moody, P. Nemes* Univeristy of Maryland, Chemistry & Biochemistry, College Park, USA	
11:10-11:30 a.m.	**Wastewater-based epidemiology: use of adulterants to estimate cocaine consumption patterns in Brasília, Brazil by LC-QToF-MS** *K. M. Da Silva, A. O. Maldaner, S. F. Fabriz* Instituto de Química, Universidade de Brasília, Brasília, Brazil	

9:30-11:30 a.m.	**WOr.03 - Reaction mechanisms and elusive intermediates** *Chairs: Scott A. McLuckey, Francesco De Angelis*	***Room 2*** ***Level 0***
9:30-10:10 a.m.	**Elucidating the chemistry of elusive gas phase radicals using distonic radical ions: Trying to get a good deal from a Faustian bargain** *S. Blanksby, D. L. Marshall, B. L. J. Poad, A. J. Trevitt* Central Analytical Research Facility (CARF), Institute for Future Environments, Queensland University of Technology, Brisbane, Australia	
10:10-10:30 a.m.	**Acetone as photo-initiator for disulfide reduction – Application to structural analysis of disulfide rich peptides and proteins** *Y. Xia, S. Adhikari, X. Yang* Tsinghua University, Chemistry, Beijing, China	
10:30-10:50 a.m.	**Kinetics of a click reaction in charged microdroplets with Time Resolved Reactive Laser Ablation Electrospray Ionization Mass Spectrometry** *F. van Geenen, S. Gangarapu, M. Franssen, M.W.F. Nielen, H. Zuilhof* Wageningen University, Laboratory of Organic Chemistry, Wageningen, Netherlands	
10:50-11:10 a.m.	**Amino-acids oxidation: a combined study of cysteine oxo-forms by mass spectrometry, IRMPD spectroscopy and simulations** *D. Scuderi, E. Bodo, S. Fornarini, B. Chiavarino, M. Crestoni, V. Macaluo, R. Spezia* Laboratoire de Chimie Physique, UMR 8000, Université Paris Sud, Orsay, France	
11:10-11:30 a.m.	**Loss of water from polyglycines and their [bn]+ ions; imidazolones and oxazolones** *K. H. B. Lam, J. K.-C. Lau, C.-K. Lai, I. K. Chu, J. Oomens, A. C. Hopkinson, K. W. M. Siu* University of Windsor, Department of Chemistry and Biochemistry, Windsor, Canada	

9:30-11:30 a.m.	**WOr.04 – Pharmaceuticals** *Chairs: Christine Eckers, Gianluca Bartolucci*	***Room 3*** ***Level 1***
9:30-10:10 a.m.	**Pharmaceutical Industry Challenges with Mass Spectrometry Solutions: from Microsampling to Monoclonal Antibodies** *W. Korfmacher* Sanofi, Drug Metabolism & Pharmacokinetics, Waltham, USA	
10:10-10:30 a.m.	**Impact of centroiding and differences in data processing on quantification using high-resolution mass spectrometry** *L. Vereyken, L. Dillen, R. Vreeken, F. Cuyckens* Janssen R&D, Discovery Sciences, Beerse, Belgium	
10:30-10:50 a.m.	**LC-ICP-MS as an alternative to radioactivity in pharmacology** *C. Enjalbal, E. Cordeau, G. Subra, D. Gagne, N. Prache, C. Arnaudguilhem, B. Bouyssiere* IBMM, University of Montpellier, Montpellier, France	
10:50-11:10 a.m.	**Sub-ppm detection and identification of in-vivo metabolites of an antibody-drug conjugate by data-independent HPLC-High-Resolution tandem MS** *A. Triolo, E. Ciuti, C. Carboni, V. Chirulli* Menarini Ricerche, Firenze, Italy	
11:10-11:30 a.m.	**New QC identity testing for acellular pertussis combination vaccines using LC-MS** *H. Zhang, R. Maharajh, S. Vydelingum, L. Yin* Sanofi Pasteur, Analytical Process and Technology, Toronto, Canada	

9:30-11:30 a.m.	**WOr.05. - Food integrity, authenticity & traceability** *Chairs: Ruud Peters, Michele Suman*	***Room 4*** ***Level 1***
9:30-10:10 a.m.	**A story on food, faith and fraud – detection of the fakes** *S. van Ruth* Wageningen University and Research, Wageningen, The Netherlands	
10:10-10:30 a.m.	**Detecting food fraud: determination of a potato´s variety and its geographical origin in one analysis via UPLC-IMS-QToF** *C. Claassen, J. Kuballa, S. Rohn* GALAB Laboratories GmbH, University of Hamburg, Hamburg, Germany	
10:30-10:50 a.m.	**Nosespace analysis by PTR-ToF-MS for the extravirgin olive oil characterization** *I. Khomenko, E. Aprea, F. Gasperi* Edmund Mach Foundation, Food quality and nutrition, San Michele all'Adige, Italy	
10:50-11:10 a.m.	**Ultra-fast identification of fish species by paperspray coupled to a benchtop Orbitrap mass spectrometer** *D. Lopez-Ferrer, G. Foster, M. Prieto* Thermo Fisher Scientific, San Jose, USA	
11:10-11:30 a.m.	**Characterization and classification of Spanish paprika with protected designation of origin by UHPLC-HRMS polyphenolic fingerprinting and chemometrics** *S. Barbosa, G. Campmajó, O. Núñez, J. Saurina, L. Puignou* University of Barcelona, Department of Chemical Engineering and Analytical Chemistry, Barcelona, Spain	

11:30 a.m. - 12:30 p.m.	Coffee Break **Poster Sessions WPS-S01 – WPS-S10** *Odd numbered abstracts*	***Exhibition hall*** ***Level 0***

12:30 - 1:45 p.m.	**Lunch Symposia**	
	AGILENT TECHNOLOGIES	**Room 2 – Level 0**
	BIOGNOSYS	**Room 3 – Level 1**
	PERKINELMER	**Room 1 – Level 0**
	THERMO FISHER SCIENTIFIC	**Room 4 – Level 1**

1:30 - 3:00 p.m.	Coffee Break **Poster Sessions WPS-S01 – WPS-S10** *Even numbered abstracts*	***Exhibition hall Level 0***

3:00-5:00 p.m.	**WOr.06 - MS tools in doping & toxicology** *Chairs: Mario Thevis, Gianluca Bartolucci*	***Plenary room Level 0***
3:00-3:40 p.m.	**Evolution and application of mass spectrometry–based analytical methods in anti-doping analyses** *T. Kuuranne* Swiss Laboratory for Doping Analyses, University Center of Legal Medicine Geneva and Lausanne, Centre Hospitalier Universitaire Vaudois and University of Lausanne, Lausanne, Switzerland	
3:40-4:00 p.m.	**LC-HRMS/MS vs. LC-MRM: screening of covalent drug-protein adducts** *T. Geib, L. Sleno* Université du Québec à Montréal, Chemistry Department, Montréal, Canada	
4:00-4:20 p.m.	**Coupling mass spectrometry and chemometrics for structural characterization of androgenic anabolic steroids** *P. Leogrande, T. De La, F. Botrè, D. Jardines, F. Marini* "Sapienza" Università di Roma, Dipartimento di Chimica; Lab. Antidoping, Federazione Medico Sportiva Italiana, Rome, Italy	
4:20-4:40 p.m.	**Detection of chemical warfare agents-related phenylarsenic compounds in marine biota and identification of their metabolites in in vitro studies by Orbitrap HRMS** *H. Niemikoski, D. Koske, P. Vanninen* Finnish Institute of Verification of Chemical Weapon Convention, University of Helsinki, Helsinki, Finland	
4:40-5:00 p.m.	**A fit-for-purpose UHPLC-MS/MS method for routine screening of SARM residues in bovine and equine serum** *E. Ventura, A. Gadaj, T. Buckley, M. H. Mooney* Institute for Global Food Security, Queen's University Belfast, School of Biological Sciences, Belfast, United Kingdom	

3:00-5:00 p.m.	**WOr.07 - MS imaging: applications** *Chairs: Martina Marchetti-Deschmann, Fulvio Magni*	***Room 1 Level 0***
3:00-3:40 p.m.	**Combining mass spectrometry imaging & microproteomics to investigate intratumor heterogeneity** *L. McDonnell* Leiden University Medical Center, Leiden, Netherlands	
3:40-4:00 p.m.	**Multisite multimodal mass spectrometry imaging of genetically engineered mouse models containing mutations linked to bowel cancer** *C. J. Nikula, R. T. Steven, E. A. Elia, A. D. Campbell, S. A. Thomas, A. Dexter, T. Murta, S. Ling, A. K. Najumudeen, A. J. Taylor, J.-L. Vorng, G. Hamm, R. Havelund, R. Filipe-Soares, D. Gay, B. Yan, A. Al-Afeef, T. Fu, R. Philip, K. N. Robinson, S. Barry, K. Brindle, I. S. Gilmore, R. J. A. Goodwin, J. F. Marshall, G. Poulogiannis, Z. Takats, M. O. Yuneva, O. J. Sansom, J. Bunch* National Physical Laboratory, NiCE-MSI, Teddington, United Kingdom	
4:00-4:20 p.m.	**Can 3D MALDI-MS Imaging be the missing piece for understanding the traumatic brain injury puzzle?** *K. Mallah, J. Quanico, F. Kobeissy, K. Zibara, M. Salzet, I. Fournier* INSERM, U1192 - Laboratoire Protéomique, Réponse Inflammatoire et Spectrométrie de Masse (PRISM), Université de Lille, Department of Biology, Lille, France	
4:20-4:40 p.m.	**DLEMMA-MS-imaging for identification of spatially localized metabolites and metabolic network map reconstruction** *Y. Dong, L. Feldberg, U. Heinig, I. Rogachev, A. Aharoni* Weizmann Institute of Science, Weizmann Institute of Science, Rehovot, Israel	

4:40-5:00 p.m.	**Silver-doped nano-DESI MSI for prostaglandin imaging** *K. Duncan, R. Fang, J. Yuan, R. Chu, S. K. Dey, K. Burnum-Johnson, I. Lanekoff* Uppsala University, Dept of Chemistry-BMC, Uppsala, Sweden	

3:00-5:00 p.m.	**WOr.08 - Gas phase ion chemistry & thermochemistry** *Chairs:* Pan Yanjiang, Giovanni Sindona	***Room 2*** ***Level 0***
3:00-3:40 p.m.	**Progress towards enzyme-like specificity in protein fragmentation** *S. A. Mcluckey, D. J. Foreman* Purdue University, Department of Chemistry, West Lafayette, USA	
3:40-4:00 p.m.	**Dissociation of hydrogen-abundant peptide radical formed by hydrogen attachment in gas phase** *D. Asakawa, H. Takahashi, S. Iwamoto, K. Tanaka, K. Kamiya* AIST, Research Institute for Measurement and Analytical Instrumentation, Tsukuba, Japan	
4:00-4:20 p.m.	**One-electron reduction of isolated metallo-supramolecular aggregates** *M. Engeser* Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Bonn, Germany	
4:20-4:40 p.m.	**Reaction dynamics of ionized 1-methylpyrene: why is the 1-methylenepyrene ion formed from H atom loss and not a tropylium-containing ion?** *P. Mayer, B. West, B. Lowe* University of Ottawa, Dept. of Chemistry and Biomolecular Sciences, Ottawa, Canada	
4:40-5:00 p.m.	**Highly charged protein ions: The strongest acids to date** *M. Zenaidee, W. Donald* UNSW, School of Chemistry, Sydney, Australia	

3:00-5:00 p.m.	**WOr.09 - FTMS and innovative methods for (bio)analyses** *Chairs: Ljiljana Pasa-Tolic, Giuliana Bianco*	***Room 3*** ***Level 1***
3:00-3:40 p.m.	**Mative top-down Fourier Transform mass spectrometry of proteins and protein complexes as a tool for structural biology and drug development** *J. A. Loo, H. Li, W. Jung, C. Lantz, M. Nshanian* University of California-Los Angeles (UCLA), Los Angeles, USA	
3:40-4:00 p.m.	**Advances in Orbitrap instrumentation for analysis of high-mass proteins and protein complexes** *A. Makarov, E. Damoc, E. Denisov, K. Fort, M. van de Waterbeemd, D. Boll, D. Grinfeld, M. Reinhardt-Szyba, M. Belov, A. Heck* Thermo Fisher Scientific, Bremen, Germany	
4:00-4:20 p.m.	**Ion traps with quadratic potentials in Fourier transform based mass spectrometry. Harmonized multi-electrode Kingdon traps and FT ICR cell** *E. Nikolaev, G. Vladimirov, O. Kharybin, V. Fernando, A. Fursova, Z. Sun, M. Sudakov, A. Lioznov* Skolkovo Institute of Science and Technology, Transnational Medicine and Space, Moscow, Russian Federation	
4:20-4:40 p.m.	**The next dimension in proteomics** *P.Y.Y. Lam, P. B. O'Connor* University of Warwick, Department of Chemistry, Coventry, United Kingdom	
4:40-5:00 p.m.	**Ultra-high resolution Orbitrap FTMS: implementation and applications** *Y. Tsybin, K. Nagornov, D. Kilgour, N. Gasilova, L. Menin* Spectroswiss, Biomolecular Mass Spectrometry, Lausanne, Switzerland	

3:00-5:00 p.m.	**WOr.10 - Food additives and contaminants** *Chairs: Jose Diana Di Mavungu, Roberta Galarini*	***Room 4*** ***Level 1***
3:00-3:40 p.m.	**Direct food analysis by (transportable) ambient ionization mass spectrometry** *M. W. F. Nielen, M. Blokland, A. Gerssen, M. van Dam, G. A. Gómez-Ríos, J. Pawliszyn* Wageningen University & Research, Wageningen, The Netherlands	

3:40-4:00 p.m.	**Gum arabic characterisation and its detection in wine using high resolution mass spectrometry** *T. Nardin, G. Ferrari, R. Larcher* Fondazione E. Mach, CTT, San Michele all'Adige, Italy
4:00-4:20 p.m.	**The fragmentation behaviour of pyrrolizidine alkaloids and its implications on food analysis** *C. Czerwenka* Austrian Agency for Health and Food Safety, Group for Contaminant and Special Analysis, Wien, Austria
4:20-4:40 p.m.	**Validation of an accurate mass screening method for pesticide residue analysis in cocoa beans and evaluation of collision cross section values using ion mobility QToF mass spectrometry** *B. H. Zainudin, S. Salleh* Malaysian Cocoa Board, Cocoa Downstream Technology Division, Nilai, Malaysia
4:40-5:00 p.m.	**The sweet deal of adding ion mobility to full scan acquisitions to profile steviol glycosides knowns and known-unknowns in food matrices** *S. Goscinny, M. Herman, W. Van Hoeck, M. McCullagh* Sciensano, Organic Contaminants and Additives, Brussels, Belgium

5:15-7:00 p.m.	**Workshops**		
	WKS-W1 -	**MS-Based Techniques for the Characterization of Nanomaterials in Food, Biological and Other Complex Matrices**	**ROOM 1 - Level 0**
	WKS-W2 -	**Mass spectrometry in Microbiology**	**ROOM 2 - Level 0**
	WKS-W3 -	**Advances in Protein Structure Analysis with Mass Spectrometry**	**ROOM 3 - Level 1**
	WKS-W4 -	**The EU_FT-ICR_MS network**	**ROOM 4 - Level 1**

THURSDAY, August 30th, 2018

8:30-9:15 a.m.	**PL05: Plenary Lecture** - **THOMSON MEDALIST** *Chair: Renato Zenobi* **Driving innovation - From a protein sequence to a proteome** ***John R. Yates*** Department of Chemical Physiology, The Scripps Research Institute La Jolla, USA	***Plenary room*** ***Level 0***
9:15-9:30 a.m.	Break	
9:30-11:30 a.m.	**ThOr.01 - Glycomics, saccharides and glycoconjugates** *Chairs: Catherine Costello, Joseph Banoub*	***Plenary room*** ***Level 0***
9:30-10:10 a.m.	**Hybridation of mass spectrometry and ion spectroscopy for glycoanalytics** *I. Compagnon* Institut Lumière Matière, Université Lyon 1/CNRS. Villeurbanne, France	
10:10-10:30 a.m.	**Application of a novel functionalized resin with phenylboronic acid for capturing of glycated and glycosylated peptides and their MS identification** *M. Wierzbicka, M. Kijewska, M. Waliczek, F. Nuti, A. Papini, P. Stefanowicz, Z. Szewczuk* University of Wrocław, Faculty of Chemistry, Wrocław, Poland	

10:30-10:50 a.m.	**Glycan isomer differentiation using a sialic acid derivatization toolbox for higher throughput mass spectrometric glycomics** *N. De Haan, K. Reiding, S. Holst, B. Heijs, D. Falck, G. Kammeijer, V. Dotz, M. Wuhrer* Leiden University Medical Center, Leiden, Netherlands
10:50-11:10 a.m.	**HILIC MS-HCD/FT-IT and hybrid search enhance the structure elucidation of oligosaccharides in NIST human milk reference material** *C. Remoroza, T. Mak, S. Stein* National Institute of Standards and Technology, Mass Spectrometry Data Center, Gaithersburg, USA
11:10-11:30 a.m.	**Competitive Universal Proxy Receptor Assay (CUPRA) for quantitative high-throughput glycan library screening** *J. Klassen, E. Kitova, P. Kitov, L. Han, Z. Li* University of Alberta, Chemistry, Edmonton, Canada

9:30-11:30 a.m.	**ThOr.02 - Probing Protein Structure and Dynamics** *Chairs: Lars Konermann, Giancarlo la Marca*	***Room 1*** ***Level* 0**
9:30-10:10 a.m.	**Probing the structures of native and pathological a-synuclein species by hydrogen/deuterium exchange mass spectrometry** *T. J. D. Jørgensen, J. B.Madsen, A. L. Hemdrup, C. Sahin, D. Otzen, P. H. Jensen* University of Southern Denmark, Department of Biochemistry and Molecular Biology, Odense M, Denmark	
10:10-10:30 a.m.	**HDX-MS reveals conformational changes of IL-23 in complex with IL-23R/IL-12RB1 and phage display peptides** *H. Broughton, L. Cano, J. Dodge, I. Gonzalez, C. Michael, F. Zhang, S. Afshar, A. Espada* Lilly, S.A., Centro de Investigación, Alcobendas, Spain	
10:30-10:50 a.m.	**Mapping conformational dynamics to binding modes in TEM-1 β-lactamase using millisecond scale ESI-MS** *R. Knox, D. Wilson* York University, Chemistry, Toronto, Canada	
10:50-11:10 a.m.	**Using mass spectrometry to examine the conformational landscape of proteins – The perfect tool to report on self solvation and the effect of charge location on structure?** *P. Barran, D. Stuchfield, L. Migas, R. Beveridge, J. Ujma, B. Bellina* The University of Manchester, School of Chemistry, Manchester Institute of Biotechnology, Manchester, United Kingdom	
11:10-11:30 a.m.	**A coarse-grained computational workflow for the elucidation of biomolecular structure and dynamics by ion mobility spectrometry-mass spectrometry** *R. D'esposito, D. Fabris* University at Albany, Chemistry and Biological Sciences, Albany, USA	

9:30-11:30 a.m.	**ThOr.03 - Organic and inorganic MS: challenges & applications - Natural substances and their complexes** *Chairs: Pascal Gerbaux, Luisa Mattoli*	***Room 2*** ***Level* 0**
9:30-10:10 a.m.	**Contextualizing metabolomics data trough multi-informative molecular networks: metabolite annotation and bioactive natural products prioritization strategies** *P. Allard* School of Pharmaceutical Sciences, EPGL, University of Geneva, University of Lausanne, CMU, Geneva, Switzerland	
10:10-10:30 a.m.	**New approach for the structure elucidation of (acyl)polyamines in spider venoms by UHPLC-HR-ESI-MS/MS** *Y. Forster, S. Bienz, L. Bigler* University of Zurich, Department of Chemistry, Zurich, Switzerland	
10:30-10:50 a.m.	**Glycoalkaloids in plants using high resolution mass - neutral loss approach** *T. Nardin, R. Larcher* Fondazione E. Mach, CTT, San Michele all'Adige, Italy	

10:50-11:10 a.m.	**Structural investigation of natural organic matter using direct fractionation and selective isotopic labeling coupled to FTICR MS** *A. Zherebker, Y. Kostyukevich, E. Shirshin, O. Kharybin, A. Kononikhin, I. Perminova, E. Nikolaev* Skolkovo Institute of Science and Technology, Translational medicine, Moscow, Russian Federation
11:10-11:30 a.m.	**Evaluation of cosmetic interest of the Yellow-legged hornet venom (Vespa velutina nigrithorax)** *N. Le Thao, D. Da Silva, C. Colas, E. Darrouzet, P. Baril, L. L. Petit, B. Maunit* Institut de Chimie Organique et Analytique (ICOA), UMR 7311, Université d'Orléans-CNRS, Orléans, France

9:30-11:30 a.m.	**ThOr.04 - Environmental MS** *Chairs: Encarnation Moyano, Cecilia Bergamini*	***Room 3*** ***Level* 1**
9:30-10:10 a.m.	**Emerging contaminants: state of the art and new discoveries** *S. D. Richardson* University of South Carolina, Department of Chemistry & Biochemistry, Columbia, USA	
10:10-10:30 a.m.	**Development and optimization of a membrane-inlet-photoionization mass spectrometer for real-time analysis of (poly)aromatic compounds in aquatic systems** *C. Gehm, T. Streibel, J. Passig, D. Schulz-Bull, R. Zimmermann* Joint Mass Spectrometry Center, University of Rostock, Rostock, Germany	
10:30-10:50 a.m.	**Selective and rapid quantification of atmospheric monoterpenes** *K. Sovová, P. Pásztor, V. Shestivska, A. Spesyvyi, M. Lacko, P. Španel* J. Heyrovský Institute of Physical Chemistry of the CAS, v. v. i., Department of Chemistry of Ions in Gaseous Phase, Prague, Czech Republic	
10:50-11:10 a.m.	**Comprehensive depth profiling of Staten Island soil by GC and petroleomics** *M. Thomas, E. Collinge, M. Witt, C. Vane, M. Barrow* MAS CDT, University of Warwick, Coventry, United Kingdom	
11:10-11:30 a.m.	**New pesticide metabolites in groundwater detected using high resolution mass spectrometry** *K. Kiefer, A. Müller, H. Singer, J. Hollender* Eawag, Environmental Chemistry, Dübendorf, Switzerland	

9:30-11:30 a.m.	**ThOr.05 - Safe & Valuable Food** *Chairs: Michel W.F. Nielen, Emanuela Gregori*	***Room 4*** ***Level* 1**
9:30-10:10 a.m.	**How far can we trust untargeted HRMS-based exposomics to assess food value and safety for the consumer: the case of exposure to pesticides** *L. Debrauwer* INRA, UMR 1331 Toxalim, Toulouse, France	
10:10-10:30 a.m.	**Novel identification of 3-epi-25-hydroxyvitamin D3 in pork and beef longissimus thoracis steaks confirms the presence of this metabolite in the human food chain** *K. G. Dowling, A. Hayes, K. Galvin, S. K. Duffy, A. K. Kelly, J. V. O'doherty, K. D. Cashman* Cork Centre for Vitamin D and Nutrition Research, School of Food and Nutritional Sciences, University College Cork, Cork, Ireland	
10:30-10:50 a.m.	**Artificial Intelligence enables the detection of pathogens in food and other complex biological matrices by mass spectrometric analysis of RNA modifications** *B. Toro, R. Nemati, M. Salehi, W. Mcintyre, C. Aldrich, D. Fabris* University at Albany, Chemistry and Biological Sciences, Albany, NY, USA	
10:50-11:10 a.m.	**Hydrogen/deuterium exchange is an effective method for the structural resolution of isomeric proanthocyanidins in wine and other dietary sources** *V. Merkyte, E. Longo, F. Rossetti, E. Boselli* Free University of Bozen - Bolzano, Faculty of Science and Technology, Bolzano, Italy	
11:10-11:30 a.m.	**MALDI-ToF mass spectrometry identification and detection of relevant pathogens in beef cattle** *G. Bacanelli, C. Mantovani, A. Louzan, T. Pasquatti, D. Bier, G. Rosinha, F. Araujo, N. Verbisck* EMBRAPA Beef Cattle, Animal Health, Campo Grande, Brazil	

11:30 a.m. - 12:30 p.m.	Coffee Break **Poster Sessions ThPS-S01 – ThPS-S13** *Odd numbered abstracts*	***Exhibition hall Level 0***

12:30 - 1:45 p.m.	**Lunch Symposia**	
	AGILENT TECHNOLOGIES	**Room 2 – Level 0**
	SHIMADZU	**Room 3 – Level 1**
	THERMO FISHER SCIENTIFIC	**Room 4 – Level 1**
	WATERS	**Room 1 – Level 0**

1:30 - 3:00 p.m.	Coffee Break **Poster Sessions ThPS-S01 – ThPS-S13** *Even numbered abstracts*	***Exhibition hall Level 0***

3:00-5:00 p.m.	**ThOr.06 - Lipidomics** *Chairs: Gavin Reid, Donatella Caruso*	***Plenary room Level 0***
3:00-3:40 p.m.	**Lipidomics analysis of cells and tissues identifies therapeutic targets** *M. Wakelam, A. Nguyen, Q. Zhang, R. Solari* Babraham Institute, Signalling, Cambridge, United Kingdom	
3:40-4:00 p.m.	**Non-subjective characterization of medulloblastoma subgroup affiliation with Desorption Electrospray Ionization Mass Spectrometry** *A. Zarrine-Afsar, M. Woolman, A. Tata, I. Ferry, C. Kuzan-Fischer, M. Wu, S. Das, M. Taylor, J. Rutka, H. Ginsberg* University of Toronto, University Health Network, TECHNA Institute, Toronto, Canada	
4:00-4:20 p.m.	**Expanding the lipidome by data-independent ozone-induced dissociation to profile complex lipid isomers** *D. Marshall, B. Poad, R. Young, S. Blanksby* Queensland University of Technology, Institute for Future Environments, Brisbane, Australia	
4:20-4:40 p.m.	**Modelling cancer lipogenesis using LA-REIMS metabolic flux analysis in breast cancer cell lines** *S. Turkseven, N. Koundouros, R. Soares, L. Doria, M. Perdones-, S. Cameron, G. Poulogiannis, Z. Takats* Imperial College London, Department of Surgery and Cancer, London, United Kingdom	
4:40-5:00 p.m.	**Relative quantification of phospholipid *sn*-Isomers using positive doubly charged lipid-metal ion complexes** *S. Heiles, S. Becher, P. Esch* Justus Liebig University Giessen, Analytical Chemistry, Giessen, Germany	

3:00-5:00 p.m.	**ThOr.07 - Developments and applications in ion mobility MS** *Chairs: Perdita Barran, Leopoldo Ceraulo*	***Room 1 Level 0***
3:00-3:40 p.m.	**IMS-MS as a means of revealing new states during the melting of proteins** *D. Clemmer, T. El Baba, D. Woodall, S. Raab* School of Public Health-Bloomington, Indiana University, USA	
3:40-4:00 p.m.	**Probing peptide conformational rearrangements with high resolution SLIM traveling wave ion mobility-MS** *R. Wojcik, I. K. Webb, Y. M. Ibrahim, S. B. V. Garimella, R. Renslow, S. Colby, D. G. Thomas, R. D. Smith* PNNL, Integrative Omics, Richland, USA	
4:00-4:20 p.m.	**Ion mobility-derived collision cross section for mycotoxins: an interlaboratory study** *L. Righetti, L. Gethings, S. Stead, C. Dall'Asta* University of Parma, Department of Food and Drug, Parma, Italy	

4:20-4:40 p.m.	**Practical two-dimensional high-resolution ion mobility separations using FAIMS integrated with trapped IMS** *K. Jeanne Dit Fouque, J. Porter, F. Fernandez-Lima, A. Shvartsburg* Wichita State University, Wichita, USA
4:40-5:00 p.m.	**Collision cross sections of phosphoric acid cluster anions and their use as calibrants** *V. Calabrese, H. Lavanant, F. Rosu, V. Gabelica, C. Afonso* Normandie Univ, UNIROUEN, INSA Rouen, CNRS, COBRA, Rouen, France

3:00-5:00 p.m.	**ThOr.08 - Petroleomics, hydrocarbons and biofuels** *Chairs: Alan G. Marshall, Giorgio Mellerio*	***Room 2*** ***Level* 0**
3:00-3:40 p.m.	**The compositional and structural continuum of petroleum revealed by FT-ICR mass spectrometry** *R. P. Rodgers, M. L. Chacón-Patiño, S. M. Rowland, S. F. Niles, D. F. Smith, G. T. Blakney, Y. E. Corilo, A. M. Mckenna, A. G. Marshall, C. L. Hendrickson* National High Magnetic Field Laboratory, Florida State University, Tallahassee, USA	
3:40-4:00 p.m.	**Evidence of island and archipelago structures in distillable and truly non-distillable fractions of vacuum residues** *D. C. Palacio Lozano, A. Guzman, O. E. Mejía, M. P. Barrow* University of Warwick, Chemistry, Coventry, United Kingdom	
4:00-4:20 p.m.	**Direct inlet probe - high resolution time-of-flight mass spectrometry for the description of high boiling petroleum fractions** *U. Käfer, M. Saraji, J. Wendt, T. Wilharm, R. Zimmermann, T. Gröger* Helmholtz Center Munich, CMA, Munich, Germany	
4:20-4:40 p.m.	**Characterization of asphaltenes precipitated at different solvent power conditions using Magnetic Resonance Mass Spectrometry (MRMS)** *M. Witt, M. Godejohann, S. Oltmanns, E. Rogel* Bruker Daltonik GmbH, MRMS Solutions, Bremen, Germany	
4:40-5:00 p.m.	**Detailed molecular characterization of the upgrading process of pyrolysis oil by ultrahigh resolution mass spectrometry** *Y. Xu, Z. Cao, F. Schüth, W. Schrader* Max-Planck Institut für Kohlenforschung, Mass Spectrometry, Mülheim an der Ruhr, Germany	

3:00-5:00 p.m.	**ThOr.09 - Materials & nanomaterials** *Chairs: Jan Preisler, Giuseppe Avellone*	***Room 3*** ***Level* 1**
3:00-3:40 p.m.	**Bioimaging of nanoparticles in cells and tissue by laser ablation inductively coupled plasma mass spectrometry** *N. Jakubowski, H. Traub* Bundesanstalt für Materialforschung und -prüfung (BAM), Inorganic Trace Analysis, Berlin, Germany	
3:40-4:00 p.m.	**Nanostructured tungsten oxide substrate with oxygen vacancies for efficient Surface-Assisted Laser Desorption/Ionization mass spectrometry analysis** *Q. Ma* Chinese Academy of Inspection and Quarantine, Chinese Academy of Inspection and Quarantine, Beijing, China	
4:00-4:20 p.m.	**Supramolecular nanoreactors studied by ion mobility mass spectrometry** *E. Kalenius, T. Lee, P. Barran* University of Jyväskylä, Department of Chemistry, Jyväskylä, Finland	
4:20-4:40 p.m.	**H_2 detection in-situ by membrane introduction mass spectrometry** *A. Rousseau, B. Luna, H. Remita, E. Louarn* Laboratoire de Chimie Physique, CNRS, Univ. Paris-Sud, Université Paris-Saclay, Orsay, France	
4:40-5:00 p.m.	**Development of isolation techniques and capillary electrophoresis mass spectrometry (CESI-MS) methods for the characterisation of nanomaterial protein coronas** *K. Faserl, A. Chetwynd, I. Lynch, J. Thorn, H. Lindner* AB Sciex UK Ltd, Separations, Warrington, United Kingdom	

3:00-5:00 p.m.	**ThOr.10 - Novel food; nanoparticles in food and beverage; future applications** *Chairs: Stefan Weigel, Giovanni Sindona*	***Room 4*** ***Level 1***
3:00-3:40 p.m.	**Mass spectrometric detection and characterisation of nanoparticles** *R. Peters, A. Undas, M. van der Lee* RIKILT Wageningen University &Research, Wageningen, The Netherlands	
3:40-4:00 p.m.	**How to manage matrix effects for accurate nanoparticle sizing using single-particle ICP-ToF MS?** *L. Hendriks, A. Gundlach-Graham, D. Günther* ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland	
4:00-4:20 p.m.	**Use of ICP-MS-based techniques for the characterization of nanomaterials used in food-related applications** *F. Aureli, F. Ferraris, S. Savini, A. Raggi, F. Cubadda* Istituto Superiore di Sanità - National Institute of Health, Rome, Italy	
4:20-4:40 p.m.	**Translating into practice the EFSA Guidance on risk assessment of the application of nanotechnologies in the food chain: the role of mass spectrometry** *F. Aureli, F. Ferraris, S. Savini, A. Raggi, F. Cubadda* Istituto Superiore di Sanità - National Institute of Health, Rome, Italy	
4:40-5:00 p.m.		

8:00 p.m.	**Conference dinner**

FRIDAY, August 31st, 2018

8:30-9:15 a.m.	**PL06: Plenary Lecture** *Chair: Simonetta Fornarini* **Mass spectrometry and theoretical chemistry in service of catalysis research: a ménage-à-trois at its best** ***Helmut Schwarz*** Institut für Chemie, Technische Universität Berlin, Berlin, Germany	***Plenary room*** ***Level 0***
9:15-9:30 a.m.	Break	
9:30-11:30 a.m.	**FOr.01 - Life sciences - Metabolomics** *Chairs: Ulf Sommer, Donatella Caruso*	***Plenary room*** ***Level 0***
9:30-10:10 a.m.	**Metabolomics and the exposome - Application to cancer epidemiology** *A. Scalbert* International Agency for Research on Cancer (IARC), Biomarkers Group, Nutrition and Metabolism Section, Lyon, France	
10:10-10:30 a.m.	**Targeted on-line breath analysis supports the hypothesis of altered collagen turnover in idiopathic pulmonary fibrosis** *M. T. Gaugg, A. Engler, S. P. Martinez-Lozano, L. Bregy, Y. Nussbaumer-Ochsner, L. Eiffert, T. Bruderer, R. Zenobi, M. Kohler* ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland	
10:30-10:50 a.m.	**Targeted metabolomic analysis of urine for improving the diagnosis of asthma and COPD** *M. Khamis, H. Awad, K. Allen, D. Adamko, A. El-Aneed* University of Saskatchewan, College of Pharmacy and Nutrition, Saskatoon, Canada	

10:50-11:10 a.m.	**In vivo real-time monitoring system for metabolites in a living mouse brain using probe electrospray ionization/tandem mass spectrometry (PESI/MS/MS)** *K. Zaitsu* Nagoya University, In Vivo Real-time Omics Laboratory, Institute for Advanced Research, Nagoya, Japan
11:10-11:30 a.m.	**Energy metabolism in age-related diseases: focus on mitochondria** *N. Mitro, D. Caruso* Università degli Studi di Milano, Department of Pharmacological and Biomelecular Sciences, Milano, Italy

9:30-11:30 a.m.	**FOr.02 - Informatics tools and data analysis** *Chairs: Peter O'Connor, Giuseppe Avellone*	***Room 1*** ***Level* 0**
9:30-10:10 a.m.	**Leveraging new algorithmics for better MS spectra** *M.-A. Delsuc* IGBMC, Illkirch, France	
10:10-10:30 a.m.	**Advanced mass spectrometry methods for unravelling the mechanisms of organophosphate toxicity** *H. Wang, M. Leeming, B. Cochran, W. Donald* University of New South Wales, School of Chemistry, UNSW, Sydney, Australia	
10:30-10:50 a.m.	**Algorithm for processing complex mixture data from hyphenated ultrahigh resolution mass spectrometry** *R. Gavard, H. Jones, D. Rossell, S. Spencer, M. Barrow* University of Warwick, MAS CDT, Coventry, United Kingdom	
10:50-11:10 a.m.	**LC-MS^1 method for protein identification and quantitation without using tandem mass spectra** *M. Ivanov, I. Tarasova, E. Solovyeva, M. Gorshkov* V.L. Talrose Institute for Energy Problems of Chemical Physics Russian Academy of Sciences, Moscow, Russian Federation	
11:10-11:30 a.m.	**Phase-constrained spectrum deconvolution-real time super-resolution processing of FTMS data** *K. Aizikov, D. Grinfeld, A. Kreutzmann, D. Mourad, E. Damoc, T. N. Arrey, O. Lange, A. Makarov* ThermoFisher Scientific, LSMS, Bremen, Germany	

9:30-11:30 a.m.	**FOr.03 - Cultural heritage and archaeology** *Chairs: Klaas Jan van den Berg, Giorgio Mellerio*	***Room 2*** ***Level* 0**
9:30-10:10 a.m.	**Art and cultural heritage natural polymers by bottom up and top down approaches** *C. Tokarski* Université de Lille 1 Sciences et Technologies, Villeneuve d'Ascq, France	
10:10-10:30 a.m.	**Fast analysis of modern oil paintings and dyes in textiles by surface acoustic wave nebulization-mass spectrometry (SAWN-MS)** *A. Astefanei, M. van Bommel, K. J. van den Berg, G. Corthals* University of Amsterdam, HIMS, Analytical Chemistry, Amsterdam, Netherlands	
10:30-10:50 a.m.	**Molecular signatures of protein aging in ancient human bones from the eruption area of Vesuvius** *G. Ntasi, P. Pucci, G. Marino, L. Birolo* University of Naples Federico II, Chemical Sciences, Naples, Italy	
10:50-11:10 a.m.	**Characterization of isobaric species and photo-degradation products of triarylmethane dyes within textiles** *F. Sabatini, C. Bracini, A. Quye, I. Degano, M. P. Colombini* University of Pisa, Department of Chemistry and Industrial Chemistry, Pisa, Italy	
11:10-11:30 a.m.	**Wine production and consumption in pre Roman times: residue analysis of a production structure an ceramic vessels from the Western Mediterranean** *A. Pecci, A. Zifferero, G. Giorgi, S. Mileto, R. Jornet, C. Belarte Franco, A. De Palmas, M. Vidale* ERAAUB, Departament Història i Arqueologia, Universitat de Barcelona, Spain	

9:30-11:30 a.m.	**FOr.04 - Atomic mass spectrometry: metallomics and isotope ratio mass spectrometry** *Chairs: Ryszard Lobinski, Federica Camin*	***Room 3*** ***Level 1***
9:30-10:10 a.m.	**New ion sources for metallomic analysis and isotope-ratio mass spectrometry** *G. M. Hieftje* Indiana University, Department of Chemistry, Bloomington, USA	
10:10-10:30 a.m.	**Element analysis with thermalized laser ablation ions from solid samples** *L. Querci, B. Hattendorf, D. Günther* ETH Zürich, Laboratory of Inorganic Chemistry, Zurich, Switzerland	
10:30-10:50 a.m.	**High-resolution and tandem mass spectrometry techniques contribute to the discovery of new arsenic metabolites of toxicological importance** *Q. Liu, X. Lu, H. Peng, E. Leslie, M. Zuidfhof, X.-F. Li, X. C. Le* University of Alberta, Analytical and Environmental Toxicology, Edmonton, Canada	
10:50-11:10 a.m.	**Isotopic techniques for studying the sources and processes of pollutants in the environment** *N. Ogrinc* Jožef Stefan Institute Department of Environmental Sciences, Ljubljana, Slovenia	
11:10-11:30 a.m.	**Potential use of the stable isotope ratios of bioelements and elemental composition to trace the origin of dairy products** *L. Bontempo, F. Camin* Fondazione E. Mach, Food Quality and Nutrition Department, San Michele all'Adige, Italy	

9:30-11:30 a.m.	**FOr.05 - Nutraceutics directions** *Chairs: Roberto Romero Gonzalez, Roberta Galarini*	***Room 4*** ***Level 1***
9:30-10:10 a.m.	**Medicinal extremophile plants: valuable source of "GRAS" and health promoting biomolecules with medical, nutraceutical and food applications** *K. Riadh* Laboratory of Aromatic and Medicinal Plants, CBBC, BP901, Hammam-Lif, Tunisia	
10:10-10:30 a.m.	**Ancient apple of Friuli Venezia Giulia region as potential new nutraceutical ingredients** *S. Sut, S. Dall'Acqua* University of Padova, Dept. of Pharmaceutical and Pharmacological Sciences, Padova, Italy	
10:30-10:50 a.m.	**Putting pigment to paper. The quantitation of bioactive anthocyanins in fruits and nutraceuticals with paper spray ionization mass spectrometry** *R. Cody, J. Tamura, K. Downard* University of New South Wales, Medicine, Sydney, Australia	
10:50-11:10 a.m.	**Reliable identification of bioactive compounds in foodstuffs through the use of a novel dual-filter mass spectral library in liquid chromatography** *F. Rigano, M. Oteri, P. Dugo, L. Mondello* Chromaleont Srl, c/o Dipartimento ChiBioFarAm, University of Messina, Messina, Italy	
11:10-11:30 a.m.	**Antioxidant activities and phytochemical profile of Azorella glabra** *I. Faraone, D. K. Ray, L. Chiummiento, A. Choudhary, D. Russo, C. Sinisgalli, E. Fernandez, L. Milella* University of Basilicata, Department of Science, Potenza, Italy	

11:30-11:45 a.m.	Break
11:45 a.m. - 12:15 p.m.	**Presentation of IMSC 2020**
12:15-1:00 p.m.	Arrivederci & farewell drinks

POSTER SESSIONS

Odd numbers: 11:30 a.m.- 1:00 p.m.

Even numbers: 1:30 p.m.- 3:00 p.m.

Poster set up: 8:00-8:30 a.m.

Poster removal: 6:00-7:00 p.m.

MONDAY, August 27th, 2018

MPS-S01 - Nucleic Acids

MP-1 **Characterization of LILBID-MS using DNA structures**
G. Hense, P. Young, N. Morgner
AK Morgner, Physical and Theoretical Chemistry at the Goethe University, Frankfurt am Main, Germany

MP-2 **The simultaneous determination of intracellular nucleoside triphosphates and cyclic dinucleotides with LC-MS/MS**
R. Oertel, R. Behrendt, A. El-Armouche
Institute of Clinical Pharmacology, GWT TU Dresden, Dresden, Germany

MP-3 **Semi-quantitative determination of oligonucleotide drug impurities: main and co-eluting species**
S. Roussis
Ionis Pharmaceuticals, ADQC, Carlsbad, USA

MP-4 **Interactions of oxaliplatin and carboplatin with DNA building blocks as studied in the gas phase: a combined experimental and theoretical study**
J.-Y. Salpin, M. E. Crestoni, D. Corinti, S. Fornarini, D. Scuderi, B. Chiavarino
CNRS, LAMBE - UMR 8587 - Université d'Evry Val d'Essonne, Evry, France

MP-5 **Development of the LC-MS method for the analysis and characterization chemically modified RNA**
D. Strzelecka, M. Smietanski, M. Warminski, P. Sikorski, J. Jemielity, J. Kowalska
University of Warsaw, Faculty of Physics, Warsaw, Poland

MP-6 **Solution and gas-phase structures of DNA G-quadruplexes: ion mobility mass spectrometry, solution spectroscopy, and collision cross section calculations**
A. Ghosh, F. Rosu, V. Gabelica
INSERM, University of Bordeaux/IECB, Pessac, France

MPS-S02 - Clinical Proteomics

MP-7 **Cluster-assembled smart surfaces for on-target processing of biological samples in MALDI-MS analysis**
E. Barborini, S. Vinati, G. Bertolini, M. Baumann
Tethis SpA, R&D, Milan, Italy

MP-8 **Proteome profiling of bronchioalveolar lavage fluid after exposure to magnetic iron and cobalt oxide nanoparticles**
A. M. Billing, K. B. Knudsen, U. Vogel, F. Kjeldsen
University of Southern Denmark, Department of Biochemistry and Molecular Biology, Odense, Denmark

MP-9 **Concurrent quantification of synaptotagmin-1 and SNAP-25 in clinically relevant volumes of CSF by immunoaffinity LC-MS/MS**
A. Brinkmalm, A. Öhrfelt, L. Frölich, L. Hausner, H. Zetterberg, K. Blennow
The Sahlgrenska Academy at University of Gothenburg, Institute of Neuroscience and Physiology, Department of Psychiatry and Neurochemistry, Mölndal, Sweden

MP-10 **Single shot DIA profiling of >1500 plasma proteomes of the weight loss and maintenance study DiOGenes**
R. Bruderer, J. Muntel, S. Müller, O. M. Bernhardt, T. Gandhi, P. Mironova, O. Walter, J. Carayol, A. Astrup, W. H.M. Saris, J. Hager, A. Valsesia, L. Dayon, L. Reiter
Biognosys AG, Schlieren, Switzerland

MP-11 **Identification of complete pool of bio active peptides in mouse brain striatum including SEPs, a novel class of non-classical bio active peptides**
H. Budamgunta
Center for proteomics, University of Antwerp/Biology, Antwerp, Belgium

MP-12 **Proteomic characterization of human platelet lysate by label-free nLC-MS/MS: towards the effectors of its beneficial effect in regenerative medicine**
C. Chinello, F. Re, C. Almici, A. James Smith, F. Paolella, G. Lisignoli, I. Piga, M. Stella, M. Mazza, V. Denti, L. Sartore, D. Russo, F. Magni
University of Milano-Bicocca, Department of Medicine and Surgery, Clinical Proteomics and Metabolomics Unit, Vedano al Lambro, Italy

MP-13 **Validation of a LC-MS assay for assessment of alpha-defensin in synovial fluid**
R. Dall'Anese, P. Pezzati, M. Quercioli, F. Balboni, G. Balato, A. Baldini, G. Bartolini
Buzzi Lab, Analytical chemistry, Prato, Italy

MP-14 **Mass spectrometry evaluation of circulating S100A8 and S100A9 proteins as prognosis biomarkers in sepsis**
C. Dubois, D. Payen, V. Faivre, S. Simon, F. Fenaille, C. Junot, N. Morel, F. Becher
Service de Pharmacologie et Immunoanalyse (SPI), Laboratoire d'Etude du Métabolisme des Médicaments (LEMM), CEA, INRA, Université Paris Saclay, Gif-sur-Yvette CEDEX, France

MP-15 **Characterization of the PIF peptide (preimplantation factor) interactome in human serum**
A. Fel, P. Czaplewska, K. Macur, M. Thiel, K. Lukaszuk, S. Oldziej
University of Gdansk, Intercollegiate Faculty of Biotechnology, and Medical University of Gdansk, Gdansk, Poland

MP-16 **Molecular fingerprinting of the interstitium proteome in the vastus lateralis muscle in women with fibromyalgia compared to healthy controls using MD-LC-MS/MS**
B. Ghafouri, M. Turkina, N. Christidis, K. Mannerkorpi, E. Kosek, M. Ernberg, B. Gerdle
Linkoping University, Department of medical and health sciences, Linkoping, Sweden

MP-17 **Deep proteomics of saw-scaled viper (Echis carinatus sochureki) venom by integrated top-down and bottom-up mass spectrometric approaches**
P. Ghezellou, V. Garikapati, S. M. Kazemi, K. Strupat, A. Ghassempour, B. Spengler
Justus Liebig Giessen University, Institute of Inorganic and Analytical Chemistry, Giessen, Germany

MP-18 **Differential proteome analysis of human neuroblastoma xenograft primary tumors and matched spontaneous distant metastases**
L. Haenel, H. Schlüter, L. Heikaus, T. Lange
University Medical Center Hamburg-Eppendorf, Institute of Clinical Chemistry and Laboratory Medicine, Hamburg, Germany

MP-19 **Biomarker candidates for acute myocardial infarction in human serum**
M.-J. Kang, Y. Seong
Korea Institute of Science and Technology, Molecular Recognition Research Center, Seoul, Republic of Korea

MP-20 **Rheumatoid factor-correlated proteins is complementary biomarker of rheumatoid arthritis**
H.-G. Kang, S. Mun, A. Park, A. Seok, Y. Lee, H. Kim, Y. Lee
Eulji University, Department of Senior Healthcare, BK21 Plus Program, Graduate School, Daejeon, Republic of Korea

MP-21 **Novel biomarker discovery in extracellular vesicles from plasma for colorectal cancer**
K. Kasahara, R. Narumi, Y. Shimizu, K. Masuda, S. Nagayama, T. Tomonaga, Y. Sakai, J. Adachi
National Institute of Biomedical Innovation, Health and Nutrition, Laboratory of Proteome Research, Osaka, Japan

MP-22 **Quantitative proteomic analysis of cervicovaginal fluid proteome using a 2D-nLC-ESI-MS/MS for early detection of preterm birth**
Y. E. Kim, K. Kim, D. Kang
Center of Bioanalysis, Korea Research Institute of Standards and Science, Daejeon, Republic of Korea

MP-23 **Antibody-free LC-MS methods for low to sub ng/mL quantification of the soluble Receptor for Advanced Glycation End-products (sRAGE) in serum**
F. Klont, S. D. Pouwels, M. Hadderingh, M. R. Joosten, J. Hermans, N.C. van de Merbel, P. Horvatovich, N.H.T. ten Hacken, R. Bischoff
University of Groningen, Department of Analytical Biochemistry, Groningen, Netherlands

MP-24 **Proteome analysis of human neuromelanin granules and neurons in the context of dementia with Lewy bodies**
S. Kösters, S. Plum, C. May, K. Marcus
Medizinisches Proteom-Center, Ruhr-University Bochum, Bochum, Germany

MP-25 **Proteomic profiling of melanoma cell lines and tissue using data independent acquisition mass spectrometry to predict treatment response and patient survival**
C. Krisp, R. Parker, D. Pascovici, N. K. Hayward, J. S. Wilmott, R. A. Scolyer, M. P. Molloy
Australian Proteome Analysis Facility, Macquarie University, Sydney, Australia

MP-26 **Unveiling the outer membrane vesicle proteome of A. salmonicida: a physiological insight**
T. Kroniger, A. Otto, B. Köllner, D. Becher
University of Greifswald, Institute for Microbiology, Greifswald, Germany

MP-27 **Quantitation of monoclonal antibody infliximab in human plasma by LC-MS/MS using Fab-selective limited proteolysis nSMOL technology**
N. Loftus, A. Barnes, A. Jaffuel
Shimadzu, MS/BU, Manchester, United Kingdom

MP-28 **Top down mass spectrometry with multiple MS/MS strategies to identify age-related proteoform changes in tear fluid**
D. Lopez-Ferrer, R. Huguet, D. Horn, P. P. M. Raus, V. Zabrouskov, A. Huhmer, P. Dem Verhaert
Thermo Fisher Scientific, San Jose, USA

MP-29 **Advances in clinical proteomics for analysis of thyroid fine needle aspiration biopsies: evaluating proteomic stability in preservative solutions**
I. Piga, G. Capitoli, S. Tettamanti, V. Denti, A. Smith, C. Chinello, M. Stella, D. Leni, M. Garancini, S. Galimberti, F. Magni, F. Pagni
University of Milano-Bicocca, Department of Medicine and Surgery - Clinical Proteomics and Metabolomics Unit, Vedano al Lambro, Italy

MP-30 **Quantification of endogenous VEGFA levels from human plasma using nanoLC/high resolution mass spectrometry combined with immunocapture enrichment**
S. Pleiner, K. Koehler, J. Hoke, S. Keller
Boehringer Ingelheim Pharma GmbH & Co. KG, DMPK, Biberach a. d. Riss, Germany

MP-31 **Characterization of the modification in mitochondrial proteome due to eIF6 depletion by SWATH-MS analysis and multivariate statistical tools**
E. Robotti, M. Manfredi, S. Martinotti, D. Brina, A. Scagliola, E. Ranzato, E. Marengo, S. Biffo
University of Piemonte Orientale, Department of Sciences and Technological Innovation, Alessandria, Italy

MP-32 **Label-free proteomic analysis of urinary exosomes from patients with cc-Renal Cell Carcinoma: stage-specific differential protein profile**
L. Santorelli, F. Raimondo, C. Chinello, F. Magni, M. Grasso, G. Bovo, M. Pitto
University of Milano-Bicocca, Department of Medicine and Surgery, Vedano al Lambro, Italy

MP-33 **Maximized throughput and analytical depth for shotgun proteomics using PASEF on a TIMS equipped QToF and a novel LC system**
T. Kosinsky, S. Koch, M. Lubeck, P. Schmit, N. Bache, O. Bjeld Horning, L. Falkenby, H. Koch, L. Woods
Bruker France, Proteomics, Wissembourg, France

MP-34 **Targeted quantitation of proteins for discriminating obese from normal-weight adolescents by liquid chromatography-mass spectrometry**
H. Shin, K. Dan, S. Song, D. Han
Seoul National University Hospital, Biomedical Research Institute, Seoul, Republic of Korea

MP-35 **Development of a sandwich ELISA for the thrombin light chain identified by serum proteome analysis**
K. Sogawa, M. Miyahara, S. Yamanaka, S. Takano, H. Yoshitomi, M. Miyazaki, M. Ohtsuka, F. Nomura
Azabu University, Biochemistry, Kanagawa, Japan

MP-36 **Use of the MALDI BioTyper system with MALDI-ToF MS for rapid identification of microorganisms causing bacterial urinary tract infection from urine samples**
M. Yano, K. Sogawa, H. Maeda
Azabu University, Biochemistry, Kanagawa, Japan

MP-37 **Topological distribution of lipid biomarkers in adipose tissue of metabolic-healthy and unhealthy subjects**
R. Tans, R. Bande, A. van Rooij, B. Molloy, R. Heeren, R. Stienstra, C. Tack, H. Wessels, A. van Gool
Radboud University Medical Venter, Translational Metabolic Laboratory, Nijmegen, Netherlands

MP-38 **LC-MS/MS-based characterization of glioblastoma cell responses to type I interferons for establishing defects in antiviral mechanisms**
I. Tarasova, A. Tereshkova, E. Solovyeva, J. Bubis, V. Gorshkov, F. Kjeldsen, I. Ilina, S. Moshkovskii, P. Chumakov, M. Gorshkov
RAS, Talrose Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation

MP-39 **Epitope identification of glycated HSA and the extracellular region of human RAGE by SPR and affinity-MS spectrometry**
A. Tramarin, M. Naldi, L. Lupu, P. Wiegand, E. Fabini, G. Degani, L. Popolo, G. Aldini, M. Przybylski, M. Bartolini
Alma Mater Studiorum, University of Bologna, Department of Pharmacy and Biotechnology, Bologna, Italy

MP-40 **The molecular pattern of plasma proteins and their correlation to pain intensity and sensitivity in women with fibromyalgia – a multi-center study**
K. Wåhlén, B. Gerdle, K. Mannerkorpi, E. Kosek, M. Ernberg, B. Ghafouri
Linköping University, Department of medical and health sciences, Linköping, Sweden

MP-41 **Therapeutic proteins in sports drug testing: detection of different ActRII inhibitors in serum by means of (immuno-)affinity purification, tryptic digestion, and LC-HRMS**
K. Walpurgis, A. Thomas, C. Reichel, F. Dellanna, M. Thevis
German Sport University Cologne, Institute of Biochemistry/Center for Preventive Doping Research, Cologne, Germany

MP-42 **A novel high-throughput antibody-free LC-MS/MS assay to quantitate Chromogranin-A in serum**
D. Weber, S. Goldman, M. Mcphaul, M. Caulfield, N. Clarke
Quest Diagnostics, R&D Mass Spectrometry, San Juan Capistrano, USA

MP-43 **Exosomes purification for new biomarkers discovery in cancer**
F. Anastasi, M. Cecchini, L. A. McDonnell
Laboratorio NEST, Scuola Normale Superiore, Pisa, Italy

MP-44 **Development of a novel LC concept for clinical proteomics**
N. Bache, P. Geyer, C. Ravnsborg, O. Hoerning, L. Falkenby, P. Treit, S. Doll, I. Paron, F. Meier, O. Vorm, M. Mann
Evosep, Odense, Denmark

MP-45 **Analysis and characterization of gastrointestinal metabolism of major soy allergens glycinin and β-conglycinin in an in-vitro model by LC-MS/MS**
J. Bräcker, N. Lok, J. Brockmeyer
University of Stuttgart, Food Chemistry, Stuttgart, Germany

MP-46 **Proteomic profiling of extracellular vesicles derived from mesenchymal stromal cells**
J. Brandi
University of Verona, Department of Biotechnology, Verona, Italy

MP-47 **Differentiation of hypertensive disorders during pregnancy based on urine peptidome profiling by high resolution mass spectrometry**
A. Bugrova, A. Kononikhin, V. Sergeeva, M. Indeykina, I. Popov, N. Starodubtseva, V. Frankevich, E. Nikolaev
Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow, Russian Federation

MP-48 **Comparative analysis of lectin based glycoproteins between yoga groups**
J. Kang, Y. Jung, W. Cho
Wonkwang University, Department of Chemistry, Iksan, Republic of Korea

MP-49 **Serum protein classifiers of ALS for disease etiology and progression**
S. Filip, T. Sosnowski, I. Dervishi, Y. A. Goo, P. H. Ozdinler
Northwestern University, Proteomics Center of Excellence, Chicago, USA

MP-50 **Blood plasma proteome and peptidome comparative screening for potential biomarkers of Alzheimer's disease**
M. Indeykina, A. Bugrova, N. Zakharova, A. Kononikhin, Y. Fedorova, A. Brhozovskiy, I. Popov, S. Gavrilova, E. Nikolaev
Emanuel Institute of Biochemical Physics of the Russian Academy of Sciences, Laboratory for Mass Spectrometry of Biomacromolecules, Moscow, Russian Federation

MP-51 **A online 2D-NCFC-RP/RPLC system for comprehensive and high-thoughput proteomics analysis**
H. Lee, S. Lee
Korea University, Chemistry, Seoul, Republic of Korea

MPS-S03 - Ion Spectroscopy & Photodissociation

MP-52 **Structural elucidation of metabolites using infrared ion spectroscopy**
H. Bentlage, J. Martens, G. Berden, R. Wevers, J. Oomens
FELIX, Radboud University, Nijmegen, Netherlands

MP-53 **Infrared ion spectroscopy of metal-ligand redox pairs generated via electron transfer reduction reactions**
M. Munshi, J. Martens, G. Berden, J. Oomens
FELIX, Radboud University, Nijmegen, Netherlands

MP-54 **Counter cation-dependent action spectroscopy of IR-797 and IR-806 cyanine dyes**
M. Herve, R. Bredy, G. Karras, B. Concina, F. Lepine, I. Compagnon
University of Lyon, Université Claude Bernard Lyon 1, CNRS, Institut Lumière Matière, Villeurbanne, France

MP-55 **Ion mobility spectrometry and gas phase spectroscopy of mass and isomer selected porphyrin anions**
K. Brendle, P. Weis, M. M. Kappes
Karlsruhe Institute of Technology, Institute of Physical Chemistry, Karlsruhe, Germany

MP-56 **REMPI and MATI spectroscopy of methyl and halo pyridines**
N. Helle, J. Grotemeyer
Institute of Physical Chemistry, CAU Kiel, Kiel, Germany

MP-57 **Action Spectroscopy without a trap: on-the-fly spectroscopy of IR-797 and IR-806 cyanine dyes**
M. Herve, R. Bredy, G. Karras, B. Concina, A. R. Allouche, F. Lepine, I. Compagnon
Institut Lumière Matière (ILM), Université Lyon 1, Lyon, France

MP-58 **IR tagging pre-dissociation spectroscopy to reveal isomeric composition**
P. Jusko, A. Simon, G. Wenzel, S. Brünken, S. Schlemmer, C. Joblin
Institut de Recherche en Astrophysique et Planétologie (IRAP), Université de Toulouse, CNRS, CNES, Toulouse, France

MP-59 **Validation of an IRMPD experimental setup and theoretical methods for IRMPD assignment**
A. F. Rodrigues-Oliveira, F. W. M. Ribeiro, G. Cervi, T. C. Correra
University of São Paulo, Institute of Chemistry, São Paulo, Brazil

MP-60 **Infrared Multiple Photon Dissociation of copper formate clusters**
T. Pascher, M. Ončák, C. Van Der Linde, J. Lengyel, M. K. Beyer
Universität Innsbruck, Institut für Ionenphysik und Angewandte Physik, Innsbruck, Austria

MP-61 **Development of a 3D ion trap mass spectrometer for IRMPD spectroscopy**
T. C. Penna, G. Cervi, A. F. Rodrigues-Oliveira, J. Menegon, T. C. Correra
Universidade de São Paulo, Instituto de Química, São Paulo, Brazil

MP-62 **Photoisomerization action spectroscopy of a ruthenium sulfoxide complex**
M. Scholz, J. Bull, E. Carrascosa, G. Kosgei, J. Rack, E. Bieske
University of Melbourne, School of Chemistry, Parkville, Australia

MP-63 **Photochemistry of $Mg^+(H_2O)_n$, n=1-5: experiment and theory**
T. Taxer, M. Oncak, C. van der Linde, E. Barwa, M. Beyer
Universität Innsbruck, Institut für Ionenphysik und Angewandte Physik, Innsbruck, Austria

MP-64 **Shedding light on structure: initial protein unfolding events revealed by 213 nm UVPD**
A. Theisen, R. Black, D. Corinti, J. Brown, B. Bellina, P. Barran
University of Manchester, Manchester Institute of Biotechnology and Photon Science Institute, Manchester, United Kingdom

MP-65 **IRMPD spectra of protonated hydroxybenzaldehydes: the evidence of the torsional barriers in carboxonium ions**
B. Chiavarino, M. E. Crestoni, O. Dopfer, P. Maitre, S. Fornarini
Università di Roma "La Sapienza", Dipartimento di Chimica e Tecnologie del Farmaco, Roma, Italy

MP-66 **Valence and core electron induced photoionization and dissociation dynamics of the thiazole molecule**
A. F. Lago, R. D. Januario, R. L. Cavasso-Filho, M. Simon, J. Z. Dávalos
Federal University of ABC (UFABC), Center for Natural Sciences and Humanities (CCNH), Santo Andre, Brazil

MP-67 **Relevance of the gas-phase studies to biology: cold ion spectroscopy of the opioid peptide drugs**
A. Y. Pereverzev, V. N. Kopysov, I. Szabo, E. Rosta, O. V. Boyarkin
EPFL, LCPM, Lausanne, Switzerland

MP-68 **The use of peptide bonds for cold ion spectroscopy**
A. Y. Pereverzev, V. N. Kopysov, O. V. Boyarkin
EPFL, LCPM, Lausanne, Switzerland

MP-69 **Action spectroscopy of flavins**
M. Stockett, L. Giacomozzi, H. Zettergren, C. Kjær, J. Langeland Knudsen, L. Andersen, S. Brøndsted Nielsen, J. Bull, E. Carrascosa, E. Bieske
Stockholm University, Department of Physics, Stockholm, Sweden

MPS-S04 - Hyphenated Techniques

MP-70 **Speeding up GC-MS analysis – From few minutes down to real-time analysis**
A. B. Fialkov, U. Keshet, T. Alon, A. Amirav
School of Chemistry, Tel Aviv University, Tel Aviv, Israel

MP-71 **Development of comprehensive steroid analysis methods using GCxGC-ToFMS**
V. Artaev, D. Alonso, J. Shiel, G. Tikhonov, A. Lebedev
LECO Corporation, St. Joseph, USA

MP-72 **Using electrokinetic injection to increase throughput and improve sensitivity in the detection of proteins by CE-MS**
W. Belloni
Sciex Spa, Separations CE, Milano, Italy

MP-73 **Multivariate study of matrix effect in the analysis of phytoestrogens in soy-food by LC-ESI-MS/MS**
B. Benedetti, M. Di Carro, E. Magi
University of Genova, Department of Chemistry and Industrial Chemistry, Genova, Italy

MP-74 **Application of SPME GC-MS to explore possible differences in free-lactose milks from the market**
R. Bottiroli, E. Aprea, E. Betta, F. Gasperi
Edmund Mach Foundation, Food Quality and Nutrition Department, San Michele all'Adige, Italy

MP-75 **Post-column in-source derivatization in LC-MS: a tool for natural products characterization and metabolomics**
A. Cirigliano, G. M. Cabrera
DQO, FCEN, Universidad de Buenos Aires, UMYMFOR-DQO,UBA-CONICET, Buenos Aires, Argentina

MP-76 **Conjugation among nucleotides and cyanocobalamin functionalized with cisplatin: a study by liquid chromatography coupled with ESI and multistage MS**
G. Ventura, C. D. Calvano, A. Viola, V. Cinquepalmi, F. Palmisano, T. Cataldi
University of Bari, Dept.of Chemistry, Bari, Italy

MP-77 **Analytical method for quantification of bixin in extract of annatto using V-EASI(-)-LC-MS a method softer than ESI-LC-MS**
L. F. C. Oliveira, D. U. Tega, M. B Coelho, D. R. Morais, M. Baptistão, M. N. Eberlin
UNICAMP, Chemistry Institute, Campinas, Brazil

MP-78 **Thin layer chromatography combined with Flame-Induced Atmospheric Pressure Chemical Ionization Mass Spectrometry (FAPCI/MS) for volatile and semi-volatile compound analysis**
S. Cheng, J. Shiea
National Sun Yat-sen University, Department of Chemistry, Kaohsiung, Taiwan, Province of China

MP-79 **Evaluation of gas chromatography coupled to electrospray-atmospheric pressure photon ionization Orbitrap mass spectrometry as an advanced strategy for polyaromatic hydrocarbon analysis**
Y. Cho, E. Cho, S. Kim
Green-Nano Material Research Center, Kyungpook National University/Chemistry, Daegu, Republic of Korea

MP-80 **Online coupling of non-denaturing chromatography to native mass spectrometry is no more an impossible marriage**
A. Ehkirch, O. Hernandez-Alba, T. Botzanowski, S. Cianférani
LSMBO/IPHC, University of Strasbourg, CNRS UMR7178, Strasbourg, France

MP-81 **Identification and time variation analysis of perfume by using GCxGC/HRToFMS with EI/FI/PI**
R. Cody, M. C. Long, A. Dane, K. Okuda
JEOL USA, Inc., Mass Spectrometry, Peabody, USA

MP-82 **Seconds-per-sample: novel acoustic hyphenated approaches to enable truly label-free ultra high-throughput ambient mass spectrometry advancing drug discovery**
S. Datwani, L. Ghislain
Labcyte, Inc - Chemistry, San Josè, USA

MP-83 **Experimental measurements of effective electric field radii of Rectilinear ion traps**
C. Ding, F. Xu
Fudan University, Chemistry Department, Shanghai, China

MP-84 **Universal electrode for quadrupole electrode systems**
M. Dubkov, M. Burobin, V. Ivanov, A. Malutin, V. Gurov
Ryazan State Radio Engineering University, Department of General and Experimental Physics, Ryazan, Russian Federation

MP-85 **Degradation studies of the antibiotic sulfamethoxazole utilizing HPLC/MS**
K. Eckey, U. Karst
University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany

MP-86 **The importance of enhanced molecular ions in GC-MS**
A. B. Fialkov, U. Keshet, T. Alon, A. Amirav
Tel Aviv University, School of Chemistry, Tel Aviv, Israel

MP-87 **GC-MS with cold EI - extending the range of compounds and applications amenable for GC-MS analysis**
A. Amirav, A. Fialkov, T. Alon, U. Keshet
Tel Aviv University, School of Chemistry, Tel Aviv, Israel

MP-88 **Study of endocrine disrupting compound release from medical devices in plasma samples of premature newborns through an on-line SPE UHPLC-MS/MS method**
F. Gosetti, B. Bolfi, M. Manfredi, E. Robotti, F. Ferrero, G. Bona, E. Marengo
University of Piemonte Orientale, Department of Science and Technological Innovation, Alessandria, Italy

MP-89 **Triode-type MCP-based ion detector enabling miniature mass spectrometers to operate at low vacuum up to 1Pa**
M. Hayashi, Y. Washiyama, K. Ishii, J. Sakakiyama
Hamamatsu Photonics K.K., Electron Tube Division, Hamamatsu, Japan

MP-90 **The dynamic behavior of nano liquid bridge during ambient sampling ionization in scanning probe electrospray ionization mass spectrometry**
B. Kamihoriuchi, Y. Otsuka, A. Takeuchi, F. Iwata, T. Matsumoto
Osaka Univ., Department of Chemistry, Toyonaka, Japan

MP-91 **Integration of a droplet microfluidic chip with mass spectrometry – A step towards high throughput cellular analysis**
E. E. Kempa, X. Li, C. A. Smith, P. E. Barran
University of Manchester, Manchester Institute of Biotechnology, Manchester, United Kingdom

MP-92 **Portable gas chromatography mass spectrometer with a rapid heating carbon nanotube paste**
B. Yi, S. Y. Kim, W. Jeong, J. Y. Eo, B. S. Lee, B. Kang, H. S. Kim
Korea Basic Science Institute, Mass Spectrometry & Advanced Instrumentation Group, Cheongju, Republic of Korea

MP-93 **Analytical procedure for determination of perfluoroalkyl acids, parabens and cotinine from a low volume human serum sample by LC-MS/MS**
J. Koponen, H. Kiviranta
National Institute for Health and Welfare (THL), Health Security, Kuopio, Finland

MP-94 **Cold vaporization of Tissues by Picosecond Infrared Laser Ablation (PIRL) - Unique access to the original proteoform composition**
M. Kwiatkowski, H. Schlüter
University of Groningen, Department of Pharmacokinetics, Toxicology and Targeting, Groningen, Netherlands

MP-95 **From niche application to essential research tool: why SFC-MS is the must have technique**
G. J. Langley, J. M. Herniman
University of Southampton, Chemistry, Southampton, United Kingdom

MP-96 **Conventional-flow liquid chromatography−mass spectrometry for exploratory proteomic analyses**
J. Lenčo
Charles University, Faculty of Pharmacy in Hradec Kralove, Department of Analytical Chemistry, Hradec Králové, Czech Republic

MP-97 **Modern mobile mass spectrometry for on-site analysis of VOCs**
A. Marcillo, A. Widdig, C. Birkemeyer
University of Leipzig, Institute of Analytical Chemistry, Research Group of Mass Spectrometry, Leipzig, Germany

MP-98 **Determination of multi-residue antibiotics in surface water by SPE and UHPLC-MS/MS**
D. J. Mattern, Y. Li, Z. Gan, R. Liao, X. Li, X. Zhou, C. Cai, Y. Xie, F. Qin, J. Wu
PerkinElmer, Chromatography Support, Rodgau, Germany

MP-99 **Evaluation of capillary electrophoresis and ion mobility for cyclic lipopeptides analysis**
A. Mc Cann, J. Far, C. Delvaux, J. Liigand, L. Quinton, E. De Pauw
MSlab, Université de Liège, Liège, Belgium

MP-100 **Tandem Ionisation for GC(×GC)-MS: Complementary soft electron ionisation for increased confidence in compound identification**
N. Bukowski, L. Mcgregor, J. Blanch, P. Grosshans
SepSolve Analytical, SepSolve Analytical, Peterborough, United Kingdom

MP-101 **Fluorous modification of peptides for mass spectrometric applications**
A. Molnár, M. Berta, A. Steckel, K. Uray, J. Rábai, G. Schlosser
ELTE Eötvös Loránd University, Department of Analytical Chemistry, Budapest, Hungary

MP-102 **Evaluating the capability of different non-targeted MS-based approaches for the comprehensive characterization of olive tree-derived matrices**
L. Olmo-García, N. Kessler, A. Bajoub, C. M. Sánchez-Arévalo, A. Muñoz de la Peña, H. Neuweger, C. Baessmann, A. Carrasco-Pancorbo, A. Fernández-Gutiérrez
University of Extremadura, Department of Analytical Chemistry, Badajoz, Spain

MP-103 **An energy-resolved tandem mass spectrometry approach towards identification of small isomeric metabolites**
T. Nakamura, T. Hama, M. Sekimoto, F. Sato
RIKEN CSRS, Molecular Structure Characterization, Wako, Saitama, Japan

MP-104 **Highly efficient on-line protein digestion and peptide analysis: exploiting new short-bed trypsin-reactors**
M. Naldi, U. Cernigojc, A. Štrancar, M. Bartolini
Alma Mater Studiorum University of Bologna, Department of Pharmacy and Biotechnology, Bologna, Italy

MP-105 **A comparison of the results obtained for the analysis of South African pinotage wines using GCxGC-ToFMS with hydrogen and helium as carrier gases**
Y. Naudé, P. C. Gorst-Allman
University of Pretoria, Pretoria, South Africa

MP-106 **Analysis of an antiparasitic fraction against gastrointestinal nematodes of sheep from leaves of Maytenus ilicifolia by LC-ESI-IT-MS^n**
M. Escobal, G. De Souza, A. Mederos, C. Olivaro
Universidad de la República, Espacio de Ciencia y Tecnología Química, Tacuarembó, Uruguay

MP-107 **First report about the structure of an immunoadjuvant saponin fraction from Quillaja brasiliensis leaves by LC-ESI-IT-MS^n**
F. Wallace, Z. Bennadji, F. Ferreira, C. Olivaro
Universidad de la República, Espacio de Ciencia y Tecnología Química, Tacuarembó, Uruguay

MP-108 **A versatile semi-preparative HPLC platform, including HRMS and NMR, to support process development in industrial biotechnology**
B. Ozalp
DSM, R&D, Delft, Netherlands

MP-109 **Various chromatography approaches hyphenated with mass spectrometry for the determination of flavonoids and their metabolites**
V. Pilarová, J. Pavlík, T. Lacmanová, E. Espinola, L. Nováková
Charles University, Faculty of Pharmacy in Hradec Králové, Department of Analytical Chemistry, Hradec Králové, Czech Republic

MP-110 **Multidimensional gas chromatography coupled to isotope ratio mass spectrometry in sports drug testing**
T. Piper, M. Putz, M. Thevis
German Sport University Cologne, Institute of Biochemistry - Center for Preventive Doping Research, Cologne, Germany

MP-111 **MEMS Time-of-Flight mass spectrometer for in situ gas mixture analysis**
F. Progent, A. Sonnette, J. Tupinier, P. Buthier, J. Lictevout, S. Vigne, T. Alava
CEA, DAM, DIF, Arpajon, France

MP-112 **Atmospheric pressure chemical ionization – constructing ionization efficiency scale and derivatization reagent suitability**
R. Rebane, P. Liigand, J. Liigand, M. Oldekop, K. Herodes, I. Leito
University of Tartu, Institute of Chemistry, Tartu, Estonia

MP-113 **Microfluidic CE-MS for newborn screening: a single system for monitoring small molecule and protein biomarkers**
E. Redman, J. Mellors
908 Devices Inc., Life Sciences, Boston, USA

MP-114 **Development of rapid screening apparatus with DIP and PI/MS for additives in polymer materials**
Y. Mishima, T. Tsugoshi
NMIJ, AIST, Tsukuba, Japan

MP-115 **Comparison of the displacement mode versus gradient mode for proteomics using an online 2D-LC-MS/MS system**
H. Schlueter
University Medical Center Hamburg-Eppendorf, Mass Spectrometric Proteomics, Hamburg, Germany

MP-116 **Low-flow atmospheric pressure chemical ionization based on a gas dynamic virtual nozzle nebulizer**
T. Strmen, V. Vrkoslav, O. Paces, J. Cvacka
Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Department of Analytical Chemistry, Faculty of Science, Charles University in Prague, Prague, Czech Republic

MP-117 **Analysis of enzymes in laundry detergent using SDS-PAGE and MALDI-ToF-MS**
Z. Talebpour, G. Abedi, A. Ghassempour
Alzahra University, Department of Chemistry, Tehran, Iran

MP-118 **Mechanistic reaction insights by in-situ monitoring of an AACVD reaction using GC-MS: studying the $ZnFe_2O_4$ thin film growth process**
I. C. Usen, U. Wijayantha-Kahagala-Gamage, J. C. Reynolds
Loughborough University, Department of Chemistry, Loughborough, United Kingdom

MP-119 **Pulsed extraction mode for off-axis time of flight mass spectrometer**
W. Guanyi, L. Zhiming, Z.Lihua, Y. Xianglong, D. Hu, S.Xiaopan, W. Wenliang
Northwest Institute of Nuclear Technology, Xi'an, China

MP-120 **Probing the limits of on-line reaction monitoring by small footprint ESI-MS and NMR**
C. Whitmore, A. Kenwright, A. Ray, S. Coombes, J. Mosely
Durham University, Department of Chemistry, Durham, United Kingdom

MP-121 **Improvement of electrostatic quadrupole zoom lens for fixed multi-collector system in LRI-MS**
X. Yuan, Z. Li, L. Zhai, J. Xu, X. Shen, H. Deng, W. Wang
Northwest Institute of Nuclear Technology, Xi'an, China

MPS-S05 - Volatile Molecules & Nose-Space Analysis

MP-122 **Overview of the volatile components of the Corsican liverwort Scapania undulata**
A. Pannequin, A. Tintaru, J.-M. Desjobert, J. Costa, A. Muselli
Université de Corse, Laboratoire de Chimie des Produits Naturels, Corte, France

MP-123 **Effect of germination time, roasting level and altitude in the aroma released by coffee powder monitored by proton transfer reaction mass spectrometry and gas chromatography mass spectrometry**
M. Bodner, K. Morozova, P. Kruathongsri, P. Thakeow, S. Angeli, M. Scampicchio
Free University of Bolzano-Bozen, Faculty of Science and Technology, Bolzano, Italy

MP-124 **Feasibility of selected Ion flow tube mass spectrometry (SIFT-MS) to real-time monitoring of exhaled breath volatile organic compounds (VOCs) in cancer patients**
G. Corona, G. Miolo, A. Carretta, A. Steffan
IRCCS National Cancer Institute, Immunopathology and Cancer Biomarkers, Aviano(PN), Italy

MP-125 **Clostridium tetani (C. tetani) cultivation process monitoring by Headspace solid-phase microextraction (HS-SPME) combined with GC-MS**
A. Es-Haghi, M. Ghader, N. Shokoufi, K. Kargosha
Razi Vaccine & Serum Research Institute, Department of Physico Chemistry, Karaj, Iran

MP-126 **SPME-GC/MOX sensor system: a new method for the evaluation of human semen quality**
V. Longo, A. Forleo, P. S. Pinto, D. D. Montagna, L. Coppola, V. Zara, A. Ferramosca, P. Siciliano, S. Capone
National Research Council, Institute for Microelectronics and Microsystems, Lecce, Italy

MP-127 **The volatile faecal metabolome in Cushing's syndrome mouse model of type 2 diabetes**
C. Lourenço, M. Cauchi, L. Bentley, R. D. Cox, C. Turner
Cranfield University, School of Aerospace, Transport and Manufacturing, Cranfield, Bedfordshire, United Kingdom

MP-128 **Investigations of VOCs present in breath using PTR-MS: preliminary studies of ketones and anaesthetics**
M. Malásková, D. Olivenza-León, F. Piel, P. Mochalski, M. Klieber, C. Mayhew
University of Innsbruck, Institute for Breath Research, Innsbruck, Austria

MP-129 **An innovative analysis method for fragrance of sake using an introducing device for volatile compounds combined with DART-MS**
C. Takei, Y. Otake, K. Yoshizawa, H. Nishimoto, T. Akashi
BioChromato, Fujisawa, Japan

MP-130 **Exploring inter-individual differences in In-vivo flavour release by SIFT-MS**
M. Pedrotti, L. Menghi, I. Khomenko, A. Caretta, E. Aprea, A. Cavazzana, T. Hummel, F. Gasperi, F. Biasioli
Foundation Edmund Mach, Wageneningen University FQD, Wageningen, Netherlands

MPS-S06 - Clinical Chemistry

MP-131 **Impact of CYP2D6 genetic polymorphism on the pharmacokinetics of tramadol and its three main metabolites in Koreans**
J. Bae, S. Lee, K. Chun, M. Je Choi, S. Hong
Keimyung University, College of Pharmacy, DAEGU, Republic of Korea

MP-132 **Individual and cyclic estrogenic profile in woman: structure and variability of the data**
C. Bozzolino, S. Vaglio, E. Amante, E. Alladio, E. Gerace, M. Vincenti
Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", University of Turin, Department of Chemistry, Turin, Italy

MP-133 **Pharmacokinetic of Myriocin in rabbit's eyes**
M. Dei Cas, F. M. Rubino, J. Rizzo, S. Paola, E. Strettoi, C. Platania, C. Bucolo, R. Pignatello, R. Ghidoni, R. Paroni
University of Milan, Department of Health Sciences, Milan, Italy

MP-134 **Comparison of ESI, APCI and APPI ionization techniques for testosterone (T), dihydrotestosterone (DHT) and estradiol (E2) LC-MS/MS assay**
R. Desai, P. Keski-Rahkonen, T. Harwood, D. Handelsman
Anzac research institute, Andrology, Concord, Sydney, Australia

MP-135 **Highly selective and fast identification of Brucella by immunoaffinity- MALDI-ToF mass spectrometry**
H. Hamidi, M. Zarrineh, I. Soleimani, N. R. Bagheri, A. Es-Haghi, A. Ghassempour
Medicinal Plants and Drugs Research Institute, Shahid Beheshti University, Tehran, Iran

MP-136 **Analysis of protein biomarkers from low sample volumes**
T. G. Halvorsen, C. Rosting, M. C. S. Levernæs, L. Reubsaet
University of Oslo, School of Pharmacy, Oslo, Norway

MP-137 **Early and non-invasive mass spectrometry tool for diagnosing aspergillosis**
R. Dobias, A. Skriba, T. Pluhacek, M. Petrik, P. Lyskova, V. Havlicek
Institute of Microbiology, Academy of Sciences of the Czech Republic, Prague, Czech Republic

MP-138 **Analysis of underivatized amino acids in exhaled breath condensate samples as monitoring therapy for children with type 1 diabetes**
M. Pyszka, L. Konieczna, M. Okońska, Ł. Szmygel, M. Myśliwiec, T. Bączek
Medical University of Gdańsk, Department of Pharmaceutical Chemistry, Gdańsk, Poland

MP-139 **Development and validation of a high sensitivity assay of estrogens in human plasma by UHPLC-MS/MS without derivatization**
M. Levi, H. Kobayashi, J. Watanabe
Shimadzu Corporation, MS BU, Kyoto, Japan

MP-140 **ICP-MS immunoassay using metal-doped nanoparticles for multiplex detection of HIV-1 p24 and HBsAg**
H. B. Lim, C. Kim
Dankook University, Chemistry, Chunan, Republic of Korea

MP-141 **Solid phase microextraction coupled to mass spectrometry via microfluidic open interface for point-of-care testing of tranexamic acid in plasma of cardiac surgical patients**
N. Looby, M. Tascon, J. Acquaro, N. Reyes-Garcés, T. Vasiljevic, G. A. Gómez-Ríos, M. Wasowicz, J. Pawliszyn
University of Waterloo, Department of Chemistry, Waterloo, Canada

MP-142 **Study of non-covalent interaction between ALS-linked mutant PFN1 protein and natural compound by mass spectrometry**
M. Nekouei, P. Ghezellou, M. Kiaei, A. Ghassempour
Shahid Beheshti University, Medicinal Plants and Drugs Research Institute, Tehran, Iran

MP-143 **Detection and quantification of carbohydrate deficient transferrin by MALDI-compatible protein chips prepared by ambient ion soft landing**
P. Novak, P. Darebna, M. Volny, V. Ruzicka, J. Spicka, R. Kucera, P. Pompach
Institute of Microbiology, Laboratory of Structural Biology, Prague, Czech Republic

MP-144 **Acetylcholine and acetylcholinestrase in a non-neuronal tissue (Corneal epithelium)**
I. Oulie, L. Reubsaet, T. G. Halvorsen, A. Ringvold
University of Oslo, School of Pharmacy, Dept. of Pharmaceutical Chemistry, Pharmaceutical analysis, Oslo, Norway

MP-145 **Development and validation of a sensitive LC-linear ion trap method for the determination of trace di-iodothyronines in human blood serum**
K. Richards, J. Köhrle, D. Rathmann, R. Monk
Charite Universitätsmedizin Berlin, Institute for Experimental Endocrinology, Berlin, Germany

MP-146 **Using data dependent acquisition to produce specifik and reliable MRM transitions for suspects on a Qtrap instrument**
S. K. Steffensen, I. Fomsgaard
Aarhus University, Department of AgroecologyFlakkebjerg, Denmark

MP-147 **Evaluation of UDP-glucuronosyltransferase 1A1 activity towards bilirubin**
A. Takeuchi
Instrumental Analysis Center, Kobe Pharmaceutical University, Kobe, Japan

MP-148 **A Biomphalaria glabrata peptide that stimulates extreme behaviour modifications in aquatic free-living Schistosoma mansoni miracidia**
T. Wang, R. Wyeth, D. Liang, U. Bose, G. Ni, D. Mcmanus, S. Cummins
University of the Sunshine Coast, School of Science and Engineering, Sippy Downs, Australia

MP-149 **Analysis of sweeteners in urine using novel stationary phase and selective LC-MS/MS method**
B. Cervinkova, R. Kay, A. Koulman
NIHR BRC Nutritional Biomarker Laboratory, University of Cambridge, Cambridge, United Kingdom

MP-150 **Pharmacokinetics and bioavailability of different acetylsalicylic acid formulations assessed by liquid chromatography-tandem mass spectrometry in healthy subjects**
J. Rizzo, M. Dei Cas, F. M. Rubino, R. C. Paroni
University of Milan, Department of Health Sciences, Milan, Italy

MP-151 **Which LC-MS/MS platform is most appropriate for the quantitative analysis of Steroids in urine, serum and oral fluid for Clinical Research**
S. Indelicato, R. M Doyle, D. McDowell
Thermo Fisher, CMD, Paris, France

MP-152 **GC-MS and LC-MS profiling of exhaled breath condensate: investigation of sampling considerations**
A. K. C. Laserna, H. F. Lim, N. S. Tan, E. Horiyanto, B. H. Ng, R. Verma, N. Paton, S. F. Y. Li
National University of Singapore, Department of Chemistry, Singapore

MP-153 **Set up of a simple, fast and flexible LC-MS/MS ID method for the simultaneous determination of steroids in different biological samples.**
G. Bartolucci, M. Pallecchi, S. Gozzo, G. Danza
University of Florence, department of experimental biomedical and clinical science, Firenze, Italy

MP-154 **Chemometric optimization of UPLC-MS/MS assay for clinical diagnosis and pharmacotherapy monitoring of patients with APRT deficiency**
M. Thorsteinsdóttir, U. A. Thorsteinsdóttir, F. F. Eiriksson, H. L. Runolfsdottir, V. O. Edvardsson, R. Palsson
University of Iceland, Faculty of Pharmaceutical Sciences, Reykjavik, Iceland

MPS-S07 - Quantitative Proteomics

MP-155 **Optimization of biotin enrichment protocol and its application for the analysis of organelle-enriched proteins by LC-MS/MS**
S. Ahmadi, D. Winter
University of Bonn, Institute of Biochemistry and Molecular Biology, Bonn, Germany

MP-156 **Sample multiplexing by isoelectric focusing (pI-Coding) for isobaric labeling and label-free quantification**
J. Astorga-Wells, C. Beusch, T. Lavold, R. A. Zubarev
Karolinska Institutet, Medical Biochemistry and Biophysics, Stockholm, Sweden

MP-157 **Differential proteomic analysis of actinic keratosis, bowen's disease and cutaneous squamous cell carcinoma by Sequential Window Acquisition of All Theoretical Mass Spectra (SWATH-MS)**
A. Azimi, M. Ali, K. Kaufman, P. Yang, G. Mann, P. Fernandez-Penas
The University of Sydney, Centre for Translational Skin Research, Westmead, Australia

MP-158 **Tape stripped stratum corneum samples prove to be suitable for comprehensive proteomic investigation of actinic keratosis**
A. Azimi, M. Ali, K. Kaufman, G. Mann, P. Fernandez-Penas
The University of Sydney, Centre for Translational Skin Research, Westmead, Australia

MP-159 **A high-resolution organellar proteomics approach to study protein subcellular distribution and dynamics in cells**
C. Steinbrueck, J. Jordan, M. Kocylowski, A. Kollewe, W. Bildl, A. Haupt, B. Fakler, U. Schulte
University of Freiburg, Institute of Physiology, Faculty of Medicine, Freiburg, Germany

MP-160 **Evaluation of proteomics quantitative methods on a reconstructed skin model**
S. Bourassa, C. Gotti, M. Scott-Boyer, J. Marcoux, I. Kelly, A. Droit
CHU de Quebec proteomics Platform, Laval University, Quebec, Canada

MP-161 **New pharmacological targets for cystic fibrosis treatment from extensive proteomic profiling of ΔF508-CFTR expressing cells**
C. Braccia, V. Tomati, N. Pedemonte, A. Armirotti
Istituto Italiano di Tecnologia, Università degli Studi di Genova, Genova, Italy

MP-162 **Straight forward phosphoproteomic analysis pipeline in CHO cells as mammalian non-model organism**
L. Brachtvogel, A. Pries, S. Walter, T. Noll, R. Hoffrogge
Cell Culture Technology, Bielefeld University, Bielefeld, Germany

MP-163 **Comparative proteomics study for elucidation of potential mechanisms underlying yeast resistance to alcohols**
J. Bubis, V. Gorshkov, F. Kjeldsen, M. Gorshkov, I. Tarasova, D. Spasskaya, D. Karpov
Talrose Institute for Energy Problems of Chemical Physics,
Moscow, Russian Federation

MP-164 **Quantitative label-free proteomics in a novel cellular knock out model of methylmalonic acidemia**
M. Costanzo, M. Caterino, A. Cevenini, I. C. Guerrera, M. Ruoppolo
University of Naples "Federico II", Department of Molecular Medicine and Medical Biotechnology, Naples, Italy

MP-165 **Inactivated Poliovirus vaccine antigen determination: a proteomics approach**
M. Creskey, D. Viel, T. Wu, T. Cyr
Health Canada, Biologics and Genetic Therapies Directorate, Ottawa, Canada

MP-166 **TMT-based quantitative approach discloses Monacolin K-induced proteome alterations in triple negative breast cancer cells**
F. del Gaudio, M. C. Monti, S. Rontogianni, K. Stecker, I. C. Guerrera, R. Riccio, A. J. R. Heck, M. A. F. Altelaar
Department of Pharmacy, University of Salerno, Salerno, Italy

MP-167 **High throughput signaling pathway monitoring based on fast LC-PRM analyses**
S. Gallien, A. Gajadhar, B. Patel, T. Arrey, D. Sarracino, Y. Xuan, E. Chen
Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, USA

MP-168 **Quantitation of amylase/trypsin-inhibitors in various wheat species**
S. Geisslitz, K. Scherf, P. Koehler
Leibniz-Institute for Food Systems Biology at the Technical University of Munich, Freising, Germany

MP-169 **Peptide migration profiles: a tool to trace proteolytic processes - Factor XII contact systhem activation**
L. Heikaus, H. Schlüter
University Medical Center Hamburg-Eppendorf, Mass Spectrometric Proteomics, Hamburg, Germany

MP-170 **Myelin proteomics 2.0: application to mouse models for myelin-related diseases**
O. Jahn, S. Siems, D. Hesse, S. Tenzer, H. Werner
Max-Planck-Institute of Experimental Medicine, Proteomics Group, Göttingen, Germany

MP-171 **Simplifying the use of ion libraries during data processing of data independent acquisition proteomics data**
M. Huebsch, D. Waidelich, A. Lau, K. Lewis, N. Morrice, J. Dojahn, D. Merkel, R. Sayers, Z. Demianova, S. Ahadi, C. Hunter, J. Jasak
Sciex, Darmstadt, Germany

MP-172 **The improvement in cognitive functions in 5XFAD Alzheimer's transgenic mouse model via natural compound administration**
M. Karayel Başar, I. Kiris, B. Gürel, T. Mroczek, K. Skalicka-Wozniak, A. T. Baykal, M. Y. Günal
Acibadem Mehmet Ali Aydinlar University, Medical Biochemistry, İstanbul, Turkey

MP-173 **Simultaneous dual proteome analysis towards understanding neutrophil interaction with the human-pathogenic fungus Aspergillus fumigatus**
T. Krüger, I. A. Shopova, T. Müller, M. Dittrich, D. J. Mattern, T. Conrad, O. Kniemeyer, A. A. Brakhage
Leibniz Institute for Natural Product Research and Infection Biology (Hans Knöll Institute), Department of Molecular and Applied Microbiology, Jena, Germany

MP-174 **Biomarker discovery of atherosclerotic stroke in individual serum sample**
J. Lee, S. Mun, A. Park, Y. Lee, A. Seok, H. Kim, Y. Lee, H. Kang
Eulji University, Department of Biomedical Laboratory Science, College of Health Sciences, Seongnam-si, Gyeonggi-do, Republic of Korea

MP-175 **Development of a simple and efficient quantification method of human follicular fluid (hFF) proteome**
A. Lewandowska, A. Fel, K. Macur, P. Czaplewska, J. Liss, K. Lukaszuk, S. Oldziej
Intercollegiate Faculty of Biotechnology UG-MUG, University of Gdansk, Gdansk, Poland

MP-176 **A target fishing and shotgun proteomics approaches to study the effect of a new drug against M. tuberculosis**
M. Manfredi, L. Chiarelli, A. Buzzi, M. Pasca, F. Gosetti, E. Barberis, E. Robotti, E. Marengo
University of Piemonte Orientale, Department of Sciences and Technological Innovation, Alessandria, Italy

MP-177 **A cost-effective approach to produce ^{15}N-labelled amino acids employing *Chlamydomonas Reinhardtii* CC503**
J. M. Marchante-Gayón, C. J. Nicolás, G. P. Rodríguez, G. L. Valledor, V. M. J. Cañal, A. J. I. García
University of Oviedo, Department of Physical and Analytical Chemistry, Oviedo, Spain

MP-178 **Characterization of protein extracts from yeast cells exposed to fermented Spirulina (*Arthrospira platensis*) using high resolution Orbitrap mass spectrometry**
J. Masten, B. Cillero-Pastor, R. Mohren, N. Ogrinc, P. Jamnik
Jožef Stefan Institute, Jožef Stefan International Postgraduate School, Department of Environmental Sciences, Ljubljana, Slovenia

MP-179 **QConCat-based absolute quantification of the lysosomal proteome by multiple reaction monitoring**
P. Mosen, R. Sakson, T. Ruppert, V. Gieselmann, D. Winter
Institute of Biochemistry and Molecular Biology, University of Bonn, Bonn, Germany

MP-180 **Validation strategies for the purity assessment of peptide standards by isotope dilution mass spectrometry**
J. Nicolas-Carcelen, A. Gonzalez-Gago, A. Suarez-Fernandez, J. M. Marchante-Gayon, P. Rodriguez-Gonzalez, J. I. Garcia-Alonso
University of Oviedo, Analytical and Physical Chemistry, Oviedo, Spain

MP-181 **Quantitative microproteomics for the characterization of central and peripheral nervous system of the Twitcher mouse**
D. Pellegrini, G. Ambra Del, L. Angella, N. Giordano, I. Tonazzini, M. Caleo, M. Cecchini, L. McDonnell
NEST, Scuola Normale Superiore, Pisa, Italy

MP-182 **Quantitaive study of metabolic pathways in C. Elegans using MS Western**
B. K. Raghuraman, A. Shevchenko
Max Planck Institute of Molecular Cell Biology and Genetics, Biological Mass Spectrometry, Dresden, Germany

MP-183 **Application of manual chromatography device for fractionation of complex peptide samples prior nanoESI-MS/MS**
P. Rehulka, H. Rehulkova, V. Franc, M. Sebela, R. Kupcik, Z. Bilkova, J. Stulik
University of Defence, Faculty of Military Health Sciences, Hradec Králové, Czech Republic

MP-184 **Discussion of the pros and cons of isobaric labelling compared to single shot data-independent acquisition**
J. Muntel, R. Bruderer, J. M. Kirkpatrick, O. M. Bernhardt, L. Verbeke, T. Gandhi, T. Huang, O. Vitek, A. Ori, L. Reiter
Biognosys, R&D, Schlieren, Switzerland

MP-185 **High speed, high sensitivity and highly reproducible and accurate label free quantification using the PASEF method on a TIMS QToF**
G. Kruppa, M. Lubeck, H. Koch, V. Tellström, P. Shan, C. Cox, S. Koch
Bruker France, Proteomics, Wissembourg, France

MP-186 **FAIMS reduces interference and improves quantitative accuracy in multiplexed proteomics**
D. Schweppe, S. Prasad, R. Huguet, P. J. Navarrete, J. Paulo, M. Jedrychowski, G. Mcalister, S. Abbatiello, M. Belford, V. Zabrouskov, S. Gygi
Harvard Medical School, Boston, USA

MP-187 **A targeted multiple reaction monitoring method for quantifying Nav1.6 protein in HEK239 cells and mouse hippocampus**
M. Tung, R. Kwan, C. Xi, J. Li, C. Dang, L. E. Sojo
Xenon Pharmaceuticals Inc., Compound Properties Group, Burnaby, Canada

MP-188 **Comparative proteogenomic analysis of colistin-dependence in Acinetobacter baumannii**
S. Chamoun, J. Welander, C. Claesson, E. Vikström, M. Turkina
Linköping University, Department of Clinical and Experimental Medicine, Linköping, Sweden

MP-189 **TMT quantification using spectral libraries in SpectroMine**
L. Verbeke, T. Gandhi, O. M. Bernhardt, L. Reiter
Biognosys AG, Bioinformatics, Schlieren, Switzerland

MP-190 **Multiplex quantitative assay of inflammation protein markers in feces samples**
V. Vidova, V. Thon, J. Klanova, Z. Spacil
Research Centre (RECETOX), Masaryk University, Faculty of Science, Brno, Czech Republic

MP-191 **Development of a quality control standard for Tandem Mass Tags (TMT) workflows**
J. Choi, A. Robitaille, T. N. Arrey, R. Viner, A. Huhmer, J. C. Rogers
Thermo Fisher Scientific, San Jose, USA

MP-192 **Solving the yellow mystery of Papaver nudicaule with an integrated -omics approach**
B. Dudek, N. Wielsch, R. C. Menezes, A. Warskulat, Y. Hupfer, S. Lorenz, H. Vogel, C. Paetz, B. Schneider, A. Svatos
Max Planck Institute for Chemical Ecology, Mass Spectrometry / Proteomics Group, Jena, Germany

MP-193 **A streamlined workflow for high-throughput, precise, and comprehensive large-scale quantitative proteomics analysis**
Y. Xuan, Y. Zhou, S. Gallien, O. Boychenko, J. J. Nicklay, J. Ho, S. Peterman, P. Navarro, E. I. Chen, K. Miller
Thermo Fisher Scientific, Chromatography and Mass Spectrometry Division (CMD), Bremen, Germany

MP-194 **Advancing mass spectrometry-based large-cohort proteomics for precision medicine – An international Cancer Moonshot multi-site study**
Y. Xuan, N. W. Bateman, Y. Chen, A. Sickmann, B. Wollscheid, C. R. Jimenez, M. R. Larsen, H. Zhou, S. Liu, Z. Chen, T. Kislinger, B. Crossett, S. Gallien, Y. Zhou, P. Navarro, R. Birhanu Kitata, C. Lorenz, S. Goetze, S. Piersma, D. Chiasserini, M. Tahir, H. Zhu, G. Hou, X. Sun, A. Macklin, A. Khoo, B. L. Parker, S. J. Cordwell, T. P. Conrads
Thermo Fisher Scientific, Chromatography and Mass Spectrometry Division (CMD), Bremen, Germany

MP-195 **Global analysis of protein complexes in Trypanosoma brucei using cross-linking mass spectrometry**
F. Almeida, M. Tinti, M. Ferguson
The University of Dundee, Biological Chemistry and Drug Discovery, Dundee, United Kingdom

MP-196 **Abundant protein depletion of human plasma samples – Sample preparation approaches for quantitative comparison studies**
R. Bomgarden, S. Snovida, K. Herting, R. Ganapathy, B. Kaboord, J. Rogers
Thermo Fisher Scientific, R&D, Rockford, USA

MP-197 **Quantification of human insulin and its analogues by immunopurification and LC-MS/MS**
J. Kooistra, J. Grzetic-Martens, Y. Lamkadam, T. Noij
Charles River Laboratories, Bioanalysis, Den Bosch, Netherlands

MP-198 **Parallel evaluation of MALDI-ToF and tandem LC-ESI mass spectrometry for rapid quantification of abrin toxin in complex matrices**
S. Livet, S. Worbs, E. Hansbauer, H. Volland, S. Simon, C. Junot, F. Fenaille, B. G. Dorner, F. Becher
CEA Saclay, DRF - Institut des sciences et du vivant Frédéric Joliot - Service de Pharmacologie et d' Immunoanalyse (SPI), Gif-su- Yvette, France

MP-199 **Proteomic analysis of unconventional protein secretion**
C. Mayrhofer, K. Nöbauer, G. Brem
University of Veterinary Medicine Vienna, Institute of Animal Breeding and Genetics, Institute of Biotechnology in Animal Production, IFA Tulln, Wien, Austria

MP-200 **Proteome of avian pathogenic E. coli during infection: methods and results.**
A. Nawrocki, A. E. Johansen, J. Møller-Jensen, J. E. Olsen, M. R. Larsen
University of Southern Denmark, Biochemistry and Molecular Biology, Odense, Denmark

MP-201 **Comparative study of three MS-based approaches for quantitative proteomics analysis**
D. Taverna, M. Gaspari, M. Catracchia
Proteomics-UMG lab, Department of Experimental and Clinical Medicine, Magna Graecia University of Catanzaro, Italy

MP-202 **Proteomic and metabolomic alterations in the rat brain after ischemic stroke**
J. Teppo, A. Vaikkinen, K. Mätlik, T. Kotiaho, M. Airavaara, R. Kostiainen
University of Helsinki, Faculty of Pharmacy, Helsinki, Finland

MP-203 **Determination of peptide purity by UV-MS and quantitative NMR**
F. A. Torma, M. Quaglia, J. Warren
LGC LTD, Chemical Measurement and Calibration, Teddinton, United Kingdom

MP-204 **Universal S-Trap sample processing: standardized reproducible sample workup from < µg to > mg scales for all sample types**
J. Wilson, D. J. Pappin
Cold Spring Harbor Laboratory, Cold Spring Harbor, USA

MPS-S08 - Chiral Discrimination

MP-205 **Self-assembled binuclear Cu(II)−histidine complex for absolute configuration and enantiomeric excess determination of naproxen by tandem mass spectrometry**
X. Yu, M. Chau, W. Kit Tang, C. Siu, Z. Yao
City University of Hong Kong, Department of Chemistry, Kowloon Tong, Hong Kong

MP-206 **Spectroscopic discrimination of diastereomeric complexes involving an axially chiral receptor**
A. Filippi, C. Fraschetti, L. Guarcini, C. Zazza, T. Ema, M. Speranza
Sapienza, University of Rome, Chemistry and Technology of Drugs Department, Rome, Italy

MP-207 **Acid-based recognition of diastereoisomeric peptides using ion mobility mass spectrometry**
M. Zimnicka
Polish Academy of Sciences, Institute of Organic Chemistry, Warsaw, Poland

MPS-S09 - Ambient MS and New Ionization Methods

MP-208 **A versatile integrated Ambient Ionization Source (iAmIS) platform and its applications**
Y. Bai, W. Ai, S. Xu, H. Liu
Peking University, College of Chemistry, Beijing, China

MP-209 **The role of new materials as sampling substrates for the DESI-HRMS determination of new psychoactive substances in saliva**
F. Bianchi, S. Agazzi, N. Riboni, M. Hakkarainen, L. Ilag, R. Cecchi, L. Anzillotti, M. Careri
University of Parma, Department of Chemistry, Life Sciences and Environmental Sustainability/ CIPACK, Parma, Italy

MP-210 **Matrix effects in Low Temperature Plasma Ionization (LTPI) mass spectrometry**
A. Kiontke, B. Scholz, W. Honscha, C. Birkemeyer
Universität Leipzig, Leipzig, Germany

MP-211 **Application of LDTD/TQMS-HRMS methods for quantification of psychoactive compounds in tissue microsamples**
A. Borik, A. Vojs Stanova, K. Grabicova, T. Randak, R. Grabic
University of South Bohemia in Ceske Budejovice, Faculty of Fisheries and Protection of Waters, Laboratory of Environmental Chemistry and Biochemistry, Vodnany, Czech Republic

MP-212 **Breath analysis with Secondary Ionization High-Resolution Mass Spectrometry (SESI-HRMS) in the clinical environment with a focus on disease specific biomarkers in children with cystic fibrosis**
T. Bruderer, N. Haas-Baumann, R. Weber, A. Baghdasaryan, S. J. Micic, S. Mueller, F. Singer, R. Zenobi, A. Moeller
University Children's Hospital Zurich, Division of Respiratory Medicine, Zurich, Switzerland

MP-213 **One size does not fit all: DART and complementary ambient ionization methods**
R. Cody
JEOL USA, Inc., Mass Spectrometry, Peabody, USA

MP-214 **Enhanced coupling of Acoustic Levitation SAII mass spectrometry for direct ionization and reaction monitoring**
E. A. Crawford, D. Dietrich, C. Esen, D. A. Volmer
Saarland University, Institute of Bioanalytical Chemistry, Saarbruecken, Germany

MP-215 **Direct Infusion Resonance-Enhanced Multiphoton Ionization Mass Spectrometry of liquid samples under vacuum conditions**
H. Czech, C. Kruth, M. Sklorz, J. Passig, S. Ehlert, A. Cappiello, R. Zimmermann
University of Rostock, Chair of Analytical Chemistry, Rostock, Germany

MP-216 **Ion chemistry fundamentals of secondary electrospray ionization mass spectrometry (SESI-MS) for VOC analyses**
K. Dryahina
J. Heyrovský Institute of Physical Chemistry, Department of Chemistry of Ions in Gaseous Phase, Prague, Czech Republic

MP-217 **SpiderMass a novel tool to tackle in-vivo mass spectrometry**
P. Saudemont, A. Baud, E. Bouchaert, Q. Pascal, M. Ziskind, D. Tierny, M. Salzet, I. Fournier
PRISM Inserm U1192, University of Lille, Lille, France

MP-218 **Molecular Surgery Navigation by the combination of mass spectrometry with molecular resonance probe desorption**
V. Frankevich, V. Chagovets, A. Kononikhin, G. Sukhikh
Federal State Budget Institution "Research Center for Obstetrics, Gynecology and Perinatology" Ministry of Healthcare and Social Development of the R, Systems Biology, Moscow, Russian Federation

MP-219 **A comparison between diathermic knife and CO$_2$-laser coupled to REIMS-ToF for instantaneous tissue classification**
M. Genangeli, R. M.A. Heeren, T. Porta
M4I, Maastricht University, Maastricht, Netherlands

MP-220 **Multi-scheme chemical ionization inlet for atmospheric pressure mass spectrometry applications**
M. P. Rissanen, J. Mikkilä, J. Hakala
Karsa Ltd, Karsa Ltd, Helsinki, Finland

MP-221 **Observable charge states in native MS: differences between ESI and LILBID**
J. Hoffmann, K. Karimi, N. Morgner
University, Goethe University Frankfurt, Institute of Physical and Theoretical Chemistry, Frankfurt, Germany

MP-222 **Performance enhancement using He buffer gas in a small-scale LIT for in-the-filed mass spectrometry**
A. Janulyte, Y. Zerega, J. Andre
Aix-Marseille University, CNRS, Laboratoires PIIM (UMR 7345), Madirel (UMR 7246), Marseille, France

MP-223 **Charaterization of cold electron ionization for portable mass spectrometers**
S. Y. Kim, W. Jeong, B. Yi, Y. Eo Jae, B. Kang, H. S. Kim, M. Yang
Korea Basic Science Institute, Mass Spectrometry & Advanced Instrumentation, Cheongju, Republic of Korea

MP-224 **Graphene layer substrate assisted laser desorption at atmospheric pressure for high spatial resolution mass spectrometry imaging**
J. Y. Kim, S. Y. Lee, H. . Lim, J. Park, D. Lim, D. W. Moon
Mass Spectrometry & Advanced Instrumentation Group, Korea Basic Science Institute, Cheongju Republic of Korea

MP-225 **Portable Time-of-flight mass spectrometer using a cold electron beam pulse**
W. Jeong, S. Y. Kim, B. Yi, J. Y. Eo, B. Kang, H. S. Kim, M. Yang
Div. of Scientific Instrumentation, Korea Basic Science Institute, Cheongju, Republic of Korea

MP-226 **Soft and hard ionization of volatile organic compounds by EI followed by MS/MS analysis**
A. Kornilova, L. Cousins, R. Javahery
PerkinElmer Inc., RND, Woodbridge, Canada

MP-227 **Ion source multiplexing on a single mass spectrometer**
Y. Kostyukevich, A. Zherebker, E. Nikolaev
Skoltech, Skoltech, Moscow, Russian Federation

MP-228 **Identification of chemicals in different objects by direct analysis in real time mass spectrometry**
Á. Kuki, B. Antal, L. Nagy, T. Nagy, G. Zelei, M. Zsuga, S. Kéki
University of Debrecen, Department of Applied Chemistry, Debrecen, Hungary

MP-229 **Explosives detection with a mobile Thermal Desorption Direct Analysis in Real Time Mass Spectrometry system (TD- DART-MS)**
F. Li, B. Laramee, P. Liang, B. Musselman
IonSense, Inc., Chemistry, Saugus, USA

MP-230 **Predicting aAgents that "supercharge"**
R. O. Loo, R. O'brien-Johnson, M. Nshanian, J. Loo
UCLA, DOE Laboratory for Genomics & Proteomics, Los Angeles, USA

MP-231 **Substrate modification for the analysis of highly volatile chemical warfare agents by paper spray mass spectrometry**
P. Mach, E. Dhummakupt, P. Demond, D. Carmany, M. Busch, T. Tovar, A. Ploskonka, J. Decoste, T. Glaros
Excet, Inc., Research & Technology Directorate, Springfield, USA

MP-232 **Laser-Ablation Rapid Evaporative Ionization Mass Spectrometry (LA-REIMS) for lipidomics analysis of living CHO cells directly from the cell culture**
S. Maneta-Stavrakaki, S. J. Cameron, J. Abda, A. Perdones-Montero, J. Maldutyte, Y. Chim, P. Diaz-Fernandez, Z. Takáts
Department of Surgery and Cancer, Sir Alexander Fleming Building, Imperial College, London, United Kingdom

MP-233 **Optical characteristics of matrix materials for matrix-assisted laser desorption/ionization**
N. Masaki, S. Okazaki
Department of Medical Spectroscopy, Hamamatsu University School of Medicine, Hamamatsu, Japan

MP-234 **Extending the polarity range for direct SPME-MS analyses by using novel capillary DBDI and APPI sources**
M. F. Mirabelli, A. K Huba, R. Zenobi
ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland

MP-235 **Combined Infrared and Ultraviolet Laser Ablation Electrospray Ionization Mass Spectrometry**
K. K. Murray, R. Lawal, F. Donnarumma
Louisiana State University, Department of Chemistry, Baton Rouge, USA

MP-236 **Rapid qualitative analysis of two flavonoids, rutin and silybin, in medical pills by direct analysis in real time mass spectrometry (DART-MS) combined with in situ derivatization**
L. Nagy, T. Nagy, Á. Kuki, M. Zsuga, S. Kéki
University of Debrecen, Department of Applied Chemistry, Debrecen, Hungary

MP-237 **A novel modular and versatile ToF platform combinable with various ion sources**
A. Jordan, F. Piel, S. Feil, E. Hartungen, G. Hanel, J. Herbig, K. Winkler, R. Gutmann, L. Märk, P. Sulzer
Ionicon Analytik GmbH, University of Innsbruck, Institute for Ion Physics and Applied Physics, Innsbruck, Austria

MP-238 **Ionization products of terpene species in LTP FT-ICR-MS measurements**
B. Raupers, J. Grotemeyer
Institute of Physical Chemistry, University of Kiel, Kiel, Germany

MP-239 **Development and application of a novel plasma ion source with GC-MS/MS**
M. Sarrafzadeh, R. Javahery, C. Jolliffe
PerkinElmer, Woodbridge, Canada

MP-240 **A novel voltage-assisted paper spray-APPI-HRMS method for the screening and quantification of semi-volatile florinated compounds**
L. R. Seró, C. J. F. Ayala, V. F. J. Santos, M. E. Moyano
University of Barcelona, Chemical Engineering and Analytical Chemistry, Barcelona, Spain

MP-241 **Advances in Selected Ion Flow-Drift Tube Mass Spectrometry, SIFDT-MS, for ambient quantification of trace volatile compounds in air**
P. Španel, A. Spesyvyi, D. Smith, K. Sovová
Czech Academy of Sciences, J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic

MP-242 **A triple reagent ion source for trace VOCs quantification by Selected Ion Flow-Drift Tube Mass Spectrometry**
A. Spesyvyi, P. Španel
J. Heyrovský Institute of Physical Chemistry of the CAS, v. v. i., Department of Chemistry of Ions in Gaseous Phase, Prague, Czech Republic

MP-243 **Airborne laser-spark ion source for direct microfluidic coupling**
S. van Wasen, A. Bierstedt, J. Riedel, D. Volmer
Humboldt-Universität zu Berlin, Department of Chemistry, Berlin, Germany

MP-244 **Development and the application of a 96 high throughput solid phase microextraction (SPME) transmission mode (TM) system for direct analysis in real time (DART) mass spectrometry (MS)**
T. Vasiljevic, G. A. Gómez-Ríos, J. Pawliszyn
University of Waterloo, Waterloo, Canada

MP-245 **Single-use poly(etheretherketone) solid-phase microextraction-transmission mode devices for rapid screening and quantitation of drugs of abuse in oral fluid and urine via direct analysis in real-time**
T. Vasiljevic, G. A. Gómez-Ríos, J. Pawliszyn
University of Waterloo, Waterloo, Canada

MP-246 **Improvements in small molecule detection via MALDI-MS using binary mixtures of novel ionless matrices**
J. Weissflog, A. Svatoš
Max-Planck-Institute for Chemical Ecology, Research Group Mass Spectrometry/Proteomics, Jena, Germany

MP-247 **Matrix-Assisted-Ionization-In-Vacuum coupled to high-resolution Fourier transform mass spectrometry (MAI-FTMS) in characterizing lipids in cooking oil and bacteria**
R. Liyanage, J. Gidden, J. O. Lay Jr., C. Wilkins
University of Arkansas, Chemistry and Biochemistry, Faywtteville, USA

MP-248 **3D-printed low-temperature plasma (3D-LTP) probe for imaging and in vivo studies**
S. Martínez-Jarquín, A. Moreno-Pedraza, H. Guillén-Alonso, H. Herrera-Ubaldo, I. Rosas-Román, C. Ovando-Vázquez, S. De Folter, R. Winkler
CINVESTAV Unidad Irapuato, Biotechnology and Biochemistry, Irapuato, Mexico

MP-249 **Identification of medulloblastoma subgroups on intrasurgical timescales with picosecond infrared laser desorption mass spectrometry**
M. Woolman, C. Kuzan-Fischer, I. Ferry, T. Kiyota, B. Luu, M. Wu, D. Munoz, S. Das, A. Aman, M. Taylor, J. Rutka, H. Ginsberg, A. Zarrine-Afsar
University of Toronto, Department of Medical Biophysics, Toronto, Canada

MP-250 **Improvement of nanoelectrospray and desorption nanoelectrospray signal by regulation of pressure in an inlet of triple quadrupole mass spectrometer**
L. Borovcová, P. Fryčák, D. Mosler, Š. Dostál, V. Havlícek, K. Lemr
Department of Analytical Chemistry, Faculty of Science, Palacký University, Olomouc, Czech Republic

MP-251 **Acoustic mist ionisation platform for high-throughput ms-based drug discovery**
P. Deland, I. Sinclair, G. Davies, D. Murray, E. Mouchet, M. Bachman, M. Rohman, J. Wingfield
Labcyte Inc., Mass Spectrometry Product Management, San Jose, USA

MP-252 **Study on the ionization mechanism of polymers under cluster ion irradiation**
M. Fujii, J. Matsuo
Yokohama National University, Graduate School of Environment and Information Sciences, Yokohama, Japan

MP-253 **A unique approach to charging ions for LC-MS**
C. Jolliffe, L. Cousins, R. Javahery, A. Kornilova, H. Gamble, M. Sarrafzadeh
PerkinElmer Inc., RND, Woodbridge, Canada

MP-254 **Development of mass spectrometry-based explosives trace detectors for secure city**
S. Kumano, M. Sugiyama, Y. Takada, H. Nagano, H. Mizuno, T. Ito, T. Nojiri, M. Iida, H. Maruyama
Hitachi, Ltd., Research & Development Group, Tokyo, Japan

MP-255 **Using automated low volume pipetting to enable high throughput DART-MS detection of drugs directly from biological matrices**
F. Li, P. Liang, B. Laramee, B. Musselman
IonSense, Inc., Chemistry, Saugus, USA

MP-256 **Toward high throughput screening of cell-material response using liquid extraction surface analysis-mass spectrometry (LESA-MS)**
J. Meurs, J. Bunch, M. Alexander, D. Barrett, D. Kim
Advanced Materials & Healthcare Technologies Division, University of Nottingham, Nottingham, United Kingdom

MP-257 **Development of a multimodal imaging platform based on photoinduced thermal desorption and analysis by atmospheric pressure chemical ionization mass spectrometry**
M. Lorenz, M. Viani, A. Labuda, S. Jesse, R. Proksch, O. Ovchinnikova
Oak Ridge National Laboraotry, Center for Nanophase Materials Sciences, Oak Ridge, USA

MP-258 **What determines the postionisation efficiency in MALDI-2: A combined soft-/hardware-based set-up to semi-automatically characterize the role of five relevant input parameters**
A. Potthoff, K. Dreisewerd, J. Soltwisch
University of Münster, Institute of Hygiene, Münster, Germany

MPS-S10 – Polymers

MP-259 **A combination of FAIMS separation with synchrotron UV-photo activation for the tandem MS analysis of synthetic polymers**
V. Legros, I. Aloui, A. Giuliani, W. Buchmann
LAMBE (CNRS-UEVE-CEA-UCP, UMR8587), Université Paris-Saclay (Univ Evry), Evry, France

MP-260 **"Advanced Kendrick mass defect analysis": a toolkit**
T. Fouquet, R. B. Cody, T. Satoh, H. Sato
National Institute of Advanced Industrial Science and Technology (AIST), Research Institute for Sustainable Chemistry (ISC), Tsukuba, Japan

MP-261 **Potential of liquid extraction surface analysis for mass spectrometric evaluation of safety and functionalization of polymer food packing materials**
A. Issart, S. Godin, H. Preud'homme, A. Allal, J. Szpunar
IPREM, UMR 5254 CNRS- UPPA, Pau, France

MP-262 **Study on the synthesis and characterization of surface activities of hydrophilic derivatives of β-sitosterol**
J. C. Lim
Dongguk University-Seoul, Department of Chemical and Biochemical Engineering, Seoul, Republic of Korea

MP-263 **Mass-Remainder Analysis (MARA): to understand mass spectra of copolymers**
T. Nagy, Á. Kuki, G. Deák, L. Nagy, M. Zsuga, S. Kéki
University of Debrecen, Department of Applied Chemistry, Debrecen, Hungary

MP-264 **Compositional analysis of high molecular weight biodegradable polymers by high-resolution MALDI-ToFMS combining on-plate degradation with resolution-enhanced KMD analysis**
S. Nakamura, T. Fouquet, H. Sato
National Institute of Advanced Industrial Science and Technology, Research Institute for Sustainable Chemistry, Tsukuba, Japan

MP-265 **Cold plasma treatment of polymer substrates for SALD ICP MS**
J. Preisler, M. Stiborek, M. Shekargoftar, V. Kanicky, J. Kelar
Masaryk University, Department of Chemistry, Brno, Czech Republic

MP-266 **Remainders of Kendrick mass: keeping the best of a Kendrick mass defect analysis for low-accuracy mass spectra of polymers**
H. Sato, T. Fouquet
National Institute of Advanced Industrial Science and Technology (AIST), Research Institute for Sustainable Chemistry, Tsukuba, Japan

MP-267 **Analysis of degraded polybutyleneterephthalate (PBT) products by Thermal Desorption and Pyrolysis combined with DART-MS (TDP/DART-MS)**
C. Takei, K. Yoshizawa
BioChromato, Inc., Application support, Fujisawa, Japan

MP-268 **Evaluation of thermal history of thermoplastic resins by Thermal Desorption and Pyrolysis Combined with DART-MS (TDP/DART-MS)**
C. Takei, K. Yoshizawa
BioChromato, Inc., Application support, Fujisawa, Japan

MP-269 **MALDI-LID-ToF/ToF analysis of statistical and diblock polyacrylate copolymers**
J. Town, G. Jones, D. Haddleton
University of Warwick, Chemistry, Coventry, United Kingdom

TUESDAY, August 28th, 2018

TPS-S01 - Therapeutic Drug Monitoring and Drug Discovery

TP-1 **Phosphoproteomics of non-small-cell lung cancer cells treated with erlotinib reveals drug-resistant signatures and potential targets**
J. Adachi, Y. Abe, M. Nagano, J. Isoyama, M. Kishida, T. Tomonaga
National Institutes of Biomedical Innovation, Health and Nutrition, Laboratory of Proteomics for Drug Discovery, Osaka, Japan

TP-2 **Comparison of methionine oxidation profiles of biosimilar TUR01 monoclonal antibody to its reference under oxidative stress**
A. E. Atik, Z. Z. Yildirim Keles, G. Güven, I. E. Gülser, Y. Erdemgil, D. Bayçin, Ö. Can, R. S. Alpan
Turgut Pharmaceuticals, Biotechnology Group, İstanbul, Turkey

TP-3 **Quantitative evaluation of adenosine 5'-tetraphosphate and other five analytes related to nicotinamide phosphoribosyltransferase by LC-MS in Melanoma cells and mouse plasma**
M. Bianchi, A. Grolla, C. Travelli, S. Garavaglia, A. Genazzani, G. Orsomando, E. Del Grosso
University of Piemonte Orientale, Department of Pharmaceutical Sciences, Novara, Italy

TP-4 **Analytical aspects of sunitinib and its geometric isomerism towards therapeutic drug monitoring in clinical routine**
M. Buzzo, B. Posocco, E. Marangon, G. Toffoli
National Cancer Institute of Aviano, University of Trieste, Aviano, Italy

TP-5 **A LC-MS-based assay for the determination of activity and inhibition of Anopheles gambiae 3-hydroxykynurenine transaminase enzyme**
R. Canavesi, U. Galli, R. Miggiano, F. Rossi, E. Del Grosso
Università del Piemonte Orientale, Department of Pharmaceutical Sciences, Novara, Italy

TP-6 **Rapid, sensitive fentanyl detection by thermal desorption PTR-MS and collision induced dissociation**
L. Cappellin, F. Lopez
TOFWERK AG, R&D, Thun, Switzerland

TP-7 **A validated and robust analytical method for pesticides measurement in cannabis by liquid chromatography tandem mass spectrometry**
C. Clarysse
Perkin Elmer, Chrom and Mass Spec. Division, Villebon Sur Yvette, France

TP-8 **Data independent acquisition modes for identification, quantification and monitoring of low-abundance host cell proteins during monoclonal antibody bioprocessing**
C. Doneanu, A. Xenopoulos, R. Skudas, Q. Yu Ying, A. Chakraborty, W. Chen
Waters, Biopharmaceutical Sciences, Milford, USA

TP-9 **Clinical validation of a UPLC/MS/MS-based assay to concurrently monitor four direct oral anticoagulants in dried blood spots**
K. I. Foerster, A. Huppertz, A. D. Meid, O. J. Müller, L. Tilemann, T. Rizos, W. E. Haefeli, J. Burhenne
Heidelberg University Hospital, Department of Clinical Pharmacology and Pharmacoepidemiology, Heidelberg, Germany

TP-10 **Development of a SPME tool for the determination of a small molecule-drug conjugate against carbonic anhydrase in cancer chemotherapy**
S. Ghiasikhou, J. Scheuermann, S. Cazzamalli, D. Neri, R. Zenobi
ETH Zurich, Switzerland

TP-11 **In vivo assessment of the contribution of surfactant replacement therapy in rabbits by stable isotopes natural abundance approach**
S. Giambelluca, F. Ricci, M. Simonato, L. Vedovelli, A. Correani, C. Casiraghi, M. Storti, P. Cogo, F. Salomone, V. P. Carnielli
Padova University Hospital, Department of Women's and Children's Health, Padova, Italy

TP-12 **BiopharmaViewTM for fast and efficient monitoring of pH induced deamidation**
F. Sanchez, L. Ji, K. Pohl, J. Dojahn, A. Uppal, S. Heidelberger
Sciex, Biologics, Warrington, United Kingdom

TP-13 **Unrevealing phase I metabolism of combretastatin A4 by a multi-tool MS-based approach**
K. Jaroch, P. Z. Goryńska, K. Goryński, T. Stefański, B. Bojko
NIcolaus Copernicus University in Torun, Collegium Medicum in Bydgoszcz, Department of Pharmacodynamics and Molecular Pharmacology, Faculty of Pharmacy, Bydgoszcz, Poland

TP-14 **Application of triple quadrupole MS for drug-to-antibody ratio and molecular weight determination of antibody-drug conjugates**
M. Källsten, R. Hartmann, M. Pijnappel, L. S. Bergström, J. Bergquist, F. Lehmann
Uppsala university, Department of Chemistry-BMC, Uppsala, Sweden

TP-15 **Drawing the activity of auranofin by an electrochemical reaction cell coupled to an ESI MS/MS**
P. Katarzyna, M. Kupiec, R. Ziolkowski
Warsaw University of Technology, Faculty of Chemistry, Chair of Analytical Chemistry, Warsaw, Poland

TP-16 **Therapeutic effect of a natural alkaloid observed in 5xFAD transgenic Alzheimer's transmodel: a proteomics study**
I. Kırış, M. Karayel Başar, B. Gürel, T. Mroczek, K. Skalicka-Wozniak, A. T. Baykal
Acibadem Mehmet Ali Aydinlar University, Medical Biochemistry, İstanbul, Turkey

TP-17 **Simultaneous determination of aripiprazole, dehydro-aripiprazole, olanzapine, risperidone, paliperidone, quetiapine and clozapine in human plasma by LC-MS/MS**
D. Koller, A. Wojnicz, F. Abad-Santos
Hospital Universitario de la Princesa, Clinical Pharmacology, Madrid, Spain

TP-18 **LC-MS identification and quantification of bleomycinin in serum and tumor tissue**
T. Kosjek, T. Gornik, D. Zigon, M. Bosnjak, S. Kranjc, M. Krzan, A. Groselj, M. Cemazar, G. Sersa
Jozef Stefan Institute, Dept. Envir. Sci., Ljubljana, Slovenia

TP-19 **Solid phase microextraction for the quantification of doxorubicin and untargeted metabolic profiling of lung tissue during in vivo lung perfusion**
N. Looby, B. Bojko, G. A. Gómez-Ríos, M. Tascon, A. Roszkowska, K. Gorynski, J. Pawliszyn
University of Waterloo, University of Waterloo, Department of Chemistry, Waterloo, Canada

TP-20 **Assessment of antibody-derived therapeutics at the intact and middle-up level by CESI-MS**
E. Domínguez-Vega, R. Haselberg, G. W. Somsen, J. Thorn, C. Lößner, S. Lock
Sciex, CE and Biopharma, Darmstadt, Germany

TP-21 **Detection and characterization of stable iminium ion reactive metabolite using high resolution mass spectrometry.**
T. Miraval
Idorsia LTD, DMPK, Allschwil, Switzerland

TP-22 **Phytochemical composition of extracts from wood and leaves of Lebanese Cedar (Cedrus libani) using GC/MS**
S. Mokh, M. Al Iskandarani, M. Locatelli, S. Carradori, C. Celia, J. Farouk
Lebanese atomic energy commission, Laboratory of analysis of organic compound, Beirut, Lebanon

TP-23 **A combination of chemical proteomics and DARST-based approaches to disclose natural products biological targets**
F. Del Gaudio, S. Ceccacci, F. Pollastro, M. Mozzicafreddo, A. Minassi, R. Riccio, M. C. Monti
Dept. of Pharmacy, University of Salerno, Fisciano (Salerno), Italy

TP-24 **Focal adhesion kinase binding partner study in human colon cancer cell HCT-116 using immunoprecipitation method coupled with nano-LC/MSMS technique**
B. T. Nguyen, M.-J. Kang
Korea Institute of Science and Technology, Korea University of Science and Technology, Seoul, Republic of Korea

TP-25 **Comprehensive *N*-glycan structure catalogue of therapeutic antibodies**
M. J. Oh, N. Seo, J. An Hyun
AGRS, Chungnam National University, Daejeon, Republic of Korea

TP-26 **Monitoring of sequence variants by MAM using high resolution mass spectrometry**
K. Pohl, Y. Li, C. Nortcliffe, A. Uppal, F. Sanchez, J. Dojahn, S. Heidelberger
Sciex, Biologics, Darmstadt, Germany

TP-27 **Epitope peptides identified by online biosensor-MS neutralize pathophysiological antibodies and open new clinical therapy approaches for lysosomal diseases**
M. Przybylski, L. Lupu, P. Wiegand, Z. Kukacka, S. Maeser, Y. Baschung, F. Völklein, A. Lazarev, A. Maria Papini, J. Hennermann, K. Schmitz
Steinbeis Centre for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany

TP-28 **Chromatography coupled to mass spectrometry for stability studies in drug discovery**
L. Queguiner, D. Speybrouck, S. Thomas
Janssen Resarch & Development, Discovery Sciences, Val de Reuil, France

TP-29 **ABCs of mABs and ADCs**
S. Reeksting, T. Chapman, B. Alkhawaja, A. Watts, A. Lubben
University of Bath, Faculty of Science, Chemical Characterisation and Analysis Facility (CCAF), Bath, United Kingdom

TP-30 **Development of a hybrid LC-MS/MS method for the quantification of antibody-conjugated payload in in-vivo and in-vitro ADC samples**
F. Riccardi Sirtori, E. Bertotti, A. Ariaudo, F. Molinaro, I. De Salve, L. Barbero, S. Kumar, S. Riva, T. Goletz
RBM-Merck group, NBE Drug Disposition, QPD, Colleretto Giacosa (TO), Italy

TP-31 **Epitope and affinity determination of recombinant Mycobacterium tuberculosis Ag85B antigen towards anti-Ag85 antibodies using proteolytic-affinity mass spectrometry and biosensor analysis**
F. Rinaldi, L. Lupu, H. Rusche, Z. Kukacka, S. Tengattini, R. Bernardini, L. Piubelli, T. Bavaro, S. Maeser, L. Pollegioni, E. Calleri, M. Przybylski, C. Temporini
University of Pavia, Department of Drug Sciences, Pavia, Italy

TP-32 **Monitoring of therapeutic doses of antipsychotic drugs in saliva and serum samples with the use of solid-phase microextraction technique**
A. Roszkowska, L. Konieczna, W. Zukowicz, M. Galewska, W. Cubala, T. Baczek
University of Waterloo, Department of Chemistry, Waterloo, Canada

TP-33 **Multi-attribute monitoring (MAM) to identify differences in Trastuzumab from 2 manufacturers.**
F. Sanchez, C. Nortcliffe, K. Pohl, J. Dojahn, S. Heidelberger
Sciex, Biologics, Barcelona, Spain

TP-34 **LC-MS/MS analysis and rat pharmacokinetics of the novel cyclin-dependent kinase inhibitors BP-14 and BP-20**
J. Široká, M. Čečková, L. Urbánek, V. Kryštof, T. Gucký, J. Hofman, M. Strnad, F. Štaud
Palacký University, Laboratory of Growth Regulators, Olomouc, Czech Republic

TP-35 **Identification of 5-fluorocytosine and its metabolites in complex samples by liquid chromatography coupled with mass spectrometry**
P. Škvára, M. Matúšková, E. Duriníková, S. Andrea Vojs
Comenius University in Bratislava, Department of Analytical Chemistry, Faculty of Natural Sciences, Bratislava, Slovak Republic

TP-36 **Efficient dereplication with high resolution high accuracy mass spectrometry for the discovery of novel bioactive natural products**
L. Song
Dept Chemistry, University of Warwick, Coventry, United Kingdom

TP-37 **Collision-induced dissociation study of antimicrobial peptide dendrimers**
A. Tintaru, L. Charles
Aix-Marseille Université - CNRS, Institut de Chimie Radicalaire UMR7273, Marseille, France

TP-38 **Mass spectrometry characterization of an NMS proprietary drug conjugated antibody (ADC)**
S. Troiani, R. Perego, U. Cucchi, P. Orsini, M. Salsa, M. Caruso, B. Valsasina
Nerviano Medical Sciences srl, Oncology/Biotechnology, Nerviano (MI), Italy

TP-39 **Assessing the drugability of PTP1B non-catalytic sites with mass spectrometry**
G. A. Villar, C. Buning, J. Czech, M. Dreyer, G. Hessler, S. Matthias Petry, N. Tennagels, S. Welte
Sanofi-Aventis Deutschland GmbH, Integrated Drug Discovery, Frankfurt am Main, Germany

TP-40 **Ultrafast detection of drugs and metabolites in urine by Flow Injection Analysis (FIA) coupled to Magnetic Resonance Mass Spectrometry (MRMS)**
M. Witt, M. Godejohann, A. Barsch
Bruker Daltonik GmbH, MRMS Solutions, Bremen, Germany

TP-41 **Efficient phospholipids removing clean-up SPE-LC-MS/MS method for simultaneous plasma quantification of 11 tyrosine kinase inhibitors and caffeine. Application to therapeutic drug monitoring**
A. Wojnicz, D. Koller, V. Vaitsekhovich, O. J. L. Steegmann, F. Abad-Santos
Hospital Universitario de la Princesa, Clinical Pharmacology Department, Madrid, Spain

TP-42 **Quantification of major peanut protein allergen isoform groups from peanut protein extracts**
K. Alving, P. DeMontigny, B. Wang
Sanofi, Analytical Research and Development, Waltham, USA

TP-43 **Validation of breath biopsy platform for longitudinal measurement of VOCs in breath using TD-GC-MS**
J. Boschmans, R. Smith, M. van der Schee, S. Kitchen, B. Boyle, M. Allsworth
Owlstone Medical Ltd., Chemistry, Cambridge, United Kingdom

TP-44 **Elimination profile of betamethasone and metabolites in urine after different administration routes**
S. Coll, X. Matabosch, N. Monfort, E. Alechaga, C. Pérez-Mañá, J. A Mateus, J. Monfort, J. Llorente-Onaindia, R. Ventura
Institut del Mar d'Investigacions Mèdiques, Catalonian anti-doping laboratory, Barcelona, Spain

TP-45 **Variability and values in glycosylation analyses of monoclonal antibodies: an interlaboratory study**
M. L. A. De Leoz, D. L. Duewer, S. E. Stein
National Institute of Standards and Technology (NIST), Material Measurement Laboratory, Gaithersburg, USA

TP-46 **Application of Acoustic Mist Ionization Mass Spectrometry (AMI-MS) for the development of kinase assays**
D. Srivastava, P. Deland, J. Wingfield, J. Tart, P. Clarkson, M. Tonge
Labcyte inc., Mass Spectrometry Product Management, San Jose, USA

TP-47 **A mass spectrometry toolbox for the optimization of K-RAS G12C covalent inhibitors**
S. Raibaud, A. Buzy, S. Hamon, P. Paul, J.-C. Guillemot, V. Lalleman, P. Didier, R. Arrebola, F. Duffieux, A. Parent, A. Rak, G. McCort, L. Debussche, F. Fassy
Sanofi, Research Platform & Oncology, Chilly-Mazarin & Vitry sur Seine, France

TP-48 **LC-MS/MS method for analysis of therapeutic peptide Axon Peptide 108 in AADVac1 drug product**
J. Galba, J. Piestansky, P. Barath, B. Kovacech, A. Kovac
Axon Neuroscience SE R&D, Proteomics & Metabolomics, Bratislava, Slovakia

TP-49 **Analysis of host cell proteins in antibody preparations using PASEF**
M. Greig, S. Pengelley, G. Tremintin, D. Suckau, W. Evers
Bruker Daltonics, San Jose, USA

TP-50 **Simultaneous determination of tramadol, *O*-desmethyltramdol, and *N*-desmethyltramadol in human plasma by liquid chromatography-tandem mass spectrometry and its application to a pharmacokinetic study**
C.-M. Lee, Y. Kim, W. Chae, E. Hyun Jung, S. Lee
Sungkyunkwan University, School of Pharmacy, Suwon, Republic of Korea

TP-51 **A rapid and highly sensitive liquid chromatography-tandem mass spectrometry method for simultaneous determination of meloxicam and 5'-carboxymeloxicam in human plasma and its application to a pharmaco**
C.-M. Lee, E. Hyun Jung, J. Lee Yun, H. Lee, J. Lee, S. Lee
Sungkyunkwan University, School of Pharmacy, Suwon, Republic of Korea

TP-52 **Investigation of amyloid-beta 1-42 reactivity and stable adduct(s) formation by mass spectrometry-based approach**
M. Naldi, A. De Simone, D. Tedesco, M. Bartolini, V. Andrisano
Alma Mater Studiorum University of Bologna, Department of Pharmacy and Biotechnology, Bologna, Italy

TP-53 **Dose-and time-dependent effects of hepatotoxicants on ADME proteins in 3D human liver spheroids by PRM**
N. Selevsek, W. E. Wolski, L. Kunz, H. Cordes, V. Baier, L. Kuepfer, O. Clayton, A. Roth, R. Schlapbach
Functional Genomics Center Zurich, ETH Zurich, Zurich, Switzerland

TPS-S02 - Single Cell

TP-54 **Function of PIWIL3 in mammalian oocytes**
M. Tan, H. Van Tol, M. Damen, T. Stout, W. Wu, B. Roelen
Utrecht University, Biomolecular Mass Spectrometry & Proteomics, Utrecht, Netherlands

TP-55 **Picoliter pressure-probe-electrospray-ionization mass spectrometry for in situ monitoring single plant cell metabolite changes under stress conditions**
R. Erra-Balsells, K. Nakata, H. Wada, H. Nonami
Departamento de Quimica Organica, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Buenos Aires, Argentina

TP-56 **Drug uptake and metabolism in single liver cells**
L. Pedro, P. Rudewicz
Novartis Institutes for BioMedical Research, GDC, Emeryville, USA

TPS-S03 - Noncovalent Interactions

TP-57 **The assembly of islet amyloid polypeptide (IAPP) and the role of the disulfide bond**
M. Bowers, A. Ilitchev, D. Bishop, S. Buratto
UCSB, Chemistry and Biochemistry, Santa Barbara, USA

TP-58 **Gas-phase complexation of α-/β-cyclodextrin with amino acids studied by ion mobility-mass spectrometry and molecular dynamics simulations**
Y. Chen, Z. Zuo, W. Wang, C. Ding
Fudan University, Chemistry Department, Shanghai, China

TP-59 **Investigating the interlocked nature of catenanes and knots with mass spectrometry and ion mobility spectrometry**
A. Kruve, C.A. Schalley
Freie Univeversität Berlin, Institut für Chemie und Biochemie, Berlin, Germany

TP-60 **Collision induced dissociation of multiply charged peptide aggregates**
M. Al-Majidi, A. Magyar, G. Schlosser
ELTE Eötvös Loránd University, Department of Analytical Chemistry, Budapest, Hungary

TP-61 **Novel, bilateral fluorous alkoxide-based clusters discovered by ambient ionization mass spectrometry**
M. Berta, T. Nagy, S. Kéki, J. Rábai, G. Schlosser
ELTE Eötvös Loránd University, Department of Analytical Chemistry, Budapest, Hungary

TP-62 **Noncovalent complexes in natural extracts**
P. Traldi, S. D'Aronco, S. Crotti, M. Agostini, L. Mattoli, M. Burico, S. Tamimi
Fondazione Istituto di Ricerca Pediatrica Città della Speranza, Città della Speranza, Padova, Italy

TP-63 **Steric structure and stability of the gas-phase complexes of macrocyclic receptors with anions**
M. Zimnicka, A. Wasilewska, K. Dabrowa, W. Danikiewicz
Polish Academy of Sciences, Institute of Organic Chemistry, Warsaw, Poland

TPS-S04 - High Resolution MS: Instrumentation, Methods & Applications

TP-64 **Towards routine intact level quantification of monoclonal antibody in plasma by HRMS**
Y. Alelyunas, M. Wrona, H. Shion, C. Dunning, J. Kirk
Waters Corp, Scientific Operations, Milford, USA

TP-65 **Progress towards implementing accurate mass ms for routine biotherapeutic analysis**
H. Shion, W. Alley, J. Pugh, R. Lewis, Q. Yu Ying, W. Chen
Waters Corp, Milford, USA

TP-66 **Multiplexed analysis of environmental samples by GCxGC-HRMS with multi-ionization capabilities**
V. Artaev, G. Tikhonov, A. Lebedev
LECO Corporation, St. Joseph, USA

TP-67 **Gas chromatography-atmospheric pressure photoionization-high resolution mass spectrometry for the determination of semi-volatile fluorinated compounds**
J. F. Ayala-Cabrera, E. Moyano, F. J. Santos
University of Barcelona, Department of Chemical Engineering and Analytical Chemistry, Barcelona, Spain

TP-68 **Determination of quantitative amounts and ratio between enzyme variants in a sample, by spiking with stable isotope labelled peptide**
T. Janne Bech
DuPont Nutrition Biosciences ApS, Advanced Analysis, Brabrand, Denmark

TP-69 **Think positive: finding the best matrix in MALDI-ToF MS for croconaine dyes investigation**
C. D. Calvano, M. Capozzi, A. Punzi, G. Farinola, F. Palmisano, T. Cataldi
University of Bari, Chemistry, Bari, Italy

TP-70 **Efficient preparation of organoimido derivatives of Lindqvist hexamolybdate in leidenfrost droplets**
J. Cao, Q. Wang
Beijing Institute of Technology, School of Chemistry and Chemical Engineering, Beijing, China

TP-71 **A novel PTR-ToF reaction cell superposing DC and RF fields leads to ten-fold improvements in sensitivities and LODs**
L. Cappellin, F. Lopez, M. Hutterli, J. E. Krechmer, S. Klee, B. Plet
ToFWERK AG, R&D, Thun, Switzerland

TP-72 **Determining acetylcholinesterase activity using paper spray mass spectrometry**
D. Carmany, G. Boyd, P. Mach, E. Dhummakupt, P. Demond, M. Busch, T. Glaros
Excet Inc, ECBC, Gunpowder, USA

TP-73 **LC-HRMS by means of untargeted data-dependent acquisition for the characterization of 'superfoods'**
F. Di Ottavio, J. Gauglitz, L. Felix Nothias, M. Panitchpakdi, P. Dorrestein, D. Compagnone, M. Sergi
University of Teramo, Faculty of Bioscience, Teramo, Italy

TP-74 **High-resolution mass spectrometry in combination with in silico prediction models to improve accuracy for compound identification**
E. Dossin, P. Diana, A. Glabasnia, M. Bentley, P. A. Guy
Philip Morris Product S.A., R&D Chemical Research, Neuchatel, Switzerland

TP-75 **High-throughput quan/qual LC-MS analysis: where is the sweet spot?**
A.-C. Dubbelman, F. Cuyckens, L. Dillen, R. J. Vreeken, T. Hankemeier
Leiden University, Leiden Academic Centre for Drug Research, Systems Biomedicine and Pharmacology, Leiden, Netherlands

TP-76 **UHPLC-HRMS method for targeted analysis of cyanotoxins in freshwater**
D. Filatova, M. Picardo, O. Núñez, M. Farré
Institute of Environmental Assessment and Water Research, Spanish National Research Council, University of Barcelona, Department of Chemical Engineering and Analytical Chemistry, Barcelona, Spain

TP-77 **Direct gas analysis using a multi-turn high-resolution mass spectrometer**
M. Hashimoto, M. J. van der Schans, J. A. Van der Meer, B. Van der Meer
JEOL(EUROPE)SAS, European Application Group, Croissy-sur-Seine, France

TP-78 **Development of an LC-HRMS method to aid in identification and confirmation of chlorinated and brominated contaminants**
A. Ionas, A. Miralles-Marco, G. Codling, S. Vojta, L. Melymuk, J. Klánová
Research Centre for Toxic Compounds in the Environment (RECETOX) Brno, Czech Republic

TP-79 **Combination of different ionization sources expands the analysis of complex mixtures**
A. Kondyli, W. Schrader
Max Planck Institut für Kohlenforschung, Mass Spectrometry, Mülheim an der Ruhr, Germany

TP-80 **Aberration-based numerical optimization of ion mirrors**
I. Kopaev, D. Grinfield, M. Monastyrskiy, M. Alexander
General Physics Institute/T8, Optoelectronics Department, Moscow, Russian Federation

TP-81 **Application of EThcD for leucine/isoleucine discrimination in peptides**
S. Kovalev, M. Tolpina, S. Zhokhov, T. Samguina, A. Lebedev
Moscow State University, Chemistry Department, Moscow, Russian Federation

TP-82 **A new LC-MS/MS method for determination of Apixaban in tablets**
M. Kozanli, Ö. Can Nafiz
Anadolu University, Faculty of Pharmacy, Department of Analytical Chemistry, Eskisehir, Turkey

TP-83 **Multiplexed operation of high resolution orthogonal multi-reflecting time-of-flight mass spectrometer**
B. Kozlov, J. Brown, V. Artaev
Waters Corporation, Wilmslow, United Kingdom

TP-84 **Screening for anthraquinones in chilean mushrooms by HPTLC - negative ion DESI high-resolution mass spectrometry**
A. Laub, A. Sendatzki, G. Palfner, N. Arnold, L. Wessjohann, J. Schmidt
Leibniz Institute of Plant Biochemistry, Bioorganic Chemistry, Halle, Germany

TP-85 **The advantages of using an MRMHR acquisition for increased sensitivity for targeted analysis using a QToF instrument**
D. Mcmillan, P. Taylor, K. Hyland, C. Borton
Sciex, Business Development, Warrington, United Kingdom

TP-86 **Contextualization of dark matter in MS1 FT-ICR MS^1 data**
F. Moritz, M. Kaling, J. Schnitzler, P. Schmitt-Kopplin
Helmholtz Zentrum Muenchen, Research Unit Analytical BioGeoChemistry, Neuherberg, Germany

TP-87 **Simultaneous determination of nine water-soluble synthetic colorants in cosmetics by LC-Q-ToF/MS and LC-MS/MS**
S. Park, H. Kim Jun, G. Kang, A. Min, H. Lee Ji, H. Park, T. Hwang, S. Heo, Y. Eom Kwon, D. Woo Shin, S. Park, H. Kang
National Institute of Food and Drug Safety Evaluation, Division of Advanced Analysis, Chungcheongbuk-do, Republic of Korea

TP-88 **SFC-ESI-QToF-MS: ddeveloping an innovative one-run method for chocolate quality and authenticity control**
M. Rektorisova, V. Hrbek, M. Tomaniova, J. Hajslova
University of Chemistry and Technology, Department of Food Analysis and Nutrition, Prague, Czech Republic

TP-89 **Using Atomic Layer Deposition (ALD) to enhance MCPs for mass spectrometry**
M. Breuer, P. Holmes, J. Harper
Photonis, Research and Development, Sturbridge, USA

TP-90 **The combination of hydrophilic interaction liquid chromatography and ion mobility mass spectrometry for diesel fuel analysis**
E. Smit, S. De Goede, E. Rohwer
University of Pretoria, Lynnwood Rd, Pretoria, South Africa

TP-91 **Applying high-resolution mass spectrometry to elucidate the formation and fate of ozonation TPs in wastewater treatment**
J. Schollee, R. Gulde, M. Bourgin, M. Rutsch, J. Fleiner, M. Boehler, J. Hollender, U. Von Gunten, C. Mcardell
Eawag, Environmental Chemistry, Duebendorf, Switzerland

TP-92 **Analysis of cationic polar pesticides in baby food using ion chromatography and MS/MS or high resolution accurate mass spectrometry**
F. Schoutsen, J. E Madden, J. S Rohrer, J. Beck
TFS, Breda, Netherlands

TP-93 **An automated workflow for high-throughput nicotine quantitation using high performance liquid chromatography coupled to high resolution accurate mass spectrometry for prototype testing**
S. Sendyk, Q. Dutertre, A. Knorr, J. Hoeng, M. Bentley
Philip Morris, Science & Innovation, Neuchatel, Switzerland

TP-94 **Characterization of stress degradation products of fosamprenavir calcium using Q Exactive™ Plus Orbitrap and LTQ XL™ mass spectrometers, and prediction of their toxicity using ADMET Predictor™**
D. K. Singh, M. K. Ladumor, C. N. Kotimoole, K. B. Batkulwar, A. Y. Deshpande, S. Giri, S. Singh
Department of Pharmaceutical Analysis, National Institute of Pharmaceutical Education and Research (NIPER), S.A.S. NAGAR, India

TP-95 **Quadrupole-resolved all ions MS/MS for reliable quantitation of pesticides in complex matrices using untargeted acquisition**
L. Tölgyesi, A. Mielcarek, C. Klein, T. Knotts, D. Yang, B. Frazer, T. Anumol, J. Lee, W. E. Barry
Agilent Technologies Sales & Services GmbH & Co. KG, Global Laboratory Solution Sales (LSS) Marketing, Waldbronn, Germany

TP-96 **Identification of electrochemical degradation products of selected pharmaceuticals by high resolution mass spectrometry**
A. Vojs Stanova, E. Medvecka, A. Borik, R. Grabic, P. Skvara, T. Mackulak, M. Marton, M. Vojs
Comenius University in Bratislava, Department of Analytical Chemistry, Faculty of Natural Sciences, Bratislava, Slovak Republic

TP-97 **Removal of isobaric interferences by laser resonance ionization mass spectrometry for determination of ^{126}Sn/^{121}Sn ratio**
W. Wang, X. Shen, L. Zhai, H. Deng, Z. Li
Northwest Institute of Nuclear Technology, Applied Physics and Chemistry Department, Xi'an, China

TP-98 **Improving coverage in transmembrane domains of integral membrane proteins with ultra-violet photodissociation**
J. Whitelegge
University of California Los Angeles, The Pasarow Mass spectrometry Laboratory, Los Angeles, USA

TP-99 **Study for mass resolution of quadrupole mass spectrometers according to the rod electrode alignment**
K. Yoshinari, Y. Terui
Hitachi, Ltd. Research & Development Group, Center for Technology Innovation, Hitachi-shi, Ibaraki-ken, Japan

TP-100 **SweEt HRMS workflow strategy for screening unhealthy substances in food**
S. Ekroth, M. Johansson
National Food Agency, Chemistry Department, Uppsala, Sweden

TP-101 **Simple workflow for proteoform separation and analysis using 2D gel electrophoresis-high resolution mass spectrometry**
M. Gaikwad, B.Dreyer, H. Schlüter
University Medical Center Hamburg Eppendorf, Mass Spectrometric Proteomics Institute for Clinical Chemistry and Laboratory Medicine, Hamburg, Germany

TP-102 **Rapid and effective multi-class analysis of antibiotics in feedingstuffs at carry-over level by LC-MS/MS techniques**
I. Di Marco Pisciottano, L. Giannetti, B. Neri, M. Fiori, C. Civitareale, P. Stacchini, P. Gallo
Istituto Zooprofilattico Sperimentale del Mezzogiorno, Department of Chemistry, Portici (NA), Italy

TP-103 **Determination of organic arsenic compounds by means of high resolution molecular MS/MS**
R. Glabonjat, K. Jensen, N. Guttenberger, K. Francesconi
University of Graz, Analytical Chemistry, Graz, Austria

TP-104 **Linear dynamic range improvement in ToF-MS/MS mode on X500 QToF system**
F. Zhong, S. Liu, W. Jin, D. Simmons, N. Bloomfield, R. Haufler
Sciex, Research, Concord, Canada

TP-105 **Applying a novel component detection algorithm to help accelerate metabolomics discovery workflows**
C. Hinz, E. G. Armitage, K. Hobby, N. Loftus, N. Gray, M. Y Schar, J. P. E. Spencer
Shimadzu UK Limited, LCMS technical department, Milton Keynes, United Kingdom

TP-106 **Comprehensive analysis of flame retardants and other halogenated contaminants in dust from an e-waste recycling centre**
A. Ionas, K. Jobst, L. Melymuk, D. Bowman, M. Diamond, V. Arrandale, M. Venier, L. Jantunen, E. Reiner, J. Klánová
Masaryk University, RECETOX, Brno, Czech Republic

TP-107 **Metabolomic and *N*-glycan characterization of skin fibroblasts from aged and young donors**
A. K. C. Laserna, B. H. Ng, J. Masilamani, T. T. Phan, S. F. Y. Li
National University of Singapore, Department of Chemistry, Singapore

TP-108 **Lean approach of automated sample preparation for LC-MS of intact proteins on a liquid handling robot**
K. List, D. Wetzel, M. Pauers
Boehringer Ingelheim GmbH & Co. KG, Biologicals Development, Biberach, Germany

TP-109 **Combination of chemical ionization (CI) and low-energy electron ionization with high-resolution GC/Q-ToFMS**
V. Lopez-Avila, S. Nieto, H. Prest, J. Kernan, G. Yefchak, R. Clark, N. Eno, J. Oppenheimer, B. Russ, N. Cimino
Agilent Technologies, Mass Spectrometry, Santa Clara, USA

TP-110 **Liquid chromatography coupled to quadrupole-Orbitrap high resolution mass spectrometry based method for target analysis and suspect screening of non-ionic surfactants in textiles**
X. Luo, Z. Niu, X. Ye, Z. Tang, L. Zhang
Qingdao Customs, Inspection and Quarantine Technical Center, Qingdao, China

TP-111 **Comprehensive analysis of multi-class hazardous chemicals in plastic products using high resolution mass spectrometry**
Z. Niu, X. Luo, X. Ye, Z. Tang, L. Zhang
Qingdao Customs, Inspection and Quarantine Technical Center, Qingdao, China

TP-112 **High resolution mass spectrometry based method for screening and identification of 48 prohibited dyes in textiles using data-dependent acquisition mode**
Z. Niu, X. Luo, Z. Tang, X. Ye, L. Qu
Qingdao Customs, Inspection and Quarantine Technical Center, Qingdao, China

TP-113 **Quantitation of serum creatinine in mice using Hydrophilic Interaction Liquid Chromatography (HILIC) coupled with high-resolution accurate-mass (HRMS) Orbitrap mass spectrometer**
H. Takada, Y. Ube, M. Sakai, Y. Hasegawa, T. Kitayama, Y. Yamazaki, T. Uchimura
Kyowa Hakko Kirin Co., Ltd, Translational Research Unit, R&D Division, Sunto-gun, Japan

TP-114 **Ultrasensitive detection of protein biomarkers by signal amplification mass spectrometry**
Y. Wang, R. Du, L. Qiao, B. Liu
Department of Chemistry, Fudan University, Shanghai, China

TPS-S05 - MS Imaging: Instrumentation

TP-115 **Development of optics of a stigmatic imaging mass spectrometer with high spatial resolution**
J. Aoki
Osaka University, Graduate School of Science, Toyonaka, Japan

TP-116 **Developing MS Imaging in the context of chemical ecology - laser ablation electrospray ionization on three-dimensional samples**
B. Bartels, D. Hölscher, P. Kulkarni, A. Svatoš
Research Group Mass Spectrometry/Proteomics, Max Planck Institute for Chemical Ecology, Jena, Germany

TP-117 **Improved sensitivity and speed of acquisition using quadrupole based mass spectrometer for DESI-MSI**
E. Claude, P. Harapanahalli, E. Jones
Waters Corporation, Scientific Operations, Wilmslow, United Kingdom

TP-118 **Atmospheric pressure MALDI imaging Orbitrap MS using a Masstech APMALDI UHR ion source**
G. Frache, D. El Assad
Luxembourg Institute of Science and Technology, Materials research and technology, Belvaux, Luxembourg

TP-119 **Hybrid SIMS: A new SIMS instrument for high resolution organic imaging with highest mass-resolving power and MS/MS**
S. Kayser, A. Pirkl, R. Moellers, D. Scurr, N. Starr, E. Niehuis
IONTOF GmbH, Sales, Muenster, Germany

TP-120 **Desorption electrospray ionization triple quadrupole mass spectrometry: Targeted drug and metabolite imaging in bioanalytical research**
L. Lamont, G. Eijkel, E. Jones, B. Flinders, S. Ellis, T. Porta, R. Vreeken, R. Heeren
Maastricht University, Maastricht Multimodal Molecular Imaging (M4I) Institute, Maastricht, Netherlands

TP-121 **Open development kit for building an ambient mass imaging robot with micrometric resolution**
A. Moreno-Pedraza, C. Ovando-Vázquez, H. Guillén-Alonso, I. Rosas-Román, S. Gibb, R. Winkler
CINVESTAV, Biotechnology and Biochemistry, Irapuato, Mexico

TP-122 **Big data post-processing for higher throughput MALDI/DESI FTMS imaging**
K. O. Nagornov, A. N. Kozhinov, P. C. Kooijman, E. Nicol, P. A. D. Kilgour, S. R. Ellis, R. M. A. Heeren, Y. O. Tsybin
Spectroswiss, Biomolecular Mass Spectrometry, Lausanne, Switzerland

TP-123 **Paternò-Büchi photo-derivatization protocol for MALDI-MS imaging of carbon-carbon double Abond positional isomers of phospho- and glycolipids in biological tissues**
A. Bednarík, S. Bölsker, J. Soltwisch, K. Dreisewerd
University of Münster, Institute for Hygiene, Biomedical Mass Spectrometry, Münster, Germany

TP-124 **Heat-assisted laser ablation electrospray ionization (HA-LAESI) for MS imaging of animal tissue**
J. Hieta, R. Räsänen, J. Kopra, H. Räikkönen, R. Kostiainen, T. Kauppila
University of Helsinki, Faculty of Pharmacy, Helsinki, Finland

TP-125 **Performance-enhanced data acquisition utilizing real-time DSP**
U. Lindblad, C. Watolla
Teledyne Signal Processing Devices Sweden AB, N/A, Linkoping, Sweden

TP-126 **Electrospray ionization/atmospheric pressure interfaces: comprehensive simulation of gas flow, space charge and electric fields**
P. Krah, L. Bernier, S. Rauschenbach, J. Reiss
Technical University Berlin, ISTA, Berlin, Germany

TPS-S06 - Post Translational Modifications

TP-127 **Improvement of proteomic analysis targeting multiple post-translational modifications using immunoprecipitation with pan-PTM antibodies**
Y. Abe, A. Tada, J. Isoyama, T. Tomonaga, J. Adachi
National Institute of Biomedical Innovation, Health, and Nutrition, Proteome Research Project, Osaka, Japan

TP-128 **The role of thiols in redox biology: HPLC-MS characterization of cysteine derivatives generated by interaction with cold plasma jets, powerful sources of nitrogen and oxygen species**
G. Bruno, J. Lackmann, S. Wenske, S. Bekeschus, K. Weltmann, T. Von Woedtke, K. Wende
Leibniz Institute for Plasma Science and Technology (INP Greifswald), ZIK plasmatis, Greifswald, Germany

TP-129 **A rapid, multiplexed kinase activity assay using iTRAQ labeling and MALDI-ToF/ToF MS**
C. Chen, Y. Liu
China Medical University, Taichung, Taiwan, Province of China

TP-130 **Using sub-ranked database matching scores for improving the peptide and protein identification performance**
Y.-R. Chen, Y.-L. Chen, W.-H. Chang
Academia Sinica, Agricultural Biotechnology Research Center, Taipei, Taiwan, Province of China

TP-131 **Separation of combinatorial PTMs on histone H3 tail with an advanced data analysis and ion mobility**
Y. Chikaoka, H. Ueda, R. Kajita, K. Yamamoto, L. Sujin, T. Tanaka, T. Kawamura
Isotope Science Center, The University of Tokyo, Tokyo, Japan

TP-132 **Quantitative phosphoproteomics identifies alterations of doublecortin-like kinase 1 (DCLK1) in neural progenitor cell differentiation**
A. Dehghani, M. Goedderz, V. Gieselmann, D. Winter
University of Bonn, Institute of Biochemistry and Molecular Biology, Bonn, Germany

TP-133 **Analysis of protein-phenolic compound modifications using electrochemistry coupled to mass spectrometry**
C. Kallinich, S. Schefer, S. Rohn
Hamburg School of Food Science, University of Hamburg, Department Food Chemistry, Hamburg, Germany

TP-134 **A new phosphoproteome enrichment strategy in small-scale using phospho-specific antibodies with online mHFER-nanoLC-ESI-MS/MS**
Y. L. Sun, K. Kim, D. Kang
Korea Research Institute of Standards and Science, Division of Chemical and Medical Metrology, Daejeon, Republic of Korea

TP-135 **Histone middle-down analysis using by multiple dissociation methods**
T. Kawamura, H. Ueda, D. Higo, Y. Chikaoka, K. Yamamoto, L. Sujin
Isotope Science Center, The University of Tokyo, Tokyo, Japan

TP-136 **Influence of digestion conditions on post-translational modifications in monoclonal antibodies**
M. Khalikova, A. Ortiz, K. Sandra
Charles University, Faculty of Pharmacy, Hradec Kralové, Czech Republic

TP-137 **Identification and characterization of O-Xylosylation and O-Glycosylation of recombinant protein therapeutics by mass spectrometry**
V. Larraillet
Roche Pharmaceutical Research and Early Development, Biochemical and Analytical Research, Roche Innovation Center, Munich, Germany

TP-138 **Specific mass tag of methylated amino acid validates the SUMOylation sites by HCD on Orbitrap mass spectrometer**
F. Li, Y. Cheng
Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan, Province of China

TP-139 **How does CE-MS compare with LC-MS in PTM analysis?**
K. Faserl, B. Sarg, H. Lindner, J. Thorn, C. Lößner, S. Lock
Sciex, CE and Biopharma, Darmstadt, Germany

TP-140 **Characterization of NIST monoclonal antibody on Intact, Subunit, and Peptide level with Monitoring of CQA's on the 6600**
C. Nortcliffe, K. Pohl, J. Dojahn, F. Sanchez
Sciex, Phoenix House, Warrington, United Kingdom

TP-141 **The PASEF method on a TIMS-QToF mass spectrometer for High Sensitivity Phosphoproteomics**
P.-O. Schmit, H. Koch, T. Kosinsky, M. Willets, M. Lubeck, S. Koch, O. Raether, G. Kruppa, A. Alving
Bruker France, Proteomics, Wissembourg, France

TP-142 **The citrulline effect in the dissociation of deiminated peptides**
A. Steckel, K. Uray, D. Papp, G. Schlosser
ELTE Eötvös Loránd University, Doctoral School of Chemistry, Department of Organic Chemistry, Budapest, Hungary

TP-143 **Chemical acetylation of histone lysine residues at the protein level using acetic anhydride**
A. van Pijkeren, M. D. Kwiatkowski, R. P. H. Bischoff
Rijksuniversiteit Groningen, Analytical Biochemistry, Groningen, the Netherlands

TP-144 **High resolution mass spectrometry based approach for the characterization of plasma proteins oxidative modifications by ROS**
A. Vasilyeva, L. Yurina, M. Indeykina, A. Bugrova, A. Kononikhin, M. Rosenfeld, E. Nikolaev
N.M. Emanuel Institute of Biochemical Physics, RAS, Laboratory of Thermodynamics of Biosystems, Moscow, Russian Federation

TP-145 **Mass spectrometry-based investigations of cold physical plasma-induced PTM's in peptides**
S. Wenske, J. Lackmann, G. Bruno, S. Bekeschus, K. Weltmann, T. Von Woedtke, K. Wende
INP Greifswald e.V., ZIK plasmatis, Greifswald, Germany

TP-146 **Next-generation proteomics insights into Bacillus cereus virulome highlights the key role of methionine oxidation of exoproteins**
B. Alpha-Bazin, J. P. Madeira, H. Omer, J. Armengaud, C. Duport
CEA, DRF/JOLIOT/DMTS, Bagnols-sur-Ceze, France

TP-147 **Identifying the disulfide bond pattern and ECM interaction site of TGFBIp**
M. V. Lukassen, C. Scavenius, I. B. Thøgersen, J. J. Enghild
Aarhus University, Interdisciplinary Nanoscience Center (iNANO), Aarhus, Denmark

TP-148 **Increasing variants in hydrophobic interaction chromatography during stability study of humanised monoclonal antibody identified by LC-MS ESI Q-ToF top down, middle down and bottom up analyses**
M. Pauers, K. List, D. Wetzel
Boehringer Ingelheim Pharma GmbH & Co KG, Pharmaceutical Development Biologicals, Biberach an der Riss, Germany

TP-149 **High resolution mass spectrometry characterization of the oxidation pattern of methionine and cysteine residues in human mitochondria voltage-dependent anion selective channel isoforms**
R. Saletti, M. G. G. Pittalà, P. Risiglione, V. Cunsolo, V. De Pinto, S. Foti
Department of Chemical Sciences, University of Catania, Catania, Italy

TP-150 **Understanding epigenetic control of histone modifications during drought acclimation in sorghum using top-down mass spectrometry**
M. Zhou, N. Malhan, A. Ahkami, K. Engbrecht, G. Myers, J. Dahlberg, J. Hollingsworth, J. Sievert, R. Hutmacher, M. Madera, P. Lemaux, K. Hixson, C. Jansson, L. Paša-Tolić
Pacific Northwest National Laboratory, Environmental Molecular Sciences Laboratory, Richland, USA

TPS-S07 - Mass Spectrometric Analysis of Forensic Science Evidence

TP-151 **Human salivary glycomics for saliva-specific signatures by nanoPGC-LC/MS**
J. B. Kim, J. Y. Park, H. J. An
Graduate School of Analytical Science and Technology & Asia-Pacific Glycomics Reference Site, Chungnam National University, Daejeon, Republic of Korea

TP-152 **Single-injection screening of 664 Forensic Toxicology Compounds using an Innovative Benchtop High Resolution Mass Spectrometer**
J. Anichina, O. G. Cabrices, X. He, H. Mccall, L. Baker, A. Wang, A. Taylor
Sciex, Product Applications Laboratory, Concord, Canada

TP-153 **Ultra-sensitive forensic analysis workflow of cocaine and metabolites in hair samples using LC-MS/MS**
J. Anichina, O. G. Cabrices
Sciex, Product Applications Laboratory, Concord, Canada

TP-154 **FT-ICR fingerprinting of human fingerprints**
A. C. Assis, M. H. Florêncio, C. Cordeiro
Laboratório de Polícia Científica da Polícia Judiciária, University of Lisbon, Laboratório de FTICR e Espectrometria de Massa Estrutural, FCUL, Lisbon, Portugal

TP-155 **A qualitative/quantitative LC-QToF-MS assay for forensic drug screening in urine – Feasibility study and basic method validation**
L. Huppertz, R. Peter, M. Schmidt, Z. Czentnar, V. Auwärter
Bruker Daltonik GmbH, Application/Applied, Bremen, Germany

TP-156 **Analysis of substances relevant to § 24a (2) of the German road traffic act using LC-MS^n – A method development as a first step to avoid immunoassay pre-screening**
J. Kempf, V. Auwärter, F. Ehrhardt, Z. Czentnar
Bruker Daltonik GmbH, Application/Applied, Bremen, Germany

TP-157 **Isolation and identification of thick skin microbiota using MALDI-ToF Biotyper**
G. De Oliveira Dias, A. M. Araújo Martins, R. Persighini Del Sarto
Polícia Civil do Distrito Federal, Universidade de Brasília, Brasília, Brasil

TP-158 **Application of ToF-SIMS technique to detection and imaging of fingerprints contaminated by cannabis**
E. Mackiewicz, J. Rogowski, A. Parczewski, M. I. Szynkowska
Lodz University of Technology, Faculty of Chemistry, Lodz, Poland

TP-159 **Validation of blood proteomic signatures for the forensic determination of blood and its provenance**
C. Heaton, L. Deininger, E. Patel, M. R Clench, V. Sears, C. Sammon, L. Cole, S. Francese
Sheffield Hallam University, Biomolecular Research Centre, Sheffield, United Kingdom

TP-160 **Development and validation of a gas-chromatography mass spectrometry method for the analysis of testosterone esters in biological matrices**
M. Iannone, C. Lattanzi, F. Botrè, X. De La Torre
Laboratorio Antidoping FMSI Rome, Dipartimento di Chimica e Tecnologia del Farmaco, Sapienza University of Rome, Rome, Italy

TP-161 **Elemental analysis of ink by laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS)**
A. Pawlaczyk, K. Zalecka, M. I. Szynkowska
Lodz University of Technology, Faculty of Chemistry, Institute of General and Ecological Chemistry, Lodz, Poland

TP-162 **Detection of ricin and abrin toxins in complex matrices by two novel galactose enrichment methods and high resolution LC-MS/MS**
A. Puustinen, M. Rapinoja, M. Karjalainen, P. Vanninen
Verifin, Dept of Chemistry, University of Helsinki, Helsinki, Finland

TP-163 **LC-HRMS vs NMR for the identification of Ketocaine in seized material**
A. M. Caputo, S. Detti, S. Napoletano, G. De Sangro, R. Sacrpone, F. Sciubba, F. Vincenti, M. Sergi, D. Compagnone
University of Teramo, Faculty of Bioscience, Teramo, Italy

TP-164 **Targeted and untargeted analyses by means of LC-MS to characterize the illicit substances on seized material of vegetal origin.**
A. M. Caputo, S. Detti, S. Napoletano, V. Fraioli, A. Possi, A. Zompanti, R. Scarpone, F. Di Ottavio, M. Sergi, F. Vincenti, L. Felix Nothias, P. Dorrestein
University of Teramo, Faculty of Bioscience, Teramo, Italy

TP-165 **Modafiendz metabolites identification by means of LC-HRMS: from in silico prediction to in vitro confirmation with rat hepatocytes**
F. Vincenti, F. Fanti, A. Gregori, A. Rita Togna, D. Compagnone, M. Sergi
Sapienza, University of Rome, Department of Chemistry, Roma, Italy

TP-166 **Identification of Fine plastic materials by Thermal Desorption and Pyrolysis combined with DART-MS (TDP/DART-MS)**
C. Takei, K. Yoshizawa
BioChromato, Inc., Application support, Fujisawa, Japan

TP-167 **ToF-SIMS determination of detection limit of amphetamine in 'street drugs' and polluted fingerprints**
M. Gajek, E. Mackiewicz, J. Rogowski, A. Parczewski, M. I. Szynkowska
Lodz University of Technology, Faculty of Chemistry, Lodz, Poland

TPS-S08 - Ion Activation and Dissociations

TP-168 **Tandem mass spectrometry to assist the design of information-containing synthetic polymers: an efficient approach to facilitate their sequencing and increase their storage density**
J. Amalian, G. Cavallo, S. Poyer, J. Lutz, L. Charles
Institut de Chimie Radicalaire, Aix-Marseille Université, Marseille, France

TP-169 **Facile electron capture dissociation on Q-ToFs and Orbitraps for top- and middle-down proteomics at chromatographic time scales**
J. Beckman, V. Voinov
e-MSion, Oregon State University, Corvallis, USA

TP-170 **The role of H_2O in the dissociation chemistry of $[W_6O_{19}]^{2-}$: a combinational study by mass spectrometry and DFT calculation**
J. Cao, C. Ci
Beijing Institute of Technology, School of Chemistry and Chemical Engineering, Beijing, China

TP-171 **Controled collision induced dissociation of large aromatic ions in a LQIT**
M. Carlos, H. Sabbah, C. Joblin
Institut de Recherche en Astrophysique et Planétologie, Université de Toulouse, CNRS, CNES, Toulouse, France

TP-172 **Ultraviolet photodissociation of peptides and proteins, generated by electrospray and matrix-assisted laser desorption/ionization, on the same Q-Exactive mass spectrometer**
M. Dilillo, E. De Graaf, A. Yadav, M. Belov, L. McDonnell
Fondazione Pisana per la Scienza - ONLUS, Proteomics Laboratory, San Giuliano Terme, Italy

TP-173 **Gas phase reactions of Indocyanine green using femtosecond-laser-pulse induced photodissociation and collision-induced dissociation**
E. Mitrofanov, T. Muskat, J. Grotemeyer
University of Kiel, Institute of Physical Chemistry, Kiel, Germany

TP-174 **Lost in phase space: fragmentation energetics in quadrupole ion traps**
T. Neugebauer, T. Drewello
Friedrich-Alexander-University Erlangen-Nuremberg, Chair of Physical Chemistry I, Erlangen, Germany

TP-175 **Collision induced dissociation of hydrogen deficient radical ions on the Omnitrap platform**
D. Papanastasiou, R. Zubarev
Fasmatech Science & Technology, Patriarchou Gregoriou, Agia Paraskevi, Athens, Greece

TP-176 **Comprehensive glycomics study by nanoLC-EED-MS/MS**
Y. Tang, J. Wei, C. Costello, C. Lin
Boston University, Boston University, Department of Chemistry, Boston, USA

TP-177 **ESI(-)MS/MS of 2-oxocarboxylate hydrazones: carboxyl group participation in two fragmentation pathways**
R. L. White, B. W. Firth, L. M. LeBlanc, J. S. Grossert
Dalhousie University, Chemistry, Halifax, Canada

TP-178 **Assessing binding affinity with LILBID-MS**
P. Young, G. Hense, N. Morgner
Institute of Physical and Theoretical Chemistry, Goethe Universität Frankfurt, Frankfurt am Main, Germany

TP-179 **Tuning mass spectrometric proteomics experiments: Collision energy dependence of Mascot score**
A. Revesz, T. A. Rokob, D. Jeanne Dit Fouque, L. Turiak, A. Memboeuf, K. Vekey, L. Drahos
Research Centre for Natural Sciences, Hungarian Academy of Sciences, MS Proteomics Research Group, Budapest, Hungary

TP-180 **Structural characterization of complex lipids by ozone-induced dissociation and ultraviolet photodissociation on high-resolution mass spectrometers**
A. Criscuolo, D. L. Marshall, M. Zeller, B. L. J. Poad, J. Hauschild, T. W. Mitchell, G. E. Reid, S. J. Blanksby
Thermo Fisher Scientific GmbH, Life Science Mass Spectrometry, Bremen, Germany

TPS-S09 - Astrochemistry

TP-181 **PIRENEA 2: a new setup to study cosmic dust in the laboratory**
A. Bonnamy, P. Jusko, M.-C. Ji, P. Moretto-Capelle, S. Zamith, J.-M. L'Hermite, M. Pellarin, C. Joblin
Institut de Recherche en Astrophysique et Planétologie, Université de Toulouse, CNRS, CNES, Toulouse, France

TP-182 **Mass spectrometry a new approach to study thunderstorms**
L. F. C. Oliveira, D. U. Tega, F. Galembeck, M. N. Eberlin
UNICAMP, Chemistry Institute, Campinas, Brazil

TP-183 **Reaction dynamics of substituted PAH ions**
P. Mayer, B. West, L. Lesniak, J. Burner
University of Ottawa, Dept. of Chemistry and Biomolecular Sciences, Ottawa, Canada

TP-184 **A multi-vendor applicable target system for (MA)LDI instruments with distinct performance characteristics for the analysis of small organic molecules related to C chondrites**
E. Rados, E. Pittenauer, J. Frank, K. Varmuza, G. Allmaier
TU Wien, Institute of Chemical Technologies and Analytics, Vienna, Austria

TPS-S10 - Metabolomics

TP-185 **Measuring trehalose 6-phosphate (Tre6P) in different plant materials – the technical challenge of working at the femtomole scale**
R. Feil, M. G. Annunziata, J. E. Lunn
Max Planck Institute of Molecular Plant Physiology, Dept. Metabolic Networks, Potsdam, Germany

TP-186 **Identification of novel long chain N-acylhomoserine lactones of chain length C20 from the marine phototrophic bacterium Rhodovulum sulfidophilum**
N. Arashida, K. Shimbo, T. Terada, T. Okimi, Y. Kikuchi, S. Hashiro, S. Umekage, H. Yasueda
Ajinomoto Co., Inc., Institute for Innovation, Kawasaki, Japan

TP-187 **Fatty acid β-oxidation fuels tricarboxylic acid cycle to sustain cell proliferation**
M. Audano, S. Pedretti, D. Caruso, N. Mitro, E. De Fabiani
Università degli Studi di Milano, Milano, Italy

TP-188 **Diagnostic performance of methylmalonic acid testing by LC-MS/MS compared to Holotranscobalamin by Immunoassay for vitamin B12 deficiency**
F. Bahadory, P. Stanford, A. R. Horvath
NSW Health Pathology, Prince of Wales Hospital, Sydney, NSW, Australia

TP-189 **Pycmetrix a framework for gas chromatography - mass spectrometry for clinical data pre-processing, analysis and feature extraction**
A. Barcaru, R. Heiner-Fokkema, P. Horvatovich
University Medical Center of Groningen, Laboratory of medicine, Groningen, Netherlands

TP-190 **The utilization of tandem mass spectrometry techniques in diagnosis of patients with homocystinurias**
J. Bártl, J. Krijt, P. Chrastina, J. Hodík, M. Paulová, R. Pinkasová, J. Sokolová, V. Kožich, K. Peškova
General University Hospital in Prague and 1st Faculty of Medicine, Charles University in Prague, Clinic of Pediatrics and Adolescent Medicine, Prague, Czech Republic

TP-191 **CESI-MS - A sensitive and versatile approach for metabolomics**
W. Belloni
Sciex Spa, Separations CE, Milano, Italy

TP-192 **Assessment of kidney graft quality by SPME-(LC)-HRMS: going beyond clinical routine**
I. Stryjak, M. Hamar, M. Selzner, B. Bojko
Nicolaus Copernicus University in Torun, Department of Pharmacodynamics and Molecular Pharmacology, Faculty of Pharmacy, Collegium Medicum in Bydgoszcz, Bydgoszcz, Poland

TP-193 **Multilayer omics strategy for tracing the metabolic routes exploited by KRAS oncogenetic mutation in NSCLC**
L. Brunelli, E. Caiola, F. Falcetta, S. Giordano, M. Marabese, M. Broggini, R. Pastorelli
IRCCS-Istituto di Ricerche Farmacologiche Mario Negri, Environmental Health Sciences, Milano, Italy

TP-194 **Conversion of coenzyme A thioesters by native chemical ligation – a new approach for characterizing an important class of biomolecules**
N. Cakic, H. Wilkes
Institute for Chemistry and Biology of the Marine Environment (ICBM), University of Oldenburg, Oldenburg, Germany

TP-195 **Enhanced metabolite identification using an Orbitrap Tribrid mass spectrometer**
K. Comstock, S. Ma, S. Sharma, H. Cardasis, Y. Chen
Thermo Fisher Scientific, 1, San Jose, USA

TP-196 **Targeted approach for determination of metabolites of flavonoids and isoflavonoids in biological samples**
L. Chrenková, V. Pilarová, L. Applová, I. Najmanová, P. Mladenka, L. Nováková
Charles University, Faculty of Pharmacy, Department of Analytical Chemistry, Hradec Králové, Czech Republic

TP-197 **Exploring serum targeted metabolomics mass spectrometry profile analysis to implement risk criteria for first-degree relatives (FDR) of gastric cancer (GC) patients**
G. Corona, R. Cannizzaro, G. Miolo, A. Steffan, V. De Re
IRCCS National Cancer Institute, Immunopathology and Cancer Biomarkers, Aviano(PN), Italy

TP-198 **Phytochemical screening of fagioli bianchi di Rotonda beans DOP (Phaseolus Vulgaris L.) and evaluation of their biological activity for functional food properties**
D. Coviello, A.Onzo, G. Bianco, R. Pascale, P. Schmitt-Kopplin, P. Iannece, C. Gaeta
Università degli Studi della Basilicata, Dipartimento di Scienze, Potenza, Italia

TP-199 **Two-dimensional gas chromatography as a powerful tool for discriminating VOCs in monovarietal and commercial extra virgin olive oil**
A. Da Ros, S. Carlin, D. Masuero, S. Riccadonna, F. Mattivi, N. Mulinacci, U. Vrhovsek
Fondazione Edmund Mach, Food quality and Nutrition, San Michele all'Adige, Italy

TP-200 **A targeted metabolomics assay to investigate steroid hormones in women during pregnancy and early postpartum period**
S. Di Palma, E. Laczko
Functional Genomics Center Zurich, University of Zurich/ETH, Zurich, Switzerland

TP-201 **EcoMetabolomics of root exudates in german grassland communities**
S. Dietz, S. Döll, K. Gorzolka, D. Scheel
Leibniz Institute of Plant Biochemistry, Stress and Developmental Biology, Halle-Saale, Germany

TP-202 **A novel labeled metabolomics workflow applying Isotope Ratio Outlier Analysis (IROA) and SWATH® acquisition for unambiguous compound identification**
P. Cyrus, C. Beecher, F. A. De Jong, B. Ubhi, J. Dojahn
Sciex, Darmstadt, Germany

TP-203 **Untargeted metabolomics in plant biochemistry**
S. Döll, H. Treutler, S. Neumann, D. Scheel
Leibniz Institute of Plant Biochemistry, Stress and Developmental Biology, Halle, Germany

TP-204 **An investigation of biomarkers in the serum of developmental disorders using an intellectual disability model mouse, which show impaired social behaviours**
K. Gamoh, M. Nishimura, T. Akashi, Y. Nishiwaki, T. Kashio, S. Mitsui
Kochi University and Gunma University Graduate School of Health Sciences, Kochi, Japan

TP-205 **Electrochemical oxidation of primary bile acids: Simulation of endogenous metabolism**
L. Navarro Suarez, L. Brückner, S. Rohn
Hamburg School of Food Science, University of Hamburg, Hamburg, Germany

TP-206 **Low invasive metabolomic phenotyping: a potential alternative for genotyping of gliomas**
P. Z. Gorynska, K. Gorynski, K. Chmara, J. Furtak, D. Paczkowski, M. Harat, B. Bojko
Faculty of Pharmacy Collegium Medicum, Department of Pharmacodynamics and Molecular Pharmacology, Nicolaus Copernicus University in Toruń, Bydgoszcz, Poland

TP-207 **$^{13}CO_2$ Isotope labelling of Arabidopsis thaliana: Tracking labelled carbon in metabolites from leaves to roots to exudates**
K. Gorzolka, G. Balcke, H. Treutler, S. Neumann, D. Scheel
Leibniz Institute of Plant Biochemistry, Stress and Developmental Biology, Halle, Saale, Germany

TP-208 **Metabolomic approach to investigate metabolite alterations attributed to a 25-hydroxyvitamin D in healthy Korean adults**
M.-R. Gwon, B. K. Kim, B. Ohk, S. Cho, S. J. Seong, Y.-R. Yoon
Cell and Matrix Research Institute, Department of Biomedical Science, School of Medicine, Kyungpook National University, DAEGU, Republic of Korea

TP-209 **An analytical framework for the exploration of endogenous peptides integrating peptide structure prediction and tandem mass spectrometry**
C. Kawano, E. Hayakawa, H. Watanabe
Okinawa Institute of Science and Technology, Okinawa, Japan

TP-210 **Towards the deciphering of the mechanism of action of an experimental drug against Chagas disease, using multi-omics platform**
K. Hennig, J. Abi-Ghanem, A. Bunescu, X. Meniche, E. Biliaut, F. Bequet, M. Lewis, J. Kelly, S. Braillard, G. Courtemanche, E. Chatelain
BIOASTER, Metabolomics and proteomics unit, Lyon, France

TP-211 **Metabolomic approach for the estimation of age of bloodstain**
H.-G. Kang, Y. Lee, A. Seok, Y. Lee, A. Park, S. Mun, H. Kim
Eulji University, Department of Senior Healthcare, BK21 Plus Program, Graduate School, Daejeon, Republic of Korea

TP-212 **Metabolomic analysis of human plasma to characterize metabolite changes associated with exposure to persistent organic pollutants**
B. K. Kim, M.-R. Gwon, B. Ohk, S. Cho, S. J. Seong, D. Lee, Y.-R. Yoon
Kyungpook National University, Department of Biomedical Science, School of Medicine, Daegu, Republic of Korea

TP-213 **A Rapid Microbore Metabolic Profiling (RAMMP) analytical platform for discovery metabolomics and lipidomics**
A. King, L. Mullin, I. Wilson, P. Rainville, R. Plumb, L. Gethings, D. Heywood, G. Maker, R. Trengove
Waters Corporation, Scientific Operations, Wilmslow, United Kingdom

TP-214 **Rapid and simultaneous determination of 23 amino acids in non-invasive and invasive biological samples from obesity patients by liquid chromatography-tandem mass spectrometry after derivatization**
L. Konieczna, A. Krawczyńska, J. Siebert, P. Gutknecht, M. Skrzypkowska, Ł. Kaska, J. Bigda, M. Proczko-Stepaniak,T. Bączek
Medical University of Gdańsk, Department of Pharmaceutical Chemistry, Gdańsk, Poland

TP-215 **Identification of internal standard metabolites for standardization bloodstains**
J. Lee, H. Kim, Y. Lee, A. Eun Seok, A. Park, S. Mun, Y. Lee, H. Kang
Eulji University, Department of Biomedical Laboratory Science, College of Health Sciences, Seongnam-si, Gyeonggi-do, Republic of Korea

TP-216 **An infusion "shotgun" approach for high-throughput untargeted metabolomics**
M. Maldini, C. Papan, Z. Demianova, J. Dojahn, B. K Ubhi
Sciex, Darmstadt, Germany

TP-217 **SWATH® acquisition improves metabolite coverage over traditional data dependent techniques for untargeted metabolomics**
M. Maldini, Z. Demianova, C. Papan, J. Dojahn, B. K. Ubhi
Sciex, Darmstadt, Germany

TP-218 **Analytical ion spectroscopy - a new route to metabolite identification**
J. Martens, G. Berden, R. Van Outersterp, L. Kluijtmans, R. Wevers, J. Oomens
FELIX Laboratory, Radboud University, Nijmegen, Netherlands

TP-219 **Microflow metabolomics differentiates pre-classified healthy and cancer samples**
D. Merkel, C. Papan, Z. Demianova, J. Dojahn, M. Maldini, K. Motamedchaboki, B. K. Ubhi, E. Lin
SCIEX Germany, Application Support, Darmstadt, Germany

TP-220 **High-throughput LC-MS/MS-based chiral metabolic profiling focusing on amino acids and related metabolites**
Y. Nakano, M. Taniguchi, E. Fukusaki
Osaka university, Advance Science and Biotechnology, Osaka, Japan

TP-221 **Study of auxin biosynthesis using in vivo labelling**
A. Pencik, P. Vonka, M. Kubes, K. Ljung, O. Novak
Institute of Experimental Botany AS CR & Palacky University, Laboratory of Growth Regulators, Olomouc, Czech Republic

TP-222 **Can obstructive sleep apnoea be diagnosed by real-time analysis of exhaled breath using secondary electrospray ionization mass spectrometry - a validation study**
N. Nowak, A. Engler, D. Schneeberger, S. Thiel, T. Gaisl, M. T. Gaugg, S. P. Martinez-Lozano, A.-S. Stöberl, M. Kohler, R. Zenobi
ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland

TP-223 **A dual separation/high resolution accurate mass spectrometry system for improved metabolome coverage and increased throughput**
I. Ntai, M. Samonig, A. Paulus, R. Tautenhahn, A. Souza, A. Huhmer
Thermo Fisher Scientific, San Jose, USA

TP-224 **Intelligent MS^n workflow for improved metabolome coverage and increased confidence in unknown identification**
I. Ntai, I. Mohtashemi, R. Tautenhahn, G. Mcalister, S. Sharma, V. Zabrouskov, A. Souza, A. Huhmer
Thermo Fisher Scientific, San Jose, USA

TP-225 **Non-target metabolomic analysis of peperoni di Senise peppers IGP (Capsicum Annuum L.) and evaluation of their nutraceutical properties**
A. Onzo, D. Coviello, G. Bianco, R. Pascale, P. Schmitt-Kopplin, P. Iannece, C. Gaeta
Università degli Studi della Basilicata, Dipartimento di Scienze, Potenza, Italy

TP-226 **Determination of metabolization of new fluorescently labeled auxin-like compounds in plant material using UHPLC-MS/MS**
B. Parízková, A. Žukauskaite, T. Vain, P. Grones, M. Kubeš, M. Kieffer, K. Doležal, S. Kepinski, M. Strnad, S. Robert, O. Novák
Centre of the Region Haná for Biotechnological and Agricultural Research, Department of Chemical Biology and Genetics, Faculty of Science, Palacký University, Olomouc, Czech Republic

TP-227 **Metabolomic approaches to investigate the role of the mitochondrial regulator Zc3h10 in adipocytes**
S. Pedretti, M. Audano, E. De Fabiani, D. Caruso, N. Mitro
Università degli Studi di Milano, Department of Pharmacological and Biomolecular Sciences, Milan, Italy

TP-228 **LC-MS/MS quantification of thiol-containing metabolites within the de novo glutathione synthesis pathway over the lifespan of Caenorhabditis elegans**
G. Ferguson, R. Pickford, W. Bridge
University of New South Wales, Bioanalytical Mass Spectrometry Facility, Kensington, Australia

TP-229 **Integration of tandem mass spectrometry molecular networking and gas-phase fragmentation reactions for structural analysis of flavonoid glycoconjugates**
A. C. Pilon, N. F. Carnevale, H. Gu, D. Raftery, V. Da Silva Bolzani, N. Peporine Lopes, G. Ian Castro
University of São Paulo, Faculty of Pharmaceutical Sciences, Ribeirão Preto, Brazil

TP-230 **Typical LC-MS metabolomics workflow for profiling urine samples of patients with colorectal cancer**
I. Plyushchenko, T. Bolotnik, D. Shakhmatov, S. Achkasov, O. Sushkov, O. Shpigun, I. Rodin
Lomonosov Moscow State University, Chemistry Department, Moscow, Russian Federation

TP-231 **Metabolomics analysis of urine in mice with prostate cancer**
L. C. Rodas Sánchez, P. Rodriguez-González, A. J. I. García, P. González-Menéndez, J. C. Mayo Barrallo, R. Sainz Menéndez, A. López- Gonzálvez, C. Barbas
University of Oviedo, Department of Physical and Analytical Chemistry, Faculty of Chemistry, Oviedo, Spain

TP-232 **A novel integrative strategy to prevent colorectal cancer within the diet-host-microbiota TRIANGLE: from organoids to human in vivo reality**
J. Rubert, F. Mattivi, A. Lunardi
Centre for Integrative Biology (CIBIO), University of Trento, Trento, Italy

TP-233 **Indolome analysis for nutraceutical and physiological studies**
F. M. Rubino, M. Dei Cas, A. Penoni, M. Iriti, R. Clara Paroni, J. Rizzo
Università degli Studi di Milano, Dipartimento di Scienze della Salute, MIlano, Italy

TP-234 **Rapid analysis of NCI60 panel metabolic and lipid profiles with an automatic well plate reader using laser assisted REIMS**
R. Schäffer, J. Balog, D. Simon, N. Kucsma, A. Lovrics, G. Szakacs, S. Pringle, Z. Takats
Waters Research Center, R&D, Budapest, Hungary

TP-235 **A wellness study using microflow targeted metabolomics to investigate the effects of diet and exercise on the metabolome**
Z. Demianova, K. Motamedchaboki, B. Ubhi, D. Schleuder
Sciex, Darmstadt, Germany

TP-236 **Fecal metabolomics of a mouse model of autism**
E. Sekera, T. Wood, H. Rudolph, S. Carro
University at Buffalo, Department of Chemistry, Buffalo, USA

TP-237 **Liquid extraction surface analysis and direct ESI/nanoESI mass spectrometry for high throughput urinary metabolomics applied to malaria**
S. Abdelrazig, C. Ortori, D. Barrett
University of Nottingham, School of Pharmacy, Nottingham, United Kingdom

TP-238 **Urinary metabolic profile of newborns with transposition of great arteries undergoing cardiac surgery with cardiopulmonary bypass**
M. Simonato, L. Vedovelli, M. Padalino, G. Stellin, S. Carollo, A. Bandini, V. Carnielli, P. Cogo
Istituto di Ricerca Pediatrica "Città della Speranza", Padova, Italy

TP-239 **Volatilome analysis for Parkinson's disease diagnostics**
E. Sinclair, D. Trivedi, Y. Xu, C. Liscio, P. Banks, J. Milne, M. Silverdale, T. Kunath, R. Goodacre, P. Barran
University of Manchester, Chemistry, Manchester, United Kingdom

TP-240 **Detection of metabolic signatures of Crohn's disease using an intelligent MS^n-based discovery workflow**
I. Ntai, A. Souza, R. Tautenhahn, G. Tan, A. Huhmer
Thermo Fisher Scientific, Metabolomics Program, San Jose, USA

TP-241 **Monoamine mapping by mass spectrometry identified brain nuclei regulating anxiety in a serotonin deficiency model**
Y. Sugiura, E. Sugiuyama
Keio University, School of Medicine, Tokyo, Japan

TP-242 **Construction and application of a high-resolution MS/MS library including retention time information for rapid identification of endogenous metabolites**
M. Szesny, S. Zhao, X. Luo, W. Chan, U. Schweiger-Hufnagel, A. Barsch, L. Li
Bruker Daltonik GmbH, Metabolomics, Bremen, Germany

TP-243 **Developing a robust LC-MS panel for assessing residual platelets and other sample quality issues in plasma**
W. Tan, C. Drum
National University of Singapore, NUS Graduate School for Integrative Sciences and Engineering, Singapore, Singapore

TP-244 **Revealing the hidden part of bacterial metabolism**
E. Dairii, P. L. Saaidi, A. Perret, M. Salanoubat
CEA - Genoscope, Evry, France

TP-245 **Assessment of the THS exposition in animal models by multiplatform metabolomics analysis**
S. Torres, S. Samino, P. Rafols, N. Adhami, M. Martins-Greens, X. Correig, N. Ramirez
Rovira y Virgili University, Department of Electronic, Electrical and Automatic Control Engineering, Tarragona, Spain

TP-246 **Simultaneous quantitative analysis method for hydroxyproline and 4-hydroxyglutamic acid using isotopologue-SRM to clarify hydroxyproline metabolism**
M. Tsuji
Daiichisankyo RD Novare Co., Ltd., Pharmaceutical and Biomedical Analysis, Tokyo, Japan

TP-247 **An untargeted metabolomics approach to go beyond Aspirin canonical effect**
L. Turnu, C. M. Manega, B. Porro, A. Di Minno, F. Veglia, D. Caruso, E. Tremoli, V. Cavalca
Centro Cardiologico Monzino IRCCS, Unit of metabolomics and cellular biochemistry of atherotrombosis, Milano, Italy

TP-248 **Evaluation of high speed, high resolution data independent acquisition for the analysis of metabolomic flux, kinetics and pathway mapping**
Z. Demianova, B. K Ubhi, L. Olson, J.-B. Vincendet
Sciex, France

TP-249 **Utilizing a standardized and targeted quantitative assay coupled to HRAM MS for the analysis of serum metabolites obtained from diabetic study subjects**
A. Kalli, S. Webb, M. Kratzke, M. Langsdorf, S. Dearth, H. Tuan Pham, T. Koal, A. Huhmer
Thermo Fisher Scientific, San Jose, USA

TP-250 **Development of a simultaneous analysis of the fat-soluble vitamin using the lithium ion**
N. Yamada, T. Matsui, H. Kuno
Japan Tobacco Inc., Toxicology Research Laboratories, Hadano, Japan

TP-251 **Human metabolite identification by searching a high quality and comprehensive tandem mass spectral library**
X. Yang, P. Neta, S. Stein
NIST, Mass Spectrometry Data Center, Gaithersburg, USA

TP-252 **TiO_2 assisted laser desorption/ionization mass spectrometry for rapid profiling of candidate metabolite biomarkers from antimicrobial resistant bacteria**
R. Zhang, Q. Qin, B. Liu, L. Qiao
Fudan University, Shanghai, China

TP-253 **Metabolic characterization of THP-1 macrophages polarization using LC-MS-based metabolite profiling**
A. Abuawad, D. Barrett, A. Ghaemmaghami, D. Kim
University of Nottingham, University of Nottingham, Advanced Materials and Healthcare Technologies, Nottingham, United Kingdom

TP-254 **Investigating the differences in the molecular effects of free and nanoparticle loaded methotrexate on proliferative and nonproliferative cancer cells using advance cell based metabolomics**
M. Al-Natour, A. Alazzo, A. Ghaemmaghami, D.-H. Kim, A. Cameron
University of Nottingham, School of pharmacy, Division of Molecular Therapeutics and Formulation, Nottingham, United Kingdom

TP-255 **Characterization of phenolic compounds and determination of anti-inflammatory and anti-cholinesterase activity in 2 Colombian fruits: Borojoa Patinoi and Bactris Gasipaes**
D. Arias Ramirez
Universidad de los Andes, Chemistry Department, Bogotá D.C., Colombia

TP-256 **Phenolic, alkaloids and lipids of Ochroma pyramidale, Tapirira guianensis and Inga edulis, host plants of the caterpillar Lonomia descimoni**
F. Benavides, C. Carazzone
Universidad de los Andes, Chemistry Department, Bogotá D.C., Colombia

TP-257 **Multi-omics profiling of pancreatic cancer stem-like cells**
C. Di Carlo
Università degli Studi di Verona, Biotechnology, Verona, Italy

TP-258 **Informed unTargeted Metabolomics using LC-MS/MS**
J. Folberth, O. Jöhren, M. Schwaninger, A. Othman
University of Luebeck, Institute for Experimental and Clinical Pharmacology and Toxicology, Luebeck, Germany

TP-259 **LC-MS analysis of nonribosomal peptidome from a Brazilian cyanobacterium Nostoc sp. CENA543**
J. Jokela, L. Heinilä, T. Keiko Shishido, M. Wahlsten, D.P. Fewer, M. Fátima Fiore, E. Haapaniemi, P. Permi, K. Sivonen
University of Helsinki, Department of Microbiology, Helsinki, Finland

TP-260 **Comparative evaluation of different ginseng berry species based on UPLC-QToF/MS and HR-MAS NMR metabolite profiles**
D. Y. Lee, J. W. Lee, B. Choi, D. Yoon, Y. C. Kim, S. Kim
National Institute of Horticultural and Herbal Science, Department of Herbal Crop Research, Eumseong, Republic of Korea

TP-261 **Untargeted metabolomics with parallel accumulation – serial fragmentation (PASEF) on a novel trapped ion mobility mass spectrometer**
F. Meier, C. Vasilopoulou, K. Sulek, A. Brunner, U. Schweiger-Hufnagel, S. Meyer, A. Barsch, M. Mann
Max Planck Institute of Biochemistry, Proteomics and Signal Transduction, Martinsried, Germany

TP-262 **Automated parallel derivatization strategy with broad metabolite coverage coupled to SWATH/MS data acquisition for qualitative and quantitative analysis**
D. Ruskic, M. F. C. Girard, R. Picenoni, M. F. Mirabelli, G. Böhm, G. Hopfgartner
CTC Analytics AG, Zwingen, Switzerland

TP-263 **Targeted metabolomics applied to heart failure patients – a pilot study**
R. Nilsson, L. Löfgren, F. Michopoulos, M. Ryaboshapkina, P. Davidsson, C. Linde, B. Persson
Astrazeneca, Translational science, Mölndal, Sweden

TP-264 **Phospholipid removal by solid phase extraction for untargeted metabolomics: improved sensitivity for polar metabolites in brain**
P. Pöhö, A. Vaikkinen, E. Scurti, M. Airavaara, T. Kotiaho, R. Kostiainen
University of Helsinki, Division of Pharmaceutical Chemistry and Technology, Helsinki, Finland

TP-265 **Coffee metabolomics by LC-HRMS and molecular networking**
C. M. Rezende, N. M. D. Sá, R. G. Costa
Federal University of Rio de Janeiro, Chemistry Institute, Rio de Janeiro, Brazil

TP-266 **Untargeted metabolomics of native tasmanian plants: comparison with their medicinally-known relatives**
K. Skraskova, R. Wilson, J. Smith
University of Tasmania, School of Chemistry, Hobart, Australia

TP-267 **Hydrophilic interaction liquid chromatography – field asymmetric waveform ion mobility spectrometry – mass spectrometry as a platform for untargeted metabolomic studies**
K. Szykula, M. Turner, C. Creaser, J. Reynolds
Loughborough University, Department of Chemistry, Centre for Analytical Science, Loughborough, United Kingdom

WEDNESDAY, August 29th, 2018

WPS-S01 - Native MS and Structural Proteomics

WP-01 **Acidic XPlex: a multiplex alternative to NHS esters for faster cross-linking reactions at lower temperatures**
B. C. Amaral, F. C. Gozzo, D. B. Lima, P. C. Carvalho
University of Campinas, Dalton Mass Spectrometry Laboratory, Institute of Chemistry, Campinas, Brazil

WP-02 **Intact mass analysis of macromolecular PEG-Fab conjugate using multi-mode native LC coupled to ultra-high mass range native MS**
A. Bailey, G. Han, J. Josephs, W. Sandoval, E. Damoc
Thermo Fisher Scientific, San Jose, USA

WP-03 **Native mass spectrometry analysis of recombinant antibodies directly from the growth medium**
G. Ben-Nissan, S. Vimer, A. Katz, S. Warszawsky, R. Diskin, S. Fleishman, M. Sharon
Weizmann Institute of Sceince, Department of Biomolecular Sciences, Rehovot, Israel

WP-04 **Coupling online separations to native MS for the characterization of designed protein complexes**
F. Busch, M. Jia, Z. Vanaernum, A. Sahasrabuddhe, Z. Chen, S. Boyken, D. Baker, V. Wysocki
The Ohio State University, Department of Chemistry and Biochemistry, Columbus, USA

WP-05 **Structural characterisation of wild-type and ΔN6 β2–microglobulin comparing HDX and FPOP chemical labelling**
O. Cornwell, J. Ault, S. Radford, A. Ashcroft
University of Leeds, Faculty of Biological Sciences, Leeds, United Kingdom

WP-06 **Double mutant cycles in the gas phase: measuring inter-protein pairwise interaction energies from crude cell lysates by native MS**
J. Cveticanin, R. Netzer, G. Arkind, S. Fleishman, A. Horovitz, M. Sharon
Weizmann Institute of Science, Department of Biomolecular Sciences, Rehovot, Israel

WP-07 **Advances in Orbitrap™ instrumentation for native top-down analysis of non-covalent protein complexes**
E. Damoc, R. Viner, A. Konijnenberg, K. Fort, M. Reinhardt-Szyba, M. Belov, A. Makarov
Thermo Fisher Scientific, Bremen, Germany

WP-08 **Architecture of eukaryotic mRNA 3′-end processing machinery - The role of cross-linking and mass spectrometry**
G. Degliesposti, M. Skehel, A. Casanal, A. Kumar, C. Hill, A. Easter, P. Emsley, Y. Gordiyenko, B. Santhanam, J. Wolf, K. Wiederhold, G. Dornan, C. V. Robinson, L. A. Passmore
Laboratory of Molecular Biology (MRC LMB), Cambridge, United Kingdom

WP-09 **The influence of substrates and nucleotides on complex formation in ABC transporters – insights from mass spectrometry**
F. Fiorentino, J. R. Bolla, S. Mehmood, C. V. Robinson
University of Oxford, Department of Chemistry, Oxford, United Kingdom

WP-10 **Chemico-structural and functional characterization of filgrastim originator and three of its biosimilar drugs**
A. Gianoncelli, M. Bertuzzi, M. Guarienti, M. Memo
University of Study of Brescia, Molecular and Translational Medicine, Brescia, Italy

WP-11 **Characterization of calcium-mediated alpha-synuclein aggregation pathway at the molecular level**
J. Y. Han, H. I. Kim
Korea University, Department of Chemistry, Seoul, Republic of Korea

WP-12 **Characterization of intact monoclonal antibodies under native and reverse phase conditions using high resolution mass spectrometry**
C. Nortcliffe, R. Yokoyama, S. Heidelberger, K. Pohl, J. Dojahn, F. Sanchez, A. Uppal
Sciex, Biologics, Warrington, United Kingdom

WP-13 **Native mass spectrometry of biomolecules: a comparison of nESI-MS and LILBID-MS**
N. Hellwig, O. Peetz, N. Morgner
Goethe-University, Institute of Physical and Theoretical Chemistry, Frankfurt, Germany

WP-14 **Evaluation of an Isotope-Labeled MS/MS-Cleavable Cross-Linker for Protein Structure Analysis**
C. Ihling, P. Springorum, M. Götze, C. Hage, M. Schäfer, A. Sinz
Martin Luther University Halle-Wittenberg, Institute for Pharmacy, Halle, Germany

WP-15 **Deep biosimilarity assessment by monitoring multiple critical quality attributes of an intact monoclonal antibody drug using native IEC and SEC coupled to native Orbitrap MS**
J. Josephs, A. Bailey, T. Zhang, S. Houel, S. Lin, G. Han, B. Gamez, K. Southwick, W. Sandoval, J. Josephs
Thermo Fisher Scientific, Chromatography and Mass Spectrometry, San Jose, USA

WP-16 **Structural comparison and epitope mapping of innovator and biosimilar therapeutic antibodies**
C. Lento, K. Brown, D. Wilson
York University, Chemistry, Toronto, Canada

WP-17 **LILBID-MS reveals influences of ThT and Coomassie on aggregation kinetics of amyloid-β (1-42) and a-synuclein**
J. Martin, R. Zangl, T. Lieblein, N. Morgner
Goethe University, Institute of Physical and Theoretical Chemistry, Frankfurt, Germany

WP-18 **Quantification of substrate and inhibitor binding to wild type and mutant isocitrate dehydrogenase (IDH1) by non-denaturing mass spectrometry**
V. Mikhailov, S. Liu, C. Schofield, J. McCullagh
University of Oxford, Department of Chemistry, Oxford, United Kingdom

WP-19 **An optimized enrichment strategy for improved mass spectrometry analysis of chemically cross-linked peptides**
R. Viner, L. Foster, E. Raja, C. Etienne, R. Bomgarden, M. Oppermann
Thermo Fisher Scientific, Europe, Stockholm, Sweden

WP-20 **Towards defining of the molecular maturation pathway of the mitochondrial sulfhydryl oxidase Erv1**
K. Pacholarz, X. Tang, H. Lu, P. Barran
Manchester Institute of Biotechnology, The University of Manchester, Manchester, United Kingdom

WP-21 **Enrichment of electrochemically cleaved peptides for middle-down proteomics applications**
H. Permentier, T. Zhang, X. Tian, R. Bischoff
University of Groningen, Analytical Biochemistry, Groningen, Netherlands

WP-22 **Heterogeneous protein complexes in synaptic vesicles mediate signal transduction in neurons**
S. Wittig, C. Haupt, M. Ganzella, S. Kostmann, R. Jahn, C. Schmidt
HALOmem, Charles Tanford Protein Center, Institute for Biochemistry and Biotechnology, Martin Luther University, Halle, Germany

WP-23 **Hydroxyl radical footprinting study for structural characterization of aluminum hydroxide-adsorbed calmodulin by mass spectrometry**
A. Vadi
GSK Vaccines S.r.l., Analytical Research and Development, Siena, Italy

WP-24 **Rapid characterization of overproduced proteins using native mass spectrometry**
S. Vimer, G. Ben-Nissan, H. Cohen-Dvashi, E. Morag, Y. Peleg, T. Unger, M. Yona, R. Diskin, M. Sharon
Weizmann Institute of Science, Department of Biomolecular Sciences, Rehovot, Israel

WP-25 **Integrative structural proteomics analysis of the 20s proteasome complex**
R. Viner, D. M. Horn, E. Damoc, A. Konijnenberg
Thermo Fisher Scientific, San Jose, USA

WP-26 **Assembly studies of Acetobacterium woodii F1FO-ATP synthase and analyzing conformational changes of TmrABby nESI**
K. Vu Huu, S. Brüchert, R. Tampé, V. Müller, N. Morgner
Goethe-University, Institute of Physical and Theoretical Chemistry, Frankfurt am Main, Germany

WP-27 **Gas-phase electrophoresis (nES GEMMA) of virus-like particles: relating particle surface-dry size and molecular weight**
V. U. Weiss, R. Pogan, S. Zoratto, C. Uetrecht, G. Allmaier
TU Wien, Inst. Chem. Technologies and Analytics, Vienna, Austria

WP-28 **Native mass spectrometry to identify stoichiometries and stability of CRISPR-cascade complexes**
S. Wittig, M. Rutkauskas, R. Seidel, C. Schmidt
HALOmem, Charles Tanford Protein Center, Institute for Biochemistry and Biotechnology, Martin Luther University, Halle, Germany

WP-29 **Characterization of deuterated alpha-crystalline using bench-top MALDI-ToFMS**
Y. Yamazaki, K. Morishima, N. Sato, R. Inoue, M. Sugiyama
Shimadzu Corp., Global application development center, Kyoto, Japan

WP-30 **Development of a cryo-stage for LESA mass spectrometry-towards truly native surface sampling of proteins**
B. Yan, A. Taylor, J. Bunch
National Physical Laboratory, National Centre of Excellence in Mass Spectrometry Imaging, Teddington, United Kingdom

WP-31 **Native mass spectrometry analysis of norovirus glycan interaction**
H. Yan, J. Lockhauserbäumer, K. Bücher, R. Creutznacher, A. Mallagaray, T. Peters, L. Hartmann, C. Uetrecht
Leibniz Institute for Experimental Virology, Heinrich-Pette-Institut, Hamburg, Germany

WP-32 **Top-down and middle down sequencing of immunoglobulin using electron capture dissociation – Time of Flight mass spectrometer combined with online disulfide bond reduction**
T. Baba, L. C. Y. Leblanc, P. Ryumin, B. Loyd
Sciex, Research, Concord, Canada

WP-33 **Cation exchange chromatography in displacement mode for online analysis of intact proteins by mass spectrometry**
S. N. Hidayah, D. Kroesser, B. Dreyer, H. Schluter
University Medical Center Hamburg Eppendorf, Institute for Clinical Chemistry and Laboratory Medicine, Mass Spectrometric Proteomics, Hamburg, Germany

WP-34 **High affinity epitopes of aptamer complexes of the multi-domain protein C-Met revealed by proteolytic affinity mass spectrometry**
L. Lupu, F. Rinaldi, Y. Baschung, M. V. Berezovski, M. Przybylski
Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, University of Rostock,Proteome Center, Rüsselsheim, Germany

WPS-S02 - Reaction Mechanisms and Elusive Intermediates

WP-35 **Analysis for reforming processes for gasoline surrogate fuel-air pre-mixtures by non-thermal plasmas using ion attachment mass spectrometry**
D. Asakawa, E. Takahashi, N. Saito
AIST, Research Institute for Measurement and Analytical Instrumentation, Tsukuba, Japan

WP-36 **Elusive monofunctional adducts of cisplatin with natural aminoacids revealed by IRMPD spectroscopy and photofragmentation kinetics**
D. Corinti, R. Paciotti, C. Coletti, N. Re, S. Piccirillo, P. Maitre, B. Bellina, P. Barran, B. Chiavarino, M. Elisa Crestoni, S. Fornarini
Sapienza, University of Rome, Dipartimento di Chimica e Tecnologie del Farmaco, Roma, Italy

WP-37 **Characterization of a nitrogen-operated dielectric barrier discharge ionization source**
L. Gyr, F. David Klute, J. Franzke, R. Zenobi
ETH Zurich, Zurich, Switzerland

WP-38 **A targeted metabolomics approach for diagnosis of Inborn Errors of Metabolism**
M. Jacob, A. Malkawi, N. Albast, S. Al Bougha, A. Lopata, M. Dasouki, A. Abdelrahman
King Faisal Hospital and Research Center, Genetics, Riyadh, Saudi Arabia

WP-39 **Steroid bisconjugates: unearthing hidden treasures of steroid metabolism**
M. Mcleod, C. Fitzgerald
Research School of Chemistry, Australian National University, Canberra, Australia

WP-40 **Investigating the reaction mechanism of the oxidation of heptafulvenes into tropones by a microreactor coupled online to mass spectrometry and density functional theory calculations**
S. M. E. Nilsson, H. Henschel, G. Scotti, M. Haapala, A. Kiriazis, G. Boije af Gennäs, T. Kotiaho, J. Yli-Kauhaluoma
University of Helsinki, Drug Research Program, Division of Pharmaceutical Chemistry and Technology, Helsinki, Finland

WP-41 **How to modify the acidity of charged droplets?**
M. Ojakivi, J. Liigand, A. Kruve
The University of Tartu, Institute of Chemistry, Tartu, Estonia

WP-42 **Studies of a L-proline catalyzed inverse electron demand Diels-Alder reaction by ESI-MS**
A. Schnell, J. A. Willms, M. Engeser
University of Bonn, Research group Engeser, Bonn, Germany

WP-43 **Fragmentation of arsenic-containing chemical warfare agents in GC–EI/MS and LC–ESI/MS**
M. Söderström, P. Vanninen
VERIFIN, University of Helsinki, Helsinki, Finland

WP-44 **Identification and interconversion of isomeric 4,5-functionalized 1,2,3-thiadiazoles and 1,2,3-triazoles in conditions of electrospray ionization**
M. Zimens, D. Mazur, V. Bakulev, A. Lebedev
Lomonosov Moscow State University, Organic Chemistry Department, Moscow, Russian Federation

WPS-S03 - Pharmaceuticals

WP-45 **Ultrasound assisted extraction parameters optimization by experimental design for steroidal saponins from plant material and cell cultures of Dioscorea deltoidea**
B. Sarvin, T. Baygildiev, D. Kochkin, A. Stavrianidi, I. Rodin
Lomonosov Moscow State University, Department of Chemistry, Moscow, Russian Federation

WP-46 **Analysis of pesticide residues in cannabis regulated by California and Oregon state using LC/MS/MS with Dual Electrospray and APCI source**
T. Becker, A. Dalmia, E. Cudjoe, T. Ruthenberg, J. Ye, M. Murphy, F. Qin, D. Welkie
PerkinElmer (LAS) Germany GmbH, BLL/FAS-Group, Rodgau-Jügesheim, Germany

WP-47 **Identification of a novel metabolite originating from JWH-015 using LCMS-IT-ToF**
O. D. Can, U. D. Ozkay, S. Levent, Y. N. Turan, T. F. Alyu, Y. Ozturk
Anadolu University, Faculty of Pharmacy, Department of Pharmacology, Eskisehir, Turkey

WP-48 **Synthesis and antifungal activity evaluation of new benzimidazole-triazole derivatives as potential ergesterol biosynthesis inhibitors using LC-MS/MS**
N. Oncu Can, C. Ulviye Acar, B. Nurpelin Saglik, S. Levent, Y. Ozkay, Z. A. Kaplancikli
Anadolu University, Faculty of Pharmacy, Department of Analytical Chemistry, Eskisehir, Turkey

WP-49 **Optimized MS^n workflow for improved structure elucidation of pharmaceutically relevant extractables and leachables**
S. Sharma, K. Comstock, D. E Kiehl, G. Mcalister, R. Komatsuzaki, C. Ding, R. Tautenhahm, D. J Bailey, L. Lin, T. Stratton, S. Eliuk, I. Mohtashemi, H. Cardasis, J. J. Josephs, V. Zabrouskov
Thermo Fisher Scientific, San Jose, USA

WP-50 **Comprehensive metabolite identification of DM4, a maytansinoid anti-tumor agent, in S100 fractions of Human Liver microsomes, by UPLC-QTof Mass Spectrometry**
E. Ciuti, F. Tavani, V. Chirulli, C. Carboni, A. Triolo
Menarini Ricerche SpA, Laboratory of Analytical Chemistry for Development, Firenze, Italy

WP-51 **Investigation of monoamine oxidase inhibitory activities of new chalcone derivatives: Comparison of LC-MS/MS and fluorometric methods**
Ü. Özkay, N. Öncü Can, S. Levent, Y. Özkay, Ö. D. Can
Anadolu University, Faculty of Pharmacy, Department of Pharmacology, Eskisehir, Turkey

WP-52 **Long term stability of Candesartan cilexetil after micronization**
A. M. A. P. Fernandes, M. Menezes, P. H. Amaral, M. N Eberlin, N. F. Höehr
State University of Campinas, Institute of Chemistry, Labmass Laboratory, Campinas, Brazil

WP-53 **Mass spectrometric characterization of a polymeric degradation product formed from the antibiotic Ceftazidime**
A. M. A. P. Fernandes, N. S. Camilo, E. P. Tessaro, M. N. Eberlin
State University of Campinas, Institute of Chemistry, Labmass Laboratory, Campinas, Brazil

WP-54 **Full validation of Metformin in human bloods using volumetric absorptive microsampling**
N. Ha, K. Jang, S. Han, S. Eui Lee, M. Kim
Center for Clinical Pharmacology and Biomedical Research Institute, Chonbuk National University Hospital, Jeonju, Republic of Korea

WP-55 **Determination of an isonicotinohydrazide derivative, a novel positive inotropic compound, in mouse plasma by LC-MS/MS and its application to a pharmacokinetics study**
R. Hui, J. Liu, B. Feng
Jiangnan University, School of Pharmaceutical Science, Wuxi, China

WP-56 **LC–MS/MS chiral method for simultaneous determination of R,S-ketamine and its metabolites in rat plasma and brain samples from pharmacokinetic studies**
M. Janicka, M. Matłoka, M. Mach, R. Moszczyński-Pętkowski, E. Tratkiewicz, J. Pieczykolan, M. Wieczorek
Celon Pharma S.A., R&D, Łomianki, Poland

WP-57 **Characterization of a novel Zetamicin impurity by LC-MS and NMR: an orthogonal techniques approach for the structural elucidation of low-level byproducts**
E. Libralesso, E. Ciuti, A. Triolo, F. Lamonaca, M. Gentili
Menarini Ricerche spa, Preclinical Development, Firenze, Italy

WP-58 **Prediction of ionisation efficiencies in complicated biological matrices**
P. Liigand, J. Liigand, F. Cuyckens, R. J. Vreeken, A. Kruve
University of Tartu, Institute of Chemistry, Tartu, Estonia

WP-59 **A Novel GC-MS Method for Simultaneous Determination of Seven Paraben Derivatives in Pharmaceutical and Cosmetic Products Consumed in Turkey**
S. Ozcan, S. Levent, A. Geven, N. O. Can
Anadolu University, Faculty of Pharmacy, Department of Analytical Chemistry, Doping and Narcotic Compounds Analysis Laboratory, Eskisehir, Turkey

WP-60 **Anticancer activity evaluation of new Phortress analogues and identification of bioactive metabolism products using LCMS-IT-ToF**
Y. Özkay, D. Osmaniye, B. N. Saglik, S. Levent, S. Ilgin, Z. A. Kaplancikli
Anadolu University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Eskisehir, Turkey

WP-61 **Investigation of isomeric metabolite structures using a combination of IMS, MS/MS and chemometrics: application to biotransformation**
C. Palaric, S. Rigaud, D. Mathiron, R. Molinié, J. Beaumal, T. Renaud, S. Pilard
University of Picardie Jules Verne (UPJV), Analytical Platform (PFA), Amiens, France

WP-62 **Complex approach for isolation and HPLC-MS determination of steroidal glycosides from plant material and suspension cell culture**
I. Rodin, B. Sarvin, A. Stavrianidi, T. Baygildiev
Lomonosov Moscow State University, Department of Chemistry, Moscow, Russian Federation

WP-63 **Use of high resolution mass spectrometry for tropane alkaloids determination and untargeted analysis in drugs and homeopathic products from Atropa Belladonna seed extracts**
R. Romero González, J. Marín Sáez, A. Garrido Frenich
University of Almería, Dept. Chemistry and Physics, Almería, Spain

WP-64 **All-in-one method for profiling and quantification of Polysorbate, by combined Data-Independent and Data-Dependent tandem MS**
S. Staccioli, A. Triolo, E. Ciuti
Menarini Ricerche, Laboratory of Analytical Chemistry for Development, Firenze, Italy

WP-65 **Rapid HPLC-MS/MS evaluation of the batch-to-batch consistency of the payloads substitution of a lysine antibody-drug-conjugates (ADCs)**
F. Tavani, A. Triolo
Menarini Ricerche SpA, Analytical Chemistry for the Development, Florence, Italy

WP-66 **MALDI ToF mass spectrometry for the characterization of antitumour ruthenium(ii) polypyridyl complexes**
R. Masnikosa, F. Veljkovic, B. Rajcic, A. Rilak, S. Velickovic
University of Belgrade, Vinča Institute of Nuclear Sciences, Belgrade, Serbia

WP-67 **Energy resolved tandem mass spectrometry experiments for resolution of isobaric compounds: a case of cis/trans isomerism**
L. Braconi, M. Menicatti, S. Dei, E. Teodori, G. Bartolucci
University of Florence, NEUROFARBA Dept., Sesto Fiorentino, Italy

WP-68 **Stability study in plasma of novel ester-linked NSAID - carbonic anhydrase inhibitor hybrids**
S. Bua, M. Menicatti, P. Gratteri, A. Nocentini, C.T. Supuran, G. Bartolucci
University of Florence, NEUROFARBA Dept., Pharmaceutical and Nutraceutical section, Sesto Fiorentino, Italy

WP-69 **Identification of dipropylaminopretadalafil using high resolution mass spectrometry under multi-stage fragmentation pathways**
A. Chin, C. L. Kee
Health Sciences Authority, Pharmaceutical Laboratory, Singapore, Singapore

WP-70 **Evaluation of small molecule drugs retention in fluorinated silica nanoparticle stabilized pickering emulsion using ESI_Mine(TM) platform**
X. Li, J. Francis, C. Pilkington, A. Clay, C. Smith
Sphere Fluidics Limited, R&D, Cambridge, United Kingdom

WP-71 **Generic method for parallel artificial liquid membrane extraction of nonpolar basic drugs from human plasma**
M. Lid, A. Gjelstad, S. Pedersen-Bjergaard
University of Oslo, Pharmaceutical Institute, Oslo, Norway

WP-72 **Application of linear equations deconvolution analysis (LEDA) algorithm in ion trap mass spectrometry: resolution of isomeric pairs of carbonic anhydrase and cyclooxygenase hybrids inhibitors**
D. Squillaci, M. Menicatti, S. Bua, C. Supuran, G. Bartolucci
University of Florence, NEUROFARBA Dept., Sezione di Scienze Farmaceutiche, Sesto Fiorentino, Italy

WPS-S04 - Food integrity, Authenticity & Traceability

WP-73 **Pigment profiling in olive oils by ultra–high performance liquid chromatography – atmospheric pressure chemical ionization–high resolution mass spectrometry**
A.Arrizabalaga-Larrañaga, P. Rodriguez, M. Medina, F. J. Santos, E. Moyano
University of Barcelona, Chemical Engineering and Analytical Chemistry, Barcelona, Spain

WP-74 **Isotopic mapping of milk and groundwater in the production area of Parmigiano Reggiano for food traceability**
M. Boito, P. Iacumin, N. Ogrinc
Università degli Studi di Parma, Dipartimento di Scienze Chimiche, della Vita e della Sostenibilità Ambientale, Parma, Italy

WP-75 **Wine traceability: "Vigneto Italia" project**
C. Brilli, B. Bronzi
Ruffino srl, Laboratory, Pontassieve, Italy

WP-76 **UHPLC-ESI-MS/MS for the determination of polyphenols in Spanish paprika (Capsicum annuum L.). Application to protected designation of origin (PDO) classification by chemometrics.**
G. Campmajó, S. Barbosa, O. Núñez, J. Saurina, L. Puignou
University of Barcelona, Department of Chemical Engineering and Analytical Chemistry, Barcelona, Spain

WP-77 **A novel multi-platform high resolution mass spectrometry non-targeted approach facing extra virgin olive oil adulteration**
D. Cavanna, K. Hurkova, Z. Dzuman, A. Serani, C. Dall'asta, J. Hajslova, M. Suman
Barilla G. & R. Fratelli S.p.A., University of Parma - Department of Food and Drug, Parma, Italy

WP-78 **Shrimp fraud: evaluating characteristic metabolomic features for authentication by high and unit mass resolution spectrometry**
O. Chevallier, N. Chatterjee, E. Wielogorska, C. Black, C. Elliott
Queens University Belfast, Mass Spectrometry Core Unit, Belfast, United Kingdom

WP-79 **Optimization, validation and application of GC-FID and GC-IRMS methods for the determination of fatty acids without derivatisation**
A. Ciric, J. Masten, L. Strojnik, N. Ogrinc
Jozef Stefan Institute, Department of Environmental Science, Ljubljana, Slovenia

WP-80 **Multi-class LC-MS and GC-MS methodologies to discriminate extra virgin olive oils from different Protected Designations of Origin**
L. Olmo-García, K. Wendt, A. Bajoub, C. M. Sánchez-Arévalo, A. Muñoz de la Peña, C. Baessmann, A. Carrasco-Pancorbo, A. Fernández-Gutiérrez
University of Granada, Department of Analytical Chemistry, Granada, Spain

WP-81 **Determination of melatonin and related compounds in beverages using liquid chromatography coupled to low and high resolution mass spectrometry**
M. L. Jiménez Medina, L. Manzano Sánchez, J. Marín Sáez, R. Romero González, A. Garrido Frenich
University of Almería, Dept. Chemistry and Physics, Almería, Spain

WP-82 **UHPLC-ESI-HRMS characterization of turmeric and curry samples based on profiling and fingerprinting approaches**
N. Núñez, O. Núñez, S. Sentellas, J. Saurina
University of Barcelona, Department of Chemical Engineering and Analytical Chemistry, Barcelona, Spain

WP-83 **Monoterpenes characterization in grape spirits using fast gas chromatography tandem mass spectrometry**
M. Paolini, S. Poli, L. Tonidandel, S. Moser, R. Larcher
Fondazione Edmund Mach, Technology Transfer Centre, San Michele all'Adige, Italy

WP-84 **Elucidation of oligosaccharides in milk reference materials by HILIC-MS/MS and the NIST tandem MS libraries**
C. Remoroza, S. Stein
National Institute of Standards and Technology, Mass Spectrometry Data Center, Gaithersburg, USA

WP-85 **Iknife, a novel ambient mass spectrometry approach for the real-time identification of food samples**
F. Rigano, D. Mangraviti, L. Mondello
Chromaleont Srl, c/o Dipartimento ChiBioFarAm, University of Messina, Messina, Italy

WP-86 **Determination of crocin isomers and isoforms by means UHPLC-MS/MS as quality marker for saffron**
R. Rocchi, M. Mascini, M. Sergi, D. Compagnone, P. Pittia
University of Teramo, Faculty of Bioscience and Technology for Food, Agriculture and Environment, Teramo, Italy

WP-87 **Real-time authentication of food and beverages Using DART-QDa LiveID analysis**
S. Stead, J. Kirk, K. Organtini
Waters Corporation, Scientific Operations, Manchester, United Kingdom

WP-88 **Evaluation of solid-phase microextraction for the isotopic analysis of volatile compounds in apple**
L. Strojnik, F. Camin, L. Ziller, N. Ogrinc
Jožef Stefan Institute, Department of Environmental Sciences, Ljubljana, Slovenia

WP-89 **Aromatic compounds profile of DOC Piedmontese wines by GC-MS with HS-SPME**
E. Bonometti, R. Rabezzana, G. Cerrato, L. Operti, E. Diana, F. Turco, E. Priola, A. Giordana
University of Turin, Department of Chemistry-CrisDi Interdepartmental Centre for Crystallography, Turin, Italy

WP-90 **Proteomics approach for the differentiation of Tuna species**
I. Brümmer, J. Brockmeyer
University of Stuttgart, Food Chemistry, Stuttgart, Germany

WP-91 **Identification and quantification of polyphenol in cocoa extract, study of the effets of fermentation**
G. Cazals, F. Guéhi Gbogbri, S. Munier, R. Boulanger, A. Michel, C. Enjalbal, P. Poucheret
LMP, Universite de Montpellier, Montpellier, France

WP-92 **Investigation into the *cis* isomers of dichlorogenic acids in coffee**
S. Colomban, E. Guercia, E. De Angelis, L. Navarini
illycaffè spa, Aromalab, Trieste, Italy

WP-93 **Comparative proteomic analysis of the metabolic fractions composition in modern and old wheat genotypes**
A. Di Francesco, R. Saletti, V. Cunsolo, V. Muccilli, P. De Vita, S. Foti
University of Catania, Department of Chemical Sciences, Catania, Italy

WP-94 **Proteomics going nuts? Proteome profiling of walnut kernels**
B. Dreyer, D. Kroesser, H. Schlueter
University Medical Center Hamburg-Eppendorf, Mass spectrometric proteomics, Hamburg, Germany

WP-95 **Untargeted high resolution mass spectrometry methods to assess salmon authenticity**
G. Maria Fiorino, M. Fresch, I. Brümmer, J. Brockmeyer, I. Losito, L. Monaci
National Research Council of Italy (CNR), Institute of Sciences of Food Production (ISPA), Bari, Italy

WP-96 **Characterization and quantitation of water-soluble vitamins in wine by liquid chromatography-high resolution and tandem mass spectrometry**
G. Inzalaco, F. Borghini, A. Cavaglioni, G. Giorgi
Università degli Studi di Siena, Dipartimento Biotecnologie, Chimica e Farmacia, Siena, Italy

WP-97 **Sample Profiler – A cloud-based application for confirming food authenticity**
S. Kailasam, R. Tautenhahn, T. Stratton
Thermofisher Scientific, LSMS, Bangalore, India

WP-98 **Rapid and direct analysis of coffee beans (green and roasted) and online monitoring of coffee roasting by SIFT-MS: focus on volatile aldehydes**
I. Khomenko, A. Caretta, V. Lonzarich, F. Biasioli, L. Navarini
Edmund Mach Foundation, Food quality and nutrition, San Michele all'Adige, Italy

WP-99 **Differential proteomic profiling of truffles**
D. Kroesser, B. Dreyer, H. Schlueter
University Medical Center Hamburg-Eppendorf, Mass Spectrometric Proteomics, Hamburg, Germany

WP-100 **A novel robust probe for the rapid, on-line characterisation of food samples using rapid evaporative ionisation mass spectrometry**
A. Marton, J. Balog, R. Schäffer, S. Pringle, Z. Takáts
Waters Research Center, R&D, Budapest, Hungary

WP-101 **Correlating consumer sensory experience of apple aroma with VOC profiles acquired by automated TD–GC–MS**
G. Roberts, D. Barden, N. Bukowski, L. Mcgregor, M. Santoro, N. D. Spadafora
SepSolve Analytical, SepSolve Analytical, Peterborough, United Kingdom

WP-102 **Food proteomics: a novel approach to food authentication using global protein signatures and species specific marker peptides**
L. Viet, P. Krimm, J. Brockmeyer
University of Stuttgart, Food Chemistry, Stuttgart, Germany

WPS-S05 - MS Tools in Doping & Toxicology

WP-103 **Development and validation of multi-target analytical procedures for the identification of potential doping agents in 'over the counter' products**
F. Comunità, F. Botrè, M. Capozzi, X. De La Torre, M. Mazzarino
Laboratorio Antidoping Federazione Medico Sportiva Italiana, Rome, Italy

WP-104 **Large volume injection: improving the detectioncapacity of endogenousanabolicsteroids by GC-C-IRMS**
L. Iannella, C. Colamonici, D. Curcio, F. Botrè, X. De La Torre
Laboratorio Antidoping Federazione Medico Sportiva Italiana, Rome, Italy

WP-105 **Is GC-MS analysis sufficient for identification of illicit drugs from festive gatherings?**
S. Magréault, C. Grondin, C. Lamoureux, E. Bourgogne
AP-HP-hopital Lariboisière/Université ParisDescartes, Laboratoire de toxicologie, Paris, France

WP-106 **Evaluation of the metabolic profile of 2-methiopropamine by LC-MS/MS in mice and in human liver microsomes**
C. Camuto, S. Pellegrini, M. Mazzarino, X. De La Torre, F. Botrè, M. Marti, F. De Giorgio
FMSI Antidoping, University La Sapienza-Department of Chemistry, Rome, Italy

WP-107 **Quantitation of five barbiturates in human urine by liquid chromatography-tandem mass-spectrometry**
A. Chulovskaya, D. Rakov, E. Mochalova
National Anti-Doping Laboratory (MSU, Moscow), Moscow, Russian Federation

WP-108 **A systems biology approach for discovering biomarkers indicative of exposure to Carfentanil**
E. Dhummakupt, B. Tran, D. Carmany, G. Boyd, P. Mach, M. Feasel, J. Sekowski, T. Glaros
Edgewood Chemical Biological Center, Research & Technology Directorate, Aberdeen Proving Grounds, USA

WP-109 **Co-exposure to silver nanoparticles and cadmium ions induces metabolic adaptation in HepG2 cells**
R. Miranda, V. Gorshkov, B. Korzeniowska, S. Kempf, F. Neto, F. Kjeldsen
University of Southern Denmark, Dept. of Biochemistry and Molecular Biology, Odense, Denmark

WP-110 **Application of dispersive liquid-liquid microextraction (DLLME) for identification of synthetic cannabinoids in plasma by LC-MS/MS**
T. Lino, I. L. Barbosa, D. O. K. Diniz, M. N. Eberlin, J. L. Costa
UNICAMP, School of Medical Sciences, Campinas, Brazil

WP-111 **Development and validation of an LC-MS/MS method for the determination of maternal and fetal tissue distribution of permethrin and its metabolites in pregnant rats**
S. Personne, A. Corona, C. Brochot, K. Chardon, S. Baltora, S. Pilard, V. Bach, F. Zeman, P. Marcelo
Universite de Picardie Jules Verne, Plateforme ICAP, Amiens, France

WP-112 **Proton transfer reaction – mass spectrometry and its applications to homeland security: detection of illicit drugs**
D. Olivenza-León, P. Watts, F. Reich, C. Mayhew
University of Birmingham, School of Physics and Astronomy, Birmingham, United Kingdom

WP-113 **Assessment of chemical trace elements in cosmetics' eyeshadows**
A. Pawlaczyk, M. Balcerek, M. I. Szynkowska
Lodz University of Technology, Faculty of Chemistry, Institute of General and Ecological Chemistry, Lodz, Poland

WP-114 **Generic extraction method for screening of 8 narcotic drugs in saliva with a quick turnaround analysis by LDTD-MS/MS**
P. Picartd, J. Lacoursiere, S. Auger
Phytronix Technologies Inc, Quebec City, Canada

WP-115 **Improvement of the Athlete Biological Passport by blood steroid profiling: challenges of a steroidomic approach**
F. Ponzetto, J. Boccard, R. Nicoli, T. Kuuranne, S. Rudaz, M. Saugy
Swiss Laboratory for Doping Analysis, CHUV - University of Lausanne, Lausanne, Switzerland

WP-116 **Analysis of removal of pesticides and drugs in waste water by plants using Flow Injection Analysis (FIA) Magnetic Resonance Mass Spectrometry (MRMS)**
M. Witt, A. Barsch, C. Villette, D. Heintz
IBMP-CNRS, University of Strasbourg, Strasbourg, France

WP-117 **Improvement for high sensitivity of the drug screening by thermal desorption and pyrolysis combined with DART-MS (TDP/DART-MS)**
H. Abe, C. Takei, K. Yoshizawa, M. Sakakura, T. Shiota, D. Yajima, H. Iwase
BioChromato, Inc., Application support, Fujisawa, Japan

WP-118 **Detection of IGF-1 in serum as a biomarker of growth hormone abuse by athletes**
M. Yunin, I. Zvereva, D. Rakov, E. Mochalova
National Anti-Doping Laboratory (MSU, Moscow)

WP-119 **Development of a LC-HRMS based strategy for the screening of conjugated steroids in equine urine**
X. Zuo, Z. Kaabia, F. Bagilet, B. Georges, M. Collard, Y. Moulard, P. Garcia, M. Popot, L. Bailly-Chouriberry
Laboratoire des Courses Hippiques (LCH), Anabolic agents anti-doping department, Paris, France

WP-120 **Fast GC-MS/MS for high throughput androgenic anabolic streoids analysis in equine urine**
K. Histel, M. Collard, B. Georges, F. Bagilet, M. Popot, Z. Kaabia, L. Bailly-Chouriberry
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WP-121 **In-vitro/vivo study of Andarine metabolism, a selective androgen receptor modulator (SARM), in the context of horse doping control**
S. Trevisiol, Y. Moulard, S. Boyer, M. Jaubert, B. Loup, P. Garcia, M. Popot, L. Bailly-Chouriberry
Laboratoire des courses hippiques, LCH, Verrière-le-Buisson, France

WPS-S06 - MS Imaging: Applications

WP-122 **Microbial MALDI-(2)-MS imaging of steam-inactivated co-cultured bacterial colonies at high mass resolution**
E. U. Brockmann, D. Steil, J. Soltwisch, K. Dreisewerd
University of Muenster, Institute for Hygiene; Interdisciplinary Center for Clinical Research (IZKF), Münster, Germany

WP-123 **Bioimaging of rat kidneys after single administration of iodinated contrast agents (ICAs)**
C. Brungs, M. Viehoff, R. Schmid, M. Sperling, U. Karst
University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany

WP-124 **Reversing the polarity – Targeted mass-spectrometry imaging analysis of fatty acids in positive detection mode**
A. Dannhorn, E. Kazanc, P. Inglese, J. Mckenzie, N. Strittmatter, R. J. A. Goodwin, Z. Takats
Imperial College London, Department of Surgery and Cancer, London, United Kingdom

WP-125 **Mass spectrometry imaging breaks the silence**
Y. Dong, P. Sonawane, G. Polturak, L. Feldberg, I. Rogachev, A. Aharoni
Weizmann Institute of Science, Rehovot, Israel

WP-126 **Mass spectrometry imaging in skin with AP-MALDI and ToF-SIMS**
D. El Assad, G. Frache
Luxembourg Institute of Science and Technology, Materials research and technology, Belvaux, Luxembourg

WP-127 **Elucidation of natural product biosynthesis in Amazon wood Sextonia rubra by in situ tandem MS identification with 100 nm-scale imaging**
G. L Fisher, T. Fu, D. Touboul, S. Della-Negra, E. Houel, N. Amusant, C. Duplais, A. Brunelle
Physical Electronics, Marketing & Applications, Chanhassen, USA

WP-128 **DESI mass spectrometry imaging of the distribution of a fluorescence marker in malignant glioblastoma brain tumours**
M. Gentry, E. Jones, D. Coope, A. Mcmahon
University of Manchester, Division of Informatics, Imaging and Data Sciences, Manchester, United Kingdom

WP-129 **Maleic anhydride proton sponge and its derivatives toward MALDI-MSI based brain tumor diagnosis**
M. Giampà, A. Zurowietz, T. Lammert, J. Fuchser, V. H. Hans, O. Gembruch, U. Kellner, T. W. Nattkemper, H. Bednarz, K. Niehaus
Bielefeld University/Proteome and metabolome research, Bielefeld, Germany

WP-130 **The effect of protein binding of drug substances in Desorption Electrospray Ionization Mass Spectrometry Imaging**
A. Handler, K. Troensegaard Nielsen, C. Janfelt
University of Copenhagen, LEO Pharma A/S, Copenhagen, Denmark

WP-131 **MS for MS; a mass spectrometry-based study into multiple sclerosis**
B. Heijs, F. De Graaff, E. Steenvoorden, M. Giera, G. Kooij
Leiden University Medical Center, Center for Proteomics & Metabolomics, Leiden, Netherlands

WP-132 **Gold-coated Black Silicon: An Efficient Substrate for Laser Desorption Ionization Mass Spectrometry**
S. A. Iakab, P. Rafols, O. Yanes, X. Correig
Universitat Rovira i Virgili, Department of Electrical Electronic Engineering and Automation, Tarragona, Spain

WP-133 **Application of isotope-labeling in whole-body DESI-MSI studies for intra-animal comparison of drug administration routes**
L. Morineau, S. C. Jacobsen, K. Kleberg, H. S. Hansen, C. Janfelt
University of Copenhagen, Department of Pharmacy, Copenhagen, Denmark

WP-134 **Single cell LiveScan mass spectrometry profiling and imaging**
F. Kaftan, M. Vallet, T. Baumeister, G. Pohnert, A. Svatoš
Max Planck Institute for Chemical Ecology, Research Group Mass Spectrometry/Proteomics, Jena, Germany

WP-135 **Evaluation of embedding strategies for fragile and small specimen in MSI analysis**
E. Kazanc, A. Danhorn, P. Inglese, J. Mckenzie, Z. Takats
Imperial College of London, Surgery and Cancer, London, United Kingdom

WP-136 **Visualizing molecular distributions across/under the human skin by 2D-DESI MS imaging of tape-stripped stratum corneum**
K. Kihara, A. Motoyama
Shiseido, Global Innovation Center, Yokohama, Japan

WP-137 **Distribution of lipids and anti-TB drugs in mouse lung tissue**
J. Kokesch-Himmelreich, A. Treu, K. Walter, C. Hölscher, A. Römpp
University of Bayreuth, Bioanalytical Sciences and Food Analysis, Bayreuth, Germany

WP-138 **Calcium and lipid imaging of regenerated bony rays of Zebrafish caudal fin using Time-of-Flight Secondary Ion Mass Spectrometry**
S. Y. Lee, J. Y. Kim, D. W. Moon
Daegu Gyeongbuk Institute of Science and Technology (DGIST), Department of New Biology, Daegu, Republic of Korea

WP-139 **ToF-SIMS imaging of rat and Drosophila brain tissue sections prepared by using the new sampling method**
T. G. Lee, H. K. Shon, U. T. Le Minh, J. G. Son, S. Yoon, J. H. Moon, C. Y. Shin, S. B. Lee
KRISS, Center for Nano-Bio Measurement, Daejeon, Republic of Korea

WP-140 **MALDI MSI and immunohistochemistry analysis of colorectal carcinoma spheroids**
M. Machálková, J. Navrátilová, B. Pavlatovská, K. A. Radaszkiewicz, A. Pruška, J. Preisler
Masaryk University, Department of Chemistry, Brno, Czech Republic

WP-141 **Multimodal imaging of undecalcified tissue sections by MALDI MS and µXRF**
A. Svirkova, A. Turyanskaya, C. Streli, M. Marchetti-Deschmann
TU Wien, Institute of Chemical Technologies and Analytics, Wien, Austria

WP-142 **Mass spectrometry imaging in liver cancer: LA-ICP and DESI analysis of cirrhosis and hepatocellular carcinoma**
P. H Vendramini, G. S Pessoa, R. M Oliveira, A. L Rennó, J. H P Garcia, M. A Arruda, M. N Eberlin, A. Sussulini, A. M A Martins
UnB / UniCeub, Medicine / Surgery, Brasilia, Brazil

WP-143 **Complementary bioimaging to determine nanoparticle and phospholipid distribution in lung tissue**
A. Niehoff, D. Dietrich, M. Sperling, U. Karst
Shimadzu Europa GmbH, Innovation Center, Duisburg, Germany

WP-144 **Distinguishing the core and penumbra by lipid profiles using Mass Spectrometry imaging in mice after experimental infarct induction**
N. Ogrinc Potocnik, I. Mulder, L. Broos, A. Prop, A. Maagdenberg, R. Heeren
Maastricht University, Maastricht MultiModal Molecular Imaging Institute (M4I), Maastricht, Netherlands

WP-145 **The management of haemoglobin interference for the MALDI-MSI analysis of in-vivo thyroid biopsies**
I. Piga, G. Capitoli, V. Denti, S. Tettamanti, S. Galimberti, F. Magni, F. Pagni
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WP-146 **High spatial resolution imaging of aged human retina tissue**
K. Schey, D. Anderson, J. Messinger, N. Heath Patterson, C. Curcio
Vanderbilt University, Biochemistry, Nashville, USA

WP-147 **Ambient mass spectrometry imaging on whole body skin for biomolecules**
J. Shiea
National Sun Yat-Sen University, Department of Chemistry, Kaohsiung, Taiwan, Province of China

WP-148 **Aldosterone specific visualization in primary aldosteronism using imaging mass spectrometry**
S. Shimma, E. Takeo, K. Nishimoto, Y. Sugiura
Osaka Univesirity, Graduate School of Engineering, Osaka, Japan

WP-149 **MALDI-MS imaging in the search for proteomic indicators of response to therapy in membranous nephropathy**
A. Smith, V. L'imperio, M. Mazza, E. Ajello, F. Pagni, F. Magni
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WP-150 **Precision medicine for diabetic nephropathy and hypertensive nephrosclerosis: a MALDI-MSI pilot study**
A. Smith, V. Iablokov, M. Stella, M. Mazza, B. Heijs, P. Van Veelen, D. Muruve, F. Magni
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WP-151 **High-resolution AP-SMALDI MS imaging of parasites**
B. Spengler, P. Kadesch, T. Hollubarsch, A. Taubert, C. Hermosilla, C. Grevelding, T. Quack, S. Gerbig, K. Strupat, M. Kompauer, M. Müller, S. Heiles
Justus Liebig University, Institute of Inorganic and Analytical Chemistry, Giessen, Germany

WP-152 **A molecular snapshot of clear cell renal cell carcinoma: multimodal MALDI-MSI and nLC-MS/MS of N-glycans and proteins**
M. Stella, F. Boyaval, A. Smith, M. Grasso, G. Bovo, B. Heijs, F. Magni
Univeristy of Milano Bicocca, Department of Medicine and Surgery, Clinical Proteomics and Metabolomics Unit, Vedano al Lambro, Italy

WP-153 **Exploring metabolic deregulation in mouse models of breast cancer with multimodal mass spectrometry imaging**
A. Taylor, T. Fu, B. Yan, A. Dexter, T. Murta, S. Thomas, Y. Panina, A. Al-Afeef, E. Elia, C. Nikula, R. Philip, R. Steven, S. Barry, K. Brindle, I. Gilmore, R. Goodwin, J. Marshall, G. Poulogiannis, O. Sansom, Z. Takats, M. Yuneva, J. Bunch
National Physical Laboratory, National Centre of Excellence in Mass Spectrometry Imaging, Teddington, United Kingdom

WP-154 **New Frontiers of MALDI-IMS and Lipidomics: An Untargeted Approach to Skin Lipids Mapping**
S. Tortorella, F. Xie, P. Tiberi, G. Cruciani, S. Castellino
Molecular Horizon, R&D, Bettona, PG, Italy

WP-155 **MALDI-mass spectrometric imaging for the investigation of metabolites in Linum usitatissimum L. roots inoculated with Fusarium oxysporum**
G. Vladimirov, N. Melnikova, A. Dmitriev, N. Bolsheva, R. Novakovskiy, A. Zherebker, A. Yablokov, E. Nikolaev
Skolkovo Institute of Science and Technology, Skoltech Center for Translational Biomedicine, Moscow, Russian Federation

WP-156 **Identification of asbestos fibres in a malignant mesothelioma model**
O. Voloaca, L. Cole, M. Clench, A. Managh, C. Greenhalgh, S. Haywood-Small
Sheffield Hallam University, Biomolecular Science Research Centre, Sheffield, United Kingdom

WP-157 **Two dimensional metabolic profile of bile acids and lipids in fibrosis of NASH-model liver using MALDI Imaging at 20 µm spatial resolution**
Y. Yamazaki, S. Yamaguchi, T. Oshikawa, D. Miura, M. Yamazaki
Shimadzu Corp., Global application development center, Kyoto, Japan

WP-158 **Matrix-assisted laser desorption/ionization-mass spectrometry imaging for direct visualization of plant wound stress phytohormones in situ**
C. Zhang, K. Doležal, O. Novák
Palacký University Olomouc, Laboratory of Growth Regulators, Olomouc, Czech Republic

WP-159 **A ToF-SIMS study of lipid changes in E. coli mutants with impaired plasmid transfer capability**
K. Dimovska Nilsson, M. Palm, A. Farewell, J. S. Fletcher
University of Gothenburg, Department of Chemistry and Molecular Biology, Gothenburg, Sweden

WP-160 **Chemical imaging of aggressive basal cell carcinoma using time-of-flight secondary ion mass spectrometry**
K. Dimovska Nilsson, M. Munem, O. Zaar, N. Neittaanmäki, J. S. Fletcher, J. Paoli
University of Gothenburg, Department of Chemistry and Molecular Biology, Gothenburg, Sweden

WP-161 **An untargeted approach to elucidate the metabolism and tissue distribution of phosphorothioate linked oligonucleotides by high resolution mass spectrometry**
B. Steinhuber, C. Husser, A. Brink
F. Hoffmann-La Roche AG, PS, Basel, Switzerland

WP-162 **A case study for demonstrating the usefulness of imaging mass spectrometry in toxicity assessment using an amiodarone-induced phospholipidosis model**
K. Tanaka, A. Kashimura, H. Sato
Mitsubishi Tanabe Pharma Corporation, DMPK Research Laboratories, Toda, Japan

WPS-S07 - Gas Phase Ion Chemistry & Thermochemistry

WP-163 **A quantum chemical tool for the prediction of mass spectra and the identification of fragmentation pathways**
J. Cautereels, F. Blockhuys
University of Antwerp, Department of Chemistry, Antwerp, Belgium

WP-164 **Isomerization and dissociation of alpha-centered and pi-centered glycylglycyltryptophan radical cations: structural, energetic, mechanistic, and spectroscopic investigations**
A. C. K. Siu, J. Martens, A. Sze, J. Oomens, I. K. Chu
The University of Hong Kong, Department of Chemistry, Hong Kong, China

WP-165 **Nitrogen oxides binding to cobalamin: ion chemistry by FT-ICR mass spectrometry**
M. E. Crestoni, A. Maccelli, S. Fornarini
Sapienza Università di Roma, Dipartimento di Chimica e Tecnologie del Farmaco, Roma, Italy

WP-166 **Tandem mass spectrometry as a tool to evaluate ligand electronic effect on Au(I) complexes**
D. Gatineau, D. Lesage, H. Dossmann, H. Clavier, A. Milet, Y. Gimbert
DCM UMR 5250, CNRS-Université Grenoble Alpes, Grenoble, France

WP-167 **Energy-resolved collision-induced dissociation study of proton-bound heterodimers of guanine and cytosine**
S. Yun Han, J. Ju Park, C. Sik Lee
Gachon University, Department of Nanochemistry, Seongnam, Republic of Korea

WP-168 **Correlation between structure and stability of gas phase oligonucleotides probed by tuned collision- and VUV-MS/MS**
S. Ickert, J. Riedel, S. Beck, M. W. Linscheid
Humboldt Universität zu Berlin, Federal Institute for Materials Research and Testing, Berlin, Germany

WP-169 **Measurement of protonated water clusters using High Kinetic Energy Ion Mobility Spectrometry (HiKE-IMS)**
A. T. Kirk, M. Allers, S. Zimmermann
Leibniz Universität Hannover, Department of Sensors and Measurement Technology, Hannover, Germany

WP-170 **Challenges of soft chemical ionization mass spectrometry: ion chemistry of glyoxal**
M. Lacko, F. Piel, A. Mauracher, A. Knížek, P. Španel
J. Heyrovský Institute of Physical Chemistry of the CAS, Prague, Czech Republic

WP-171 **Walk-on-sphere rearrangement and retro-Bingel reaction of gas-phase fullerene malonate ions**
J. Oschwald, M. B. Minameyer, K. L. Maxouti, A. Hirsch, T. Drewello
Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Chemie und Pharmazie, Erlangen, Germany

WP-172 **Gas phase structures and thermochemical parameters of protonated 5-HMF isomers**
F. Pepi, S. Garzoli, P. Giacomello, G. De Petris, A. Troiani, R. Ragno, A. Patsilinakos, L. Antonini, A. Ricci, C. Salvitti
"Sapienza" University of Rome, Department of Chemistry and Drugs Technologies, Rome, Italy

WP-173 **Selective conversion of protonated D-fructose to 5-HMF and 2-FA: a nitrogen-base assisted dehydration process in the gas-phase**
A. Troiani, G. De Petris, F. Pepi, S. Garzoli, M. Rosi, A. Ricci, C. Salvitti
Università della Campania "L. Vanvitelli", Dip. di Matematica e Fisica, Caserta, Italy

WP-174 **Sulfur dioxide uptake by sodium carbonate cluster anions in the gas-phase**
C. Salvitti, A. Troiani, G. De Petris
"Sapienza" University of Rome, Department of Chemistry and Technology of Drugs, Rome, Italy

WP-175 **Development of tuner integrated microwave driven radical beam sources for radical induced dissociation molecular structural analysis**
Y. Shimabukuro, H. Takahashi, S. Iwamoto, K. Tanaka, M. Wada
Doshisha University, Plasma Physics Laboratory, Kyotanabe, Japan

WP-176 **Controlled reactions of methyl cation with oxygen compounds and hydrocarbons**
R. Thissen, C. Romanzin, C. Alcaraz
Université Paris Saclay, Laboratoire Chimie Physique, Orsay, France

WP-177 **Two molecules are better than one: cooperative effects of two sulfur dioxide and sulfur dioxide/water in bond forming and hydrolysis reactions of polyvanadate dianions in the gas phase**
A. Troiani, M. Rosi, S. Garzoli, C. Salvitti, G. De Petris
"Sapienza" University of Rome, Dipartimento di Chimica e Tecnologie del Farmaco, Rome, Italy

WP-178 **Gas-phase fragmentation mechanisms studies of doubly-protonated peptide ions containing basic amino acid residues by mass spectrometry**
T. Yalcin, A. Emin Atik
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WPS-S08 - FTMS and Innovative Methods for (Bio)Analyses

WP-179 **Top-down analysis of endogenous tau fragments in human cerebrospinal fluid using immunoprecipitation and Fourier Transform Mass Spectrometry**
G. Brinkmalm, C. Cicognola, J. Gobom, E. Portelius, H. Zetterberg, K. Blennow, K. Höglund
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WP-180 **Extreme resolution FT-ICR-MS top-down analysis of glycated proteins**
C. Cordeiro
Universidade de Lisboa, Laboratório de FT-ICR e Espectrometria de Massa Estrutural, Faculdade de Ciências, Lisboa, Portugal

WP-181 **Identification of new ligand-protein complex for Mycobacterium Tuberculosis using Fourier Transform Mass Spectrometry**
A. Di Capua, P. Myler, R. Quinn
Griffith Institute for Drug Discovery, Nathan, Australia

WP-182 **Coupling gas-phase fractionation and proton-transfer reaction for improved top-down proteomics**
L. Fornelli, R. Huguet, C. Mullen, R. Fellers, R. Melani, J. Syka, N. Kelleher
Northwestern University, Molecular biosciences/Chemistry, Evanston, USA

WP-183 **Detailed analysis of temporal ion cloud distributions undergoing Coulomb interactions in FT-ICR mass spectrometry: a many-particle simulation**
M. Fujiwara, H. Takahashi, N. Happo, K. Tanaka
Hiroshima City University, Grad School of Information Sciences, Hiroshima, Japan

WP-184 **FT-ICR MS with absorption-mode data acquisition: method development and high-resolution applications**
A. N. Kozhinov, K. O. Nagornov, Y. O. Tsybin
Spectroswiss Sàrl, EPFL Innovation Park, Lausanne, Switzerland

WP-185 **Factor Xa anticoagulant bioactive proteins derived from scorpion venom**
M. Li, Y. P. Y. Lam, P. Chen, R. Gavard, C. K. C. Chiu, C. A. Wootton, Q. Wu, M. P. Barrow, H. Fu, P. B. O'connor
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WP-186 **Microchip capillary electrophoresis-ESI-MS for rapid, multi-level analysis of complex proteins**
J. Scott Mellors, E. Redman
908 Devices Inc., Life Sciences, Boston, USA

WP-187 **Flavonoid annotation using a product ion-dependent MS^n data acquisition method on a Tribrid Orbitrap mass spectrometer**
R. Kiyonami, I. Sakane, S. Sharma, G. Mcalister, A. Souza, C. Ding, A. Huhmer
Thermo Fisher Scientific, Metabolomics Program, San Jose, USA

WP-188 **Fundamentals of FT-ICR MS at the cyclotron frequency**
O. Tsybin, K. Nagornov, A. Kozhinov, Y. Tsybin
Peter the Great Saint-Petersburg State Polytechnic University, Ion Physics Laboratory, Saint-Petersburg, Russian Federation

WP-189 **Use of SIFT-MS in the analysis of volatile compounds arising from the addition of sodium hypochlorite as an irrigant in infected root canal treatment**
K. Ioannidis, S. Niazi, S. Deb, F. Mannocci, D. Smith, C. Turner
The Open University, School of Life, Health & Chemical Sciences, Milton Keynes, United Kingdom

WP-190 **Optimal signal-to-noise and peak assignment for two-dimensional mass spectrometry**
A. Maria Van, R. Gavard, A. Lynch, T. Morgan, C. Wootton, L. Chiron, M. Delsuc, M. Barrow, P. O'Connor
University of Warwick, Department of Chemistry, Coventry, United Kingdom

WP-191 **Signal amplification mass spectrometry bioassay for attomolar detection of genes**
S. Xu, Y. Bai, H. Liu
Peking University, College of chemistry, Beijing, China

WP-192 **Two-dimensional (2D) FT-ICR MS at high resolution on precursor ions**
C. Rolando, F. Bray, J. Bouclon, P. Pelupessy, M. Delsuc
CNRS, University of Lille, Villeneuve d'Ascq, France

WPS-S09- Food Additives and Contaminants

WP-193 **Determination of undesired substances in edible oils by UHPLC-MS/MS**
A. Baldi Talini, Y. Gao, Z. Zhen, M. Zhu, F. Qin, J. Ye
PerkinElmer Inc, Mass Spectrometry, Shelton, USA

WP-194 **Development and validation of an LC-MS/MS method to quantify fumonisins and hydrolysed fumonisins in porcine serum**
G. Bichl, T. Czabany, H. Schwartz-Zimmermann, D. Schatzmayr, I. Dohnal
Biomin, Research Center, Tulln, Austria

WP-195 **Identification of synthetic food dyes by nanoelectrospray ionization**
L. Borovcová, E. Mácalová, K. Lemr
Palacký University, Department of Analytical Chemistry, Faculty of Science, Olomouc, Czech Republic

WP-196 **Acrylamide determination in potato and/or cereals based food by LC-MS/MS method: one year of monitoring in North-West Italy**
V. Ciccotelli, L. A. Masiello, V. Savio, B. Vivaldi, C. Ercolini
Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle D'Aosta (sezione di Genova), N.R.L. for pesticides in cereals and feed, Genova, Italy

WP-197 **Determination of pesticides in fruit, vegetables and feed by multiresidue methos: one year of monitoring in North-West Italy**
V. Ciccotelli, R. Nappi, B. Rutigliano, A. Galleggiante Crisafulli, E. Poma Genin, E. Alesso, B. Vivaldi
Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle D'Aosta (sezione di Genova), N.R.L. for pesticides in cereals and feed, Genova, Italy

WP-198 **Robust multiresidue pecticide analysis in baby food with enhanced sensitivity GC-MS/MS technology**
E. Ciceri, R. Law, T. Anderson, C. I. Cojocariu
Thermo Fisher Scientific, CMD, Milan, Italy

WP-199 **Sensitive and robust determination of phthalates in cooking oil using advanced electron ionization single quadrupole GC-MS technology**
E. Ciceri, A. Lamb, C. I. Cojocariu
Thermo Fisher Scientific, CMD, Milan, Italy

WP-200 **Bee pollen and pyrrolizidine alkaloids: a contamination profile analysis using LC-MS/MS**
L. De Jesus Inacio, L. Lucatello, V. Bisutti, A. Sartorato, R. Merlanti, F. Capolongo
University of Padua, Department of Comparative Biomedicine and Food Science, Legnaro - PD, Italy

WP-201 **Towards untargeted chemical food safety assessment**
G. Delaporte, M. Cladière, V. Camel
Ingénierie Procédés Aliments, AgroParisTech, INRA, Université Paris-Saclay, Massy, France

WP-202 **Characterisation and quantification of known/unknown migrating substances in food using LC & GC high resolution mass spectrometry**
Y. Hammel, B. Bodet, S. Koster
Nestle Research Center, Institute Food Safety & Analytical Science, Lausanne, Switzerland

WP-203 **Mercaptomic: towards the profiling of reactive metabolites in toxicology**
E. Jamin, R. Costantino, J. Martin, L. Debrauwer, F. Guéraud
INRA, MetaboHUB-MetaToul-AXIOM platform, Toulouse, France

WP-204 **Fast and automatic data processing for targeted and non-targeted pesticide analysis**
J. Jasak, J. Meltretter, J. Stahl-Zeng, V. Raguvaran, D. Cox
Sciex, Darmstadt, Germany

WP-205 **Simultaneous determination of propoxycarbazone and its metabolite in food by UHPLC-MS/MS, applying a QuEChERS extraction based method**
M. Vargas-Pérez, J. Marín-Sáez, M. L. Jiménez Medina, F. J. Egea González, A. Garrido Frenich
University of Almería, Dept. Chemistry and Physics, Almería, Spain

WP-206 **Sensitive determination of 44 toxic pyrrolizidine alkaloids in spices and culinary herbs using liquid chromatography tandem-mass spectrometry**
F. Kaltner, M. Rychlik, M. Gareis, C. Gottschalk
Ludwig Maximilian University of Munich, Chair of Food Safety, Oberschleissheim, Germany

WP-207 **Analytical method development of multi residue pesticides in Livestock Products by Gas chromatography-mass spectrometry(GC-MS/MS)**
H. S. Kang, E. J. Kim, M. Lim, E. J. Chang, K. No, D. M. Choi, H. Choi
Gyeongin Regional Office of Food and Drug Safety, Division of Hazardous Substances Analysis, Incheon, Republic of Korea

WP-208 **Limitations of gas chromatography–single quadropole mass spectrometry in the identification of compounds migrating from food contact materials**
C. Kirchkeszner, Z. Eke, Z. Nyiri, N. Petrovics
Joint Research and Training Laboratory on Separation Techniques, Eötvös Loránd University, Budapest, Hungary

WP-209 **Multi-analyte method based on liquid chromatography coupled with single quadrupole mass analyzer for fast and effective control of food additives**
A. Krmela, V. Schulzova, J. Pulkrabova, J. Hajslova
UCT Prague, Department of Food analysis and nutrition, Prague, Czech Republic

WP-210 **Aflatoxin M1 residues detection in milk, infant food and cheese by LC-MS/MS**
G. L. Ferro, S. Massafra, P. Stella, E. Pennazio, M. Leporati, D. Marchis, M. Gili
Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle d'Aosta, S.S. Igiene dei Mangimi, Torino, Italy

WP-211 **Analytical method based on UHPLC-ESI-MS/MS for quantification of plant toxins in herbal food supplements**
S. Malysheva, J. Picron, B. Huybrechts
Sciensano, Organic contaminants and additives, Brussels, Belgium

WP-212 **Comparison between HPLC-ESI-QqQ-MS/MS and SPME-GC-MS technique for acrylamide determination in potatoes chips**
S. Marzocchi, S. Marziali, M. Fiorenza Caboni
University of Bologna, Department of Agro-Food Science, Cesena, Italy

WP-213 **A multi-residue confirmatory method for the determination of sedatives by HPLC-MS/MS**
P. Metalnikov, I. Batov, R. Selimov, A. Komarov, V. Nikulin
VGNKI, Food Safety, Moscow, Russian Federation

WP-214 **Determination of Fenpyroximate from four types of honey by LC/MS/MS**
S. Myung, J. Kim, S. Lee
Kyonggi University, Chemistry, Suwon, Republic of Korea

WP-215 **Supercritical fluid chromatography – mass spectrometry as a new tool for determination of synthetic food dyes**
V. Pauk, M. Uhrová, K. Lemr
RCPTM, Department of Analytical Chemistry, Palacky University in Olomouc, Olomouc, Czech Republic

WP-216 **Simultaneous screening of 6 different antibiotic families in meat using LDTD-MS/MS quantitation at 9 seconds per sample**
P. Picard, J. Lacoursiere, S. Auger
Phytronix Tehcnologies Inc, Quebec, Canada

WP-217 **NDL-PCBs, PBDEs, HBCDs levels and temporal trends in mussels (Mytilus galloprovincialis) from Middle Adriatic Sea**
A. Piersanti, T. Tavoloni, T. Stecconi, A. Stramenga, R. Galarini
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WP-218 **Automated Solid Phase Microextraction (SPME) with UHPLC-MS/MS to determine veterinary drugs in chicken meat**
J. Wu, A. Khaled, F. Qin, J. Pawliszyn
PerkinElmer, Woodbridge, Canada

WP-219 **Simultaneous quantitation of fat soluble vitamins in infant milk formulae using 5500 QTRAP LC-MS/MS system**
A. Sage, J. Stahl-Zeng, A. Verma, A. Kumar, M. Pillai
Sciex, Market Development, Warrington, United Kingdom

WP-220 **Multiclass method for the quantitative analysis of 108 veterinary drugs in meat and milk by liquid-chromatography quadrupole-orbitrap mass spectrometry**
G. Saluti, I. Diamanti, R. Rossi, C. Barola, D. Giusepponi, S. Moretti, R. Galarini
Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche "Togo Rosati", Centre for Development and Validation of Methods, Perugia, Italy

WP-221 **Fungicides in red wines produced in South America**
T. Vargas, N. Salustriano, B. Klein, S. Da Silva, W. Romão, R. Wagner, R. Scherer
University of Vila Velha, Vila Velha, Brazil

WP-222 **A robust and sensitive method for the direct analysis of polar pesticides in food and environmental samples**
D. Schleuder, U. Chiuminatto, W. Broer
AB SCIEX Germany GmbH, Support, Darmstadt, Germany

WP-223 **Non-targeted fast screening of hundreds residual pesticides on fruits, eggs and soil using ambient mass spectrometry**
J. Shiea
National Sun Yat-Sen University, Department of Chemistry, Kaohsiung, Taiwan, Province Of China

WP-224 **The time trend of PBDE in breast milk from Beijing within the first six months postpartum**
S. Song
National Research Center for Geoanalysis, Department of Organic Analysis, Beijing, China

WP-225 **Screening and quantitation for food matrices using scanning SWATH acquisition**
J. Stahl-Zeng, D. M. Cox, J. Rivera, H. Lee, V. Raguvaran
Sciex, MDM, Darmstadt, Germany

WP-226 **LC-MS/MS versus GC-MS/MS for hexabromocyclododecanes (HBCDs) analysis in food**
A. Stramenga, T. Tavoloni, T. Stecconi, A. Piersanti
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WP-227 **GC-MS/MS and LC-MS/MS applied to the analysis of brominated flame retardants (PBDEs and HBCDs) in fish species from Italian market**
T. Tamara, A. Stramenga, G. Scortichini, T. Stecconi, A. Piersanti
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WP-228 **Organic (PBDEs,NDL-PCBs) and inorganic (Pb, Cd, Hg, As, Ni, Mn) contaminants assessment in wild boar (Sus scrofa) by GC-MS/MS and ICP-MS**
T. Tavoloni, A. Stramenga, V. Castro, M. Ciriaci, M. Conquista, F. Griffoni, P. Palombo, G. Scortichini, T. Stecconi, A. Piersanti
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WP-229 **Screening and quantitative analysis of non intentionally added substances eluted from polyethylene terephthalate bottle by high-resolution mass spectrometry**
A. Yamamoto, T. Murakami, M. Shizuma, E. Kishi, A. Ozaki
Tottori University of Environmental Studies, Faculty of Environment, Tottori, Japan

WP-230 **Development of a rapid method for analysis of heterocyclic aromatic amines by QuEChERS extraction and UHPLC-APCI-MS/MS assay**
S. Chevolleau, J. François, A. Bouville, L. Debrauwer
INRA /Toxalim, Metatoul-AXIOM Platform, Toulouse, France

WP-231 **In vivo efficacy of a YCW-based product in reducing oral bioavailability of zearalenone in pigs**
V. D'Ascanio, A. Catteuw, E. Santovito, V. Marquis, S. Croubels, D. Greco, A. Logrieco, G. Avantaggiato
Institute of Sciences of Food Production (ISPA), National Research Council (CNR), Bari, Italy

WP-232 **Exploiting the potential of HRMS for deciphering mycotoxin modification in micropropagated wheat: the case of deoxynivalenol**
T. Damiani, L. Righetti, E. Rolli, M. Suman, R. Bruni, C. Dall'Asta
University of Parma, Department of Food and Durg, Parma, Italy

WP-233 **Sensitive mass spectrometric method for the detection of palytoxins in shellfish using lithium cationization**
A. Gerssen, M. D. Klijnstra
RIKILT, Wageningen University and Research, Wageningen, Netherlands

WP-234 **Development of a simple multi-residue determination method of 80 veterinary drugs in fish tissues by liquid chromatography coupled to quadrupole Orbitrap mass spectrometry**
X. Luo, Z. Tang, Z. Niu, X. Ye, F. Zhao
Qingdao Customs, Inspection and Quarantine Technical Center, Qingdao, China

WP-235 **Comparison of different strategies for the determination of veterinary drug residues in food by UPLC-MS/MS using Orbitrap Elite**
P. Metalnikov, R. Selimov, A. Efimov, I. Batov, A. Dzhatdoeva, A. Komarov
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WP-236 **UHPLC-HRMS analysis of theobromine in Costa Rican Theobroma cacao**
K. Mladenovic, Y. Root, D. Ramanathan
Kean University, STEM, Union, USA

WP-237 **LC-MS/MS method to evaluate the presence of exogenous glycerol in wines**
L. Tonidandel, S. Moser, D. Trainotti, R. Larcher
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WP-238 **Approaches to minimize and control external contamination during sample handling and analysis of ubiquitous environmental phenolic compounds in food samples**
M. A. Zuberovic Muratovic, U. Rybinska, K. Hellenäs
National Food Agency, Department of Chemistry / Division of Science, Uppsala, Sweden

WP-239 **A study on migration of heavy metals from ceramics and glassware using inductively coupled plasma mass spectrometry (ICP-MS)**
K. C. Cho, Y. E. Cho, Y. C. Park, D. M. Choi
Gyeongin Regional Food and Drug Administration, Center for Food and Drug Analysis, Incheon, Republic of Korea

WPS-S10 - Atomic Mass Spectrometry: Metallomics and Isotope Ratio Mass Spectrometry

WP-240 **Isotopic niche space of songbirds migrating through the Southern Alps**
A. Franzoi, F. Camin, P. Pedrini, L. Bontempo
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WP-241 **Experimental evaluation of TIMS-based detection methods for isotopic analysis of uranium at ultra-trace level**
J. Park, K. Jeong
Korea Atomic Energy Research Institute, Nuclear Chemistry Research Division, Daejeon, Republic of Korea

WP-242 **C and H stable isotope ratio analysis using GC-IRMS for vanillin authentication**
M. Perini, S. Pianezze, F. Camin
Fondazione Edmund Mach, Technology Transfer Centre, San Michele all'Adige, Italy

WP-243 **Stable isotope ratio analysis for authentication of chitosan**
M. Perini, T. Nardin, M. Venturelli, S. Pianezze, R. Larcher
Fondazione Edmund Mach, Technology Transfer Centre, San Michele all'Adige, Italy

WP-244 **Development of novel compact carbon dating instrument based on Collinear Resonance Ionisation Spectroscopy (CRIS)**
G. Edwards, K. Flanagan, B. Cooper, S. Alsufyani, C. Ricketts, C. Binnersley
The University of Manchester, School of Physics & Astronomy, Manchester, United Kingdom

THURSDAY, August 30th, 2018

ThPS-S01 - Glycomics, Saccharides and Glycoconjugates

ThP-1 **Reductive alkaline release of *N*-glycans generates a variety of unexpected, useful products**
R. Figl, F. Altmann
University of Natural Resources and Life Sciences, Chemistry, Glycobiology, Vienna, Austria

ThP-2 **Analysis of mouse brain *N*-glycans by (PGC-)LC-ESI-MS using isotopically labeled standards**
C. Grünwald-Gruber, A. Thader, J. Urteil, D. Maresch, F. Altmann
University of Natural Resources and Life Sciences, Department of chemistry, Vienna, Austria

ThP-3 **Assignment of linkage, anomeric configuration, and branch location of oligosaccharides via a logically derived MS^n approach**
H. C. Hsu, C. Y. Liew, S. Huang, S. Tsai, C. Ni
Institute of Atomic and Molecular Sciences, Academia Sinica, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan, Province of China

ThP-4 **Fragmentation of oligosaccharides and suppression of metal-salt induced adducts using electrospray ionization**
V. Iwan, J. Grotemeyer
Christian-Albrechts-University Kiel, Institute of Physical Chemistry, Kiel, Germany

ThP-5 **MALDI-MS analysis of sucrose using a charcoal matrix**
J. Kim
Chungnam National University, Yuseong-Gu, Daejeon, Republic of Korea

ThP-6 **Multiplexed isotope labeled standards for isomeric analysis of *N*-glycans**
D. Maresch, C. Grünwald-Gruber, A. Thader, F. Altmann
University of Natural Resources and Life Sciences, Department of Chemistry, Vienna, Austria

ThP-7 **N-glycan analysis of various Chlorella strains by MALDI-ToF and LC-ESI-MS**
R. T. Mocsai, R. Figl, E. Svehla, F. Altmann
University of Natural Resources and Life Sciences, Department of Chemistry, Vienna, Austria

ThP-8 **Semi-targeted analysis of metabolites in Saponaria officinalis by LC-MS**
K. Pawlak, K. Lech, K. Wojciechowski, I. Goral, P. Bartosz, P. Kosior, T. Kiehl, A. Ornoch, K. Kaczmarczyk
Warsaw University of Technology, Faculty of Chemistry, Chair of Analytical Chemistry, Warsaw, Poland

ThP-9 **Semi-automatic site specific quantitative analysis of high mannose and hybrid type glycosylation in liver tissue associated with HCC and cirrhosis**
M. Sanda, J. Benicky, Z. Brnakova, L. Zhang, R. Goldman
Georgetown University, Department of Oncology, Washington, USA

ThP-10 **Integrating ion spectroscopy with mass spectrometry for the structural analysis of carbohydrates**
B. Schindler, G. Renois-Predelus, I. Compagnon
Institut Lumière Matière, Université de Lyon, Lyon, France

ThP-11 **Isomer-specific MRM profiling of serum *N*-glycome for Behcet disease monitoring**
N. Seo, K. H. Kim, J. K. Ahn, H. S. Cha, J. Kim, J. An Hyun
Chungnam National University, Graduate School of Analytical Science and Technology,
Daejeon, Republic of Korea

ThP-12 **Glycosaminoglycan analysis of prostate cancer tissue microarrays**
G. Tóth, O. Ozohanics, A. Ács, Á. Révész, K. Vékey, L. Drahos, L. Turiák
MS Proteomics Group, Research Center for Natural Sciences, Hungarian Academy of Sciences,
Budapest, Hungary

ThP-13 **Thin-layer chromatography coupled with nano-matrix based MALDI-ToF mass spectrometry for structural elucidation of glycans**
E. Gizaw, M. Tseng, Y. Chen
Academia Sinica, Institute of Chemistry, Taipei, Taiwan, Province Of China

ThP-14 **Glycolipidomics of human brain by combined modern mass spectrometry methods: chip nano ESI MS and ESI IMS MS^n**
M. Sarbu, Z. Vukelic´, D. Clemmer, A. D. Zamfir
National Institute for Research and Development in Electrochemistry and Condensed Matter,
Department of Condensed Matter, Timisoara, Romania

ThP-15 **Top down proteomics of human α-acid-glycoprotein: fast and unambiguous glycan analysis**
M. Bärenfänger, B. Meyer
University of Hamburg, Department of Organic Chemistry, Hamburg, Germany

ThP-16 **Development of a new method for the identification of Follicle Stimulating Hormone (FSH) glycoforms involved human fertility**
C. Melchiorre, CA. Illiano, G. Pinto, A. Carpentieri, A. Amoresano
University of Naples Federico II, Department of Chemical Science, Napoli, Italy

ThPS-S02 - Probing Protein Structure and Dynamics

ThP-17 **Structural diversity of nucleosomes characterized by nanoESI-MS and structural calculation**
K. Saikusa, A. Osakabe, D. Kato, S. Fuchigami, A. Nagadoi, Y. Nishimura, H. Kurumizaka, S. Akashi
Yokohama City University, Grad. Sch. of Med Life Science, Yokohama, Japan

ThP-18 **Native state organization of outer membrane porins unraveled by HDX-MS**
D. Donnarumma, C. Maestri, P.I. Giammarinaro, L. Capriotti, E. Bartolini, D. Veggi, R. Petracca, M. Scarselli, N. Norais
GSK Vaccines, Siena, Italy

ThP-19 **Effects of oxidative stress on the conformational stability of hemoglobin measured by variable temperature nESI-IMS-MS**
D. Woodall, T. El-Baba, C. Brown, D. Fuller, S. Raab, D. Clemmer
Indiana University, Bloomington, USA

ThPS-S03 - Natural Substances and Their Complexes

ThP-20 **Development of LC-MS/MS analytical protocol for artemisinin and its derivative compounds quantification in the Artemisia annua L. extracts for cosmetic applications**
R. M. Alberici, E. C. Cabral, G. C. Nogueira, R. Vardanega, M. A. A. Meireles, M. N. Eberlin
University of Campinas, Thomson Mass Spectrometry Laboratory, Campinas, Brazil

ThP-21 **Metabolomic UHPLC-qToF method to analyze tannins in natural complex products using All-Ions fragmentation acquisition**
M. Burico, L. Mattoli, P. Traldi
Aboca Spa Società Agricola, Sansepolcro, Italy

ThP-22 **Characterization of beta amino acid esters in Ononis species**
N. Gampe, A. Darcsi, L. Ladocsi, L. Kursinszki, S. Béni
Semmelweis University, Department of Pharmacognosy, Budapest, Hungary

ThP-23 **Investigation of plant extracts for medical research**
M. Gronbach, C. Oppermann, J. M. Modenbach, M. Sendler, M. Lerch, U. Kragl
University of Rostock, Department of Chemistry, Rostock, Germany

ThP-24 **MS analysis of protein interactions relevant for the biosynthesis of APE**
K. Karimi, G. L. C. Grammbitter, H. B. Bode, N. Morgner
Goethe University Frankfurt am Main, Institute of physical and theoretical chemistry, Frankfurt am Main, Germany

ThP-25 **Analytical authentication of Ophiogopon japonicus samples: an essential step to secure its supply and its use for the development of a safe and effective dermo-cosmetic ingredient**
S. Richer, D. Laporte, L. Verzeaux, D. Boudier, I. Fourasté, M. Howes, M. Simmonds, B. Closs
SILAB, R&D Department, Brive la Gaillarde, France

ThP-26 **LC-ESI-MS/MS analysis of short-chain peptides with anti-aging properties**
M. Shamshiddinova, Y.-M. Lee
Chungbuk National University, College of Pharmacy, Cheongju, Republic of Korea

ThP-27 **From massive chicken death to insect poison diet through the mass spectrometry prism**
E. Stashenko, J. R. Martinez, F. Prada, J. Lozano, Y. Bautista, J. Zambrano, N. Ñäñez
Universidad Industrial de Santander, School of Chemistry, Bucaramanga, Colombia

ThP-28 **Characterization of environmental microorganisms by proteins and lipids MALDI-ToF fingerprints**
V. Guérineau, M. Barthélemie, V. Eparvier, D. Touboul
CNRS-ICSN, Université Paris Saclay, Gif sur Yvette, France

ThP-29 **Mass spectrometry technique for studying the peptides cyclisation by native chemical ligation**
M. Wierzbicka, O. Skwara, S. D. Ozan, P. Stefanowicz
University of Wrocław, Faculty of Chemistry, Wrocław, Poland

ThP-30 **An unusual TMS artifact in EI mass spectrometry - Perrhenic acid TMS**
W. G. Mallard, Y. Zheng, S. P. Markey, J. L. Little
NIST, MSDC, Gaithersburg, USA

ThP-31 **Comparing the profiles of yellow-legged hornet venom (Vespa velutina nigrithorax) to evaluate the influences of seasonal variations**
T. N. Le, D. Da Silva, C. Colas, E. Darrouzet, P. Baril, L. Petit Leseurre, B. Maunit
Institut de Chimie Organique et Analytique(ICOA), UMR 7311, Université d'Orléans-CNRS, Orléans, France

ThP-32 **GC-MS/MS determination of cis and trans-Δ9-THC isomers in Cannabis sativa L**
S. Valera, G. Allegrone, F. Pollastro
Università Piemonte Orientale, Dipartimento di Scienze del Farmaco, Novara, Italy

ThPS-S04 - Environmental Mass Spectrometry

ThP-33 **Strategy to identify industrial peak emissions based on long-term HRMS data time series**
S. Anliker, M. Loos, M. Ruff, R. Comte, K. Fenner, H. Singer
Eawag, Environmental Chemistry, Dübendorf, Switzerland

ThP-34 **Transformation product formation in drinking water treatment**
A. M. Brunner, D. Vughs, W. Siegers, C. Bertelkamp, A. Kolkman, T. Ter Laak
KWR Watercycle Research Institute, Chemical Water Quality and Health, Nieuwegein, Netherlands

ThP-35 **Molecular level investigation of oil contaminated soils generated during the Gulf War with two-dimensional gas chromatography (GCxGC) and ultra-high resolution mass spectrometry**
E. Cho, M. Park, Y. H. Kim, G. Kang, Y. Cho, S. Kim
Kyungpook National University, Department of Chemistry, Daegu, Republic of Korea

ThP-36 **Occurrence of organophosphate flame retardants in swimming pools and their endocrine disrupting potential**
P. Chou, W. Shih
National Cheng Kung University, Department of Environmental Engineering, Tainan City, Taiwan

ThP-37 **Assessment of BPA and DEHP metabolites in urine samples from mother-child pairs of LIFE PERSUADED project**
V. Della Latta, F. Carli, E. Buzzigoli, D. Ciociaro, M. Gaggini, A. Paola Pala, A. Raffaelli, R. Conte, L. Busani, F. Maranghi, S. Tait, S. Cianfarani, C. La Rocca, A. Gastaldelli
CNR, Consiglio Nazionale delle Ricerche, Institute of Clinical Physiology, IFC, Pisa, Italy

ThP-38 **Duloxetine: degradation processes, transformation products elucidation by mass spectrometry and in silico analysis**
R. Osawa, M. Conceição, O. Monteiro, M. H. Florêncio
Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal

ThP-39 **Multi-mode ionization techniques for efficient MS/MS analysis of pesticides**
H. Gamble, C. Jolliffe, A. Dalmia
Perkin Elmer, R&D, Woodbridge, Canada

ThP-40 **Multiclass analysis of antibiotics in sediments by LC-Q-Orbitrap HRMS. Application to the Nera River**
D. Giusepponi, F. Scoppetta, M. Sargenti, G. Saluti, S. Moretti, R. Rossi, M. Capuccella, R. Galarini
Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche "Togo Rosati", Centre for Development and Validation of Methods, Perugia, Italy

ThP-41 **Determination of 16 polycyclic aromatic hydrocarbons by core-shell molecularly imprinted polymers prepared by reversible addition fragmentation chain transfer polymerization with APGC-MS/MS**
A. Golbabanezhad-Azizi, F. Shahhoseini, C. Bottaro
Memorial University of Newfoundland, Department of Chemistry, St. John's, Canada

ThP-42 **Fate and behavior of oil sands naphthenic acids in a pilot-scale treatment wetland as characterized by negative-ion electrospray ionization Orbitrap mass spectrometry**
C. Ajaero, K. Peru, M. Simair, V. Friesen, S. Hughes, D. Mcmartin, G. O'sullivan, J. Headley
Watershed Hydrology & Ecology Research Division, Water Science & Technology Directorate, Environment & Climate Change Canada, Saskatoon, Canada

ThP-43 **Photocatalytic activity of titanium dioxide films under visible light evaluated by ESI(-)-MS**
D. Holanda Pereira de Souza, T. Carita Correra, V. de Moraes Zamarion
Universidade de São Paulo, Institute of Chemistry, São Paulo, Brazil

ThP-44 **Study on the degradation mechanism of atrazine in sewage by UHPLC-MS/MS**
J. Li, J. Yan, B. Lai, X. Lia, K. Kahen, J. Wu
PerkinElmer, Woodbridge, Canada

ThP-45 **Comparison of organic mixtures from particulate matters collected in Korea and China by using GCxGC/High resolution mass spectrometry**
M. Park, G. Bang, K. Jang, K. Park, S. Kim, Y. Hwan Kim
Korea Basic Science Institute, Biomedical Omics Group, Cheongju, Republic of Korea

ThP-46 **Biocide spray product exposure: measured gas, particle and surface concentrations compared with spray model predictions**
V. Kofoed-Sørensen, A. Nørgaard, M. Frederiksen, P. Wolkoff, P. A. Clausen
National Research Center for the Working Environment, Chemical working environment, Copenhagen, Denmark

ThP-47 **Occurrence and human exposure to brominated and organophosphate flame retardants from Finnish household dust**
E. Kumar, P. Rantakokko, J. Braber, J. Koponen, T. Huang, H. Kiviranta
National Institute for Health and Welfare (THL), Health Security, Kuopio, Finland

ThP-48 **Novel drinking water disinfection by-products**
A. Lebedev, D. Kosyakov, N. Ul'yanovskii, M. Popov, T. Latkin
Lomonosov Moscow State University, Chemistry Department, Moscow, Russian Federation

ThP-49 **A comparative study of ultra-trace-level uranium by thermal ionization mass spectrometry with continuous heating: static and peak-jumping modes**
C. G. Lee, J. Park, S. H. Lim, S. H. Han
Korea Atomic Energy Research Institute, Nuclear Chemistry Research Division, Daejeon, Republic of Korea

ThP-50 **Analysis of natural radionuclides concentrations in monazite using acid digestion by quadrupole ICP-MS**
J. Lee, S. Yi
Korea Institute of Nuclear Safety, Department of Natural Radiation Safety, Daejeon, Republic of Korea

ThP-51 **Determination of global DNA methylation and oxidation of DNA and Lipid biomarkers in metal oxide nanomaterial-handling workers by liquid chromatography-tandem mass spectrometry**
H. Lee, S. Liou
Fu Jen Catholic University, Chemistry, New Taipei City, Taiwan, Province Of China

ThP-52 **Mass spectrometry identification of halogenated peptdies in treated drinking water**
P. Jiang, G. Huang, L. Blackstock, X.-Fang Li
University of Alberta, Faculty of Medicine and Dentistry, Edmonton, Canada

ThP-53 **Iodine distribution and bioavailability in soil from Fenyang, Shanxi province, China**
W. Liu, J. Hu
Chinese Academy of Geological Sciences, National Research Center for Geoanalysis, Beijing, China

ThP-54 **Determination of Ag nanoparticles in Vltava river (Prague, Czech Republic) by single particle ICP-MS**
M. Loula, A. Kana, O. Mestek
University of Chemistry and Technology Prague, Department of Analytical Chemistry, Prague, Czech Republic

ThP-55 **Antibiotics in waters along the Grand Canal, China**
G. Lu, H. Piao, S. Chen, X. Jiao, Y. Yang
Chinese Academy of Geological Sciences, National Research center for Geoanalysis, Beijing, China

ThP-56 **GC×GC-MS in environmental analysis: from efficient separation to introduction of retention index data base**
D. Mazur, I. Zenkevich, V. Artaev, O. Polyakova, A. Lebedev
Lomonosov Moscow State University, Organic Chemistry Department; Lomonosov Northern (Arctic) Federal University, Core Facility Center "Arktika", Moscow, Arkhangelsk, Russian Federation

ThP-57 **The analysis of environmental samples using high resolution mass spectrometry to identify novel PFAS compounds**
D. Mcmillan, S. Roberts, C. Butt, C. Borton
Sciex, Business Development, Warrington, United Kingdom

ThP-58 **Characterization of organic compounds in aquatic sediment by ion profiles obtained using GC-MS system**
Z. Moldovan
National Institute of Research and Development for Isotopic and Molecular Technology, Mass Spectrometry, Cluj-Napoca, Romania

ThP-59 **Study of pharmaceuticals removal rates in wastewater treatment plant using GC-MS analytical technique**
Z. Moldovan, O. Marincas, I. Feher
National Institute of Research and Development for Isotopic and Molecular Technology, Mass Spectrometry, Cluj-Napoca, Romania

ThP-60 **Citalopram photodegradation: Identification of transformation products by mass spectrometry**
R. Osawa, M. Conceição, O. Monteiro, M. H. Florêncio
Universidade de Lisboa, Faculdade de Clências, Lisboa, Portugal

ThP-61 **A novel analytical integrated approach based on mass spectrometry for the evaluation of imidacloprid exposure during CNS development**
A. Passoni, R. Bagnati, M. De Paola, E. Davoli, A. Mariani
IRCCS - Istituto di Ricerche Farmacologiche Mario Negri, Environmental Health Sciences Department, Milan, Italy

ThP-62 **Non-targeted approach for the study of labile dissolved organic matter**
C. Patriarca, P. J.R. Sjöberg, J. Bergquist, L. J. Tranvik, J. A. Hawkes
Uppsala University, Department of Chemistry, Uppsala, Sweden

ThP-63 **Screening of pharmaceutical and their metabolites in fish by HRMS using data-base support**
J. M. Peña-Herrera, N. Montemurro, S. Pérez, D. Barceló
IDAEA-CSIC, Environmental Chemistry, Barcelona, Spain

ThP-64 **Suspected screening of natural toxins in surface water by liquid chromatography high resolution mass spectrometry**
M. Picardo, D. Filatova, O. Nuñez, M. Farré
Spanish Council for Scientific Research (CSIC), University of Barcelona, Analytical Chemistry, Barcelona, Spain

ThP-65 **Airbone measurement of organic gases and particles in the atmosphere with PTR-MS**
F. Piel, T. Mikoviny, M. Müller, S. A. Schiller, S. Feil, G. Hanel, P. Mutschlechner, A. Jordan, L. Märk, P. Sulzer, A. Wisthaler
Ionicon Analytik GmbH, University of Innsbruck, Institute for Ion Physics and Applied Physics, Innsbruck, Austria

ThP-66 **Dissipation studies of dimethachlor and metabolites in soil and water by UHPLC-Orbitrap-MS**
R. López Ruiz, R. Romero González, J. L. Martínez Vidal, A. Garrido Frenich
University of Almería, Dept. Chemistry and Physics, Almería, Spain

ThP-67 **Paving the way for the analysis of trace compounds in metallurgical gases by proton-transfer-reaction time-of-flight mass spectrometry. Importance of background**
J. I. Salazar Gómez, C. Klucken, M. Sojka, H. Ruland, K. Kähler, L. Masliuk, T. Lunkenbein, R. Schlögl
Max-Planck Institute for Chemical Energy Conversion, Department of Heterogeneous Reactions, Mülheim a.d. Ruhr, Germany

ThP-68 **Novel application of molecularly imprinted polymers with gas chromatography-atmospheric pressure ionization-mass spectrometry for high through-put determination of 16 PAHs**
F. Shahhoseini, A. Golbabanezhad-Azizi, S. Egli, C. Bottaro
Memorial university of Newfoundland, Department of Chemistry, St. John's, Canada

ThP-69 **New analysis method for organotin compounds by Tandem-LC/MS without the derivatization step**
J. E. An, Y. C. Song, Y. S. Kim, K. C. Yi
Korea Apparel Testing and Research Institute, Environment analysis center, Anyang city, Republic of Korea

ThP-70 **Continuous-introduction aerosol-to-liquid sampler and its coupled use with ICP-MS for on-line sensitive analysis of atmospheric aerosol**
Y. Su, Z. Li, W. Wang, S. Fang
Northwest Institute of Nuclear Technology, Xi'an, China

ThP-71 **Acetone degradation in a plasma reactor studied in real-time by PTR-MS**
S. Thomas, M. Heninger, N. Blin-Simiand, L. Magne, H. Mestdagh, S. Pasquier, E. Louarn
Univ. Paris Sud, CNRS, Univ. Paris Saclay, Laboratoire de Chimie Physique, Orsay, France

ThP-72 **Uptake of dioctyl phthalate by Populus alba Villafranca**
F. Vannucchi, E. C. Pierattini, A. Raffaelli, A. Francini, L. Sebastiani
Biolabs, Institute of Life Science, Scuola Superiore Sant'Anna, Pisa, Italy

ThP-73 **Identification of degradation products of selected pharmaceuticals in soils by high resolution mass spectrometry**
A. Vojs Stanova, K. Grabicova, A. Borik, R. Kodesova, A. Klement, R. Grabic
University of South Bohemia in České Budějovice, Faculty of Fisheries and Protection of Waters, South Bohemian Research Center of Aquaculture and Biodiversity of Hydrocenoses, Vodňany, Czech Republic

ThP-74 **The study of sampling pipeline effect for gases partial pressure measure with mass spectrometer**
R. Yan
Beijing Institute of Spacecraft Environment Engineering, CAST, Beijing, China

ThP-75 **Direct analysis of 17 perfluorinated compounds in water at low parts-per-trillion levels by LC-MS/MS workflow**
J. Ye Sha, J. Wu, F. Qing, F. Kero, L. Piatti, S. Edler, D. Mattern, M. Gori
Perkin Elmer, Woodbridge, Canada

ThP-76 **Molecular composition of dissolved organic matter in the TALDICE ice core**
R. Zangrando, V. Zanella, O. Karroca, E. Barbaro, N. M. Kehrwald, D. Battistel, A. Gambaro, C. Barbante
Consiglio Nazionale delle Ricerche, Institute for the Dynamics of Environmental Processes, Mestre-Venezia, Italy

ThP-77 **Investigations on the adsorption of REEs by GO with different sizes: mechanism and application**
W. Zhao
Chinese Academy of Geological Sciences, National Research Center for Geoanalysis, Beijing, China

ThP-78 **HILIC-MS (non-)target screening, monitoring and toxicological evaluation of highly polar compounds in drinking water and sources**
A. Kolkman, R. Sjerps, P. Kooij, K. Baken, P. De Voogt
KWR Watercycle Research Institute, Laboratory for Materials Research and Chemical Analysis, Nieuwegein, Netherlands

ThP-79 **Direct analysis of phenolic compounds in cork wastewater by HPLC-QToF**
C. F. J. Yuste, C. B. Godoy
Cicytex, ICMC, Mérida, Spain

ThPS-S05 - Safe & Valuable Food

ThP-80 **A new analytical method for the quantification of three lignans in espresso coffee by using HPLC-MS/MS triple quadrupole**
S. Angeloni, G. Caprioli, G. Khamitova, L. Navarini, G. Sagratini, S. Vittori
University of Camerino, School of Pharmacy, Camerino, Italy

ThP-81 **Catabolic markers 24,25-dihydroxyvitamin D2/D3 in bovine and porcine sera show inter-species differences between vitamin D2 and vitamin D3 metabolism**
K. G. Dowling, G. L. J. Hull, A. Hayes, S. K. Duffy, A. K. Kelly, J. V. O'Doherty, K. D. Cashman
University College Cork, Cork Centre for Vitamin D and Nutrition Research, School of Food and Nutritional Sciences, Cork, Ireland

ThP-82 **Evaluation of oxidative stress markers in human biological matrices by means of UHPLC-MS/MS**
F. Fanti, F. Vincenti, N. Bernabò, M. Serafini, D. Compagnone, M. Sergi
University of Teramo, Faculty of Bioscience and Technology for Food, Agriculture and Environment, Teramo, Italy

ThP-83 **Comprehensive characterization of Minimas, a natural complex food supplement, by different mass spectrometry techniques**
E. Flamini, G. Fodaroni, S. Tamimi, S. Bedont, D. Decarli, M. Burico, A. Gaetano, L. Mattoli, P. Traldi
Aboca Spa Società Agricola, Area Ricerca Fitochimica, Sansepolcro, Italy

ThP-84 **The synergism of MALDI LIFT-ToF/ToF MS and ESI-Q-ToF MS instruments to discover new isoforms of allergens from hazelnut oleosin extract**
S. Nebbia, C. Lamberti, M. Manfredi, E. Marengo, L. Cavallarin, M. G. Giuffrida
CNR, ISPA, Colleretto Giacosa, Italy

ThP-85 **Determination of pyrrolizidine alkaloids in plant material using on-line SPE coupled to UHPLC-MS/MS**
A. Grüning, J. Sander, S. Vedder
Shimadzu Europa, CIPS, Duisburg, Germany

ThP-86 **Free fatty acids and hexanal as shelf life markers in cheese: evaluation of food packaging efficiency through a quantitative HS-SPME-GC-MS method**
A. F. Kamgang Nzekoue, E. Vittori, S. Vittori, G. Caprioli, G. Sagratini
University of Camerino, Camerino, Italy

ThP-87 **Bioactive compounds of brazilian green coffee beans collected in different levels of maturation by ESI-LTQ-ORBITRAP**
M. Lemos, C. Perez, D. Ifa, R. Scherer
Universidade Vila Velha, Natural Products, Vila Velha, Brazil

ThP-88 **Development of a LC-MS/MS method for the detection of species-specific muscle peptides in PAPs**
D. Marchis, M. Leporati, A. Altomare, G. Aldini, C. Casalone
Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle d'Aosta, S.S. Igiene dei Mangimi, Torino, Italy

ThP-89 **Metabolic survey of Italian vegetables: FTICR-MS and NMR-based untargeted analyses**
A. Maccelli, A. P. Sobolev, D. Capitani, B. Chiavarino, S. Fornarini, L. Mannina, M. Elisa Crestoni
Sapienza Università di Roma, Dipartimento di Chimica e Tecnologie del Farmaco, Roma, Italy

ThP-90 **GC-MS monitoring of volatiles in grappa during aging in two different wood barrels**
M. De Rosso, C. M. Mayr, R. Castagner, R. Sonego, R. Flamini
Council for Agricultural Research and Economics - Research Center for Viticulture & Enology CREA, Conegliano, Italy

ThP-91 **Sensitive and specific allergen screening analysis using LC-MS/MS**
A. Sage, J. Stahl-Zeng, C. Borton, L. New
Sciex, Market Development, Warrington, United Kingdom

ThP-92 **LC-MS/MS: a useful tool to investigate marine lipophilic toxins in mussels**
M. Siracusa, S. Bacchiocchi, S. Evangelista, A. Piersanti
Centro Referenza Nazionale controllo microbiologico e chimico molluschi bivalvi, Istituto Zooprofilattico Sperimentale Umbria e Marche "Togo Rosati", Perugia, Italy

ThP-93 **Advances in mass spectrometry for food safety and authenticity**
D. Tsipi, H. Botitsi
General Chemical State Laboratory, Food Safety & Quality Laboratories, Athens, Greece

ThP-94 **Development of infant formula certified reference material for nutrient element analysis**
K. Lee, J. Ki Suh, S. W.Heo, S. H. Kim, Y. Lim, M. S. Han, M. C. Lim, H. S. Min, E. Hwang, Y. Yim
KRISS, Center for Analytical Chemistry, Daejeon, Republic of Korea

ThP-95 **Analysis of penta-*O*-galloyl-β-D-glucose in functional foods by LC-MS/MS**
S. Yong-Woon
Ministry of Food and Drug Safety, Nutrition and Functional Research Team, Cheongju-si, Republic of Korea

ThP-96 **Lipid fingerprint to determine *Fusarium* contamination in melon**
D. Zampieri, R. Dantas, K. R. Belaz, M. N. Eberlin, A. H. Oster, E. D. O. Silva, G. J. Zocolo
Federal University of Ceara, Organic and Inorganic Department, Fortaleza, Brazil

ThP-97 **Investigation of the gliadin fraction composition in old and modern wheat genotypes**
V. Cunsolo, M. A. De Santis, A. Di Francesco, R. Saletti, M. M. Giuliani, Z. Flagella, S. Foti
University of Catania, Department of Chemical Sciences, Catania, Italy

ThP-98 **Non-targeted characterization of the degradation products of soybean oil after frying process by HS-SPME-GC-MS and LLE-LC-HRMS**
M. Lee, C. Chen, Y. Tsai
National Chung Hsing University, Chemistry, Taichung, Taiwan, Province Of China

ThP-99 **Metabolites from cafestol - a coffee diterpene- by Zebrafish tank model and LC-MS/MS**
C. M. Rezende, C. V. Andriolo, H. M. G. Pereira, V. F. Sardela, F. J. M. Novaes
Federal University of Rio De Janeiro, Chemistry Institute, Rio De Janeiro, Brazil

ThPS-S06 – Lipidomics

ThP-100 **Novel skin lipid biomarkers associated with atopic dermatitis**
E. Berdyshev, E. Goleva, I. Bronova, J. Jung, M. A Seibold, D. Ym Leung
National Jewish Health, Department of Medicine, Denver, USA

ThP-101 **Quantum chemical mass spectrometry as a tool for the prediction of mass spectra and the identification of fragmentation pathways - Peptides and lipids**
F. Blockhuys, J. Cautereels
University of Antwerp, Department of Chemistry, Antwerp, Belgium

ThP-102 **A new UHPLC/MS-QToF method to evaluate effects of environmental metabolic disruptors on hepatic lipidomic profile**
F. Carli, M. Gaggini, V. Della Latta, S. Tait, F. Maranghi, R. Tassinari, C. La Rocca, A. Gastaldelli
CNR, Institute of Clinical Physiology, Pisa, Italy

ThP-103 **A quantum chemical tool for the identification of fragmentation pathways: additional insight into lipid-specific fragmentation mechanisms**
J. Cautereels, F. Blockhuys
University of Antwerp, Department of Chemistry, Antwerp, Belgium

ThP-104 **Robust and sensitive LC-MS/MS based plasma lipid profiling on a Thermo Scientific™ Q Exactive™ HF-X mass spectrometer**
T. N. Array, E. Sokol, A. Criscuolo, C. Dauly, A. Harder
Thermo Fisher Scientific, CMD, Villebon sur Yvette, France

ThP-105 **Verified HILIC LC-MS/MS assay for high-throughput targeted lipdomics analysis**
C. Papan, K. K. S. Gorti, L. Fu, B. Ubhi, M. J Pearson, L. Xiong, P. Baker, J. Dojahn
Sciex, Darmstadt, Germany

ThP-106 **Structure elucidation of Gram-negative microbial glycolipids by energy-resolved tandem mass spectrometry**
A. Dornyei, V. Sandor, A. Kilar, N. Eros, B. Kocsis, F. Kilar
University of Pecs, Department of Analytical and Environmental Chemistry and Szentágothai Research Center, Pecs, Hungary

ThP-107 **Development of a comprehensive panel of eicosanoids and related fatty acid metabolites for high-sensitivity and quantitative LC-MS/MS analysis**
Y. Fujito, M. Yamada, H. Lin, S. Fujita
Shimadzu Corporation, Global Application Development Center, Kyoto, Japan

ThP-108 **Rapid targeted LC-MS/MS assay for ESKAPE pathogen identification direct from biological fluids**
D. Goodlett, T. Liang, B. Oyler, C. Chandler, S. Hwan Yoon, R. Ernst
UMB, Pharmacy, Baltimore, USA

ThP-109 **Biomarker research and short time chromatography: a utopia?**
L. Hahnefeld, G. Geisslinger, N. Ferreirós
Goethe University Frankfurt, Institute of Clinical Pharmacology, Frankfurt, Germany

ThP-110 **Investigation into the bleaching of vegetable oils using high resolution mass spectrometry**
A. Hambly, J. Van Duijneveldt, P. Gates
University of Bristol, School of Chemistry, Cantock's Cl, Bristol, United Kingdom

ThP-111 **Analysis of a complex lipid profile in human sebum by using GCxGC-HRToFMS**
M. Hashimoto, K. Okuda, A. J. Dane, R. B. Cody, B. van der Meer
JEOL(EUROPE)SAS, European Application Group, Croissy-sur-Seine, France

ThP-112 **Applicability of MALDI-Orbitrap-MS for the early diagnosis of renal cell carcinoma based on the lipidomic analysis of blood and urine samples**
R. Jirásko, D. Wolrab, I. Brabcová, M. Holcapek, D. Vrána, V. Študent, B. Melichar
University of Pardubice, Department of Analytical Chemistry, Pardubice, Czech Republic

ThP-113 **Changes of specific sphingomyelins depending on the severity of nonalcoholic fatty liver disease**
Y. Jung, J. Seo, G. Hwang
KBSI, Seodaemun-gu, Seoul, Republic of Korea

ThP-114 **A comprehensive method for total lipid analysis in biological matrices by hydrophilic interaction liquid chromatography electrospray ionization mass spectrometry HILIC/ESI-MS**
S. Khoury, S. Cabaret, E. A. Y. Masson, O. Berdeaux
UMR CSGA - INRA - CNRS, University of Bourgogne Franche-Comté, Dijon, France

ThP-115 **Graphical identification of lipids using three-dimensional Kendrick mass plots**
A. Korf, C. Vosse, H. Hayen
University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany

ThP-116 **Analysis of polyglycerophospholipids using isotope-labeled methylation by nUPLC-ESI-MS/MS**
J. Lee, M. Moon
Yonsei University, Chemistry, Seoul, Republic of Korea

ThP-117 **Plasma lipidomic profiling of five different types of cancer by nUPLC-ESI-MS/MS**
G. Lee, J. Lee, M. Moon
Yonsei Univ.,Chemistry, Seoul, Republic of Korea

ThP-118 **MALDI-ToF/MS analyses determined urinary phospholipids as a potential biomarker for prostate cancer**
X. Li, K. Nakayama, T. Goto, S. Akamatsu, K. Shimizu, O. Ogawa, T. Inoue
Kyoto University, Department of Urology, Kyoto, Japan

ThP-119 **Investigation of one novel oxidized 1-palmitoyl-2-arachidonoyl-sn-glycero-3-phosphocholine molecule on human aortic endothelial cells by LC-MS/MS**
Y. Chen, H. Tsou, Y. Shieh, M. Liu
National Changhua University of Education, Department of Chemistry, Changhua, Taiwan

ThP-120 **A translational pilot study of global lipid profile as risk marker in coronary plaque: mass spectrometry approach on asymptomatic patients**
M. U. B. Paiva, D. V. N. Paiva, L. J. S. R. Alves, H. L. Machado, H. J. B. De Souza, F. N. dos Santos, M. N. Eberlin, R. M. De Oliveira, M. M. Martins, F. A. Atik, A. M. A. Martins
UnB / UniCeub, Medicine / Surgery, Brasilia, Brazil

ThP-121 **Lipid profiling of non-steroidal anti-inflammatory drugs (NSAIDs) on prostate cancer cell lines with ToF-SIMS and DESI-MS**
D. J. McDougall, E. Jones, C. Hart, M. Brown, A. Mcmahon, N. Lockyer
University of Manchester, Department of Chemistry, Manchester, United Kingdom

ThP-122 **Defining structural differences in cardiolipins from an actinomycete marine sponge symbiont and S. aureus**
B. Oyler, C. Chandler, F. Zhang, R. Ernst, R. Hill, D. Goodlett
University of Maryland, Baltimore, School of Medicine, Baltimore, USA

ThP-123 **Untargeted lipidomics for the assessment of arsenic exposure in rice (Oryza sativa japonica)**
M. C. Pérez Cova, F. R. Tauler, S. J. Jaumot
CSIC-IDAEA, Química Ambiental. Quimiometría, Barcelona, Spain

ThP-124 **High-resolution multiple reaction monitoring method development for quantification of steroidal hormones in plasma**
A. P. F. Peti, G. A. Locachevic, M. K. B. Prado, L. A. B. De Moraes, L. H. Faccioli
Universidade de São Paulo - USP, DACTB, Ribeirão Preto, Brazil

ThP-125 **Micro-UPLC-MS high-throughput screening assay for sphingolipids pathway analysis**
K. Randall, H. Klodnitsky, D. Tietz, C. Phaneuf, M. Olszewski, E. Makino, K. Murphy, A. Belenky
Sanofi, Pre-development sciences, Waltham, USA

ThP-126 **Ceramidome plasticity through iso-energetic precursor and neutral loss discovery scans**
F. M. Rubino, M. Dei Cas, P. Signorelli, R. C. Paroni, R. Ghidoni, J. Rizzo
Università degli Studi di Milano, Dipartimento di Scienze della Salute, Milano, Italy

ThP-127 **Serum lipidomic changes in Zika and Dengue virus infection reveals potential targets for assertive clinical diagnosis**
F. Santos, A. Martins, K. Magalhães, M. Eberlin
University of Campinas, Analytical Chemistry, Campinas, Brazil

ThP-128 **Fishing for lactones: method development for selective identification of lactone-containing lipids**
E. Slutsky Smith, S. Khatib, A. Szuchman-Sapir
Migal--Galilee Research Institute, Laboratory of Vascular Signaling Research, Kiryat Shmona, Israel

ThP-129 **Challenges of lipid isomers and isobars in mass spectrometry-based biomarker research**
U. Sommer, H. Pham-Tuan, T. Koal
Biocrates Life Sciences AG, R&D, Innsbruck, Austria

ThP-130 **Applying Trapped Ion Mobility Separation (TIMS) in combination with Parallel Accumulation Serial Fragmentation (PASEF) for analysis of lipidomics samples**
M. Szesny, S. Götz, S. Meyer, U. Schweiger-Hufnagel, A. Barsch, N. S. Meitei
Bruker Daltonik GmbH, Metabolomics, Bremen, Germany

ThP-131 **How to ensure quality in the analysis of endogenous compounds in biological samples**
D. Thomas, S. C. Fleck, R. Gurke, G. Geisslinger, N. Ferreirós
Goethe University, Institute of Clinical Pharmacology, Frankfurt, Germany

ThP-132 **Study of acetogenins in a natural extract using SFC-HRMS/MS and post-column metal cationisation**
L. Laboureur, P. Champy, D. Touboul
CNRS, ICSN, Gif-sur-Yvette, France

ThP-133 **Improved lipid annotation utilizing positive and negative ion MS^2 / MS^3 HCD and CID spectra**
D. Peake, R. Kiyonami, D. Gachotte, Y. Yokoi, S. Webb, A. Huhmer
Thermo Fisher Scientific, San Jose, USA

ThP-134 **A Simple and Rapid Extraction of Lipids in Plasma Using Spin Column with Superabsorbent Polymer Beads**
G. Bang, J. H. Choi, Y. J. H. Park, J. A. Kim, Y. H. Kim
Korea Basic Science Institute, Biomedical Omics Group, Cheong-ju, Republic of Korea

ThP-135 **Lipidomic approach for algal oil characterization by FTICR mass spectrometry**
S. Chiaberge, R. Miglio, D. Deriu, S. Perucchini, A. Siviero
eni s.p.a., Renewable Energy & Environmental R&D, Novara, Italy

ThP-136 **Dual mass spectrometry as a tool to improve annotation and quantification in targeted plasma lipidomics**
L. Gao, A. Cazenave-Gassiot, B. Burla, M. Wenk, F. Torta
National University of Singapore, Life Sciences Institute, Singapore, Singapore

ThP-137 **New peak alignment software: MetaboAlign improving issues of LC-MS/MS lipidomics enables highthroughput data analysis for thousands of lipids in biological materials**
A. Hayashi, T. Matsuzaka, H. Shimano
ONO Pharmaceutical Co.,LTD., Minase Research Institute, Mishima-gun, Japan

ThP-138 **Structural analysis of lipids from cells of Bacteria of the Good, the Bad and of the Ugly**
F. Hsu, C. Frankfater, W. Henson, A. Haas, J. Turk, G. Purdy, R. Tatituri
Washington University School of Medicine, St. Louis, USA

ThP-139 **Joint application of ESI and MALDI lipidomic profiles for classification of brain tumors**
D. Ivanov, A. Sorokin, E. Zhvansky, V. Shurkhay, S. Pekov, I. Popov, E. Nikolaev
Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russian Federation

ThP-140 **Development and application of an enhanced lipidomic profiling method using LC-MS**
M. Jaber, D. Barrett, D. Kim
University of Nottingham, Advanced Materials and Healthcare Technologies, Nottingham, United Kingdom

ThP-141 **UPLC-QqQ/MS-based lipidomics analysis of high glucose induced HepG2 cells treated with herbal medicine extracts**
J. Lee, D. Choi, B. Choi, Y. Lee, G. Kim, D. Lee
National Institute of Horticultural and Herbal Science, Department of Herbal Crop Research, Eumseong, Republic of Korea

ThP-142 **Construction of novel lipidomics platform combinated of targeted and non-targeted analysis**
Y. Yokoi, H. Kuwabara, T. Hoshino, A. Hayashi
Mitsui Knowledge Industry Co., Ltd., Bioscience Department, Tokyo, Japan

ThPS-S07 - Developments and Applications In Ion Mobility MS

ThP-143 **A high-resolution ion mobility spectrometer coupled to a time-of-flight mass spectrometer**
M. Allers, L. Timoumi, A. T. Kirk, F. Schlottmann, S. Zimmermann
Leibniz Universität Hannover, Institute of Electrical Engineering and Measurement Technology, Department of Sensors and Measurement Technology, Hannover, Germany

ThP-144 **Application of PASEF MS/MS scans to monoclonal antibody peptide mapping**
A. Alving, S. Pengelley, G. Trementin, D. Sukau
Bruker Daltonics, Biopharma, Billerica, USA

ThP-145 **A clip on ion mobility device. Enabling gas phase ions separation and collision cross section measurements to any mass spectrometers**
B. Bellina, J. Commandeur, P. Barran
University of Manchester, Manchester Institute of Biotechnology, Manchester, United Kingdom

ThP-146 **Exploring the chemical coverage and structural assignment of natural products by ion mobility spectrometry combined with ultra-performance liquid chromatography/mass spectrometry**
F. Carnevale Neto, J. M. Egan, L. V. Costa-Lotufo, N. P. Lopes, R. G. Linington
Faculdade de Ciências Farmacêuticas da Universidade de São Paulo, Ribeirão Preto, São Paulo, Brazil

ThP-147 **Influence of protomers on dissociation of sequence-defined oligo(alkoxyamine amide)s**
C. Chendo, S. Poyer, D. Siri, J. Lutz, L. Charles
Fédération des Sciences Chimiques, Aix Marseille Université, Marseille, France

ThP-148 **Trapped ion mobility spectrometry as novel separation technique for the investigation on isomer formation during the simulation of Phase I Metabolism by means of Electrochemistry/Mass Spectrometry**
J. Fangmeyer, S. Gereon Scheeren, R. Schmid, U. Karst
University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany

ThP-149 **Prion protein conformational landscape studied by mass spectrometry and ion mobility**
F. Halgand, G. Van der Rest, H. Rezaei
CNRS, Chemistry, Orsay, France

ThP-150 **Secondary structure of ionized peptoids by ion mobility mass spectrometry**
E. Halin, S. Hoyas, J. De Winter, V. Lemaur, J. Cornil, S. Laurent, P. Gerbaux
UMONS, Université de Mons, Mons, Belgium

ThP-151 **Collision cross section (CCS) as a complementary parameter to characterize human and veterinary drugs: creation of a database**
C. Tejada-Casado, M. Hernández-Mesa, F. Monteau, F. J. Lara, M. del Olmo-Iruela, A. M. García-Campaña, B. Le Bizec, G. Dervilly-Pinel
École nationale vétérinaire, agroalimentaire et de l'alimentation de Nantes-Atlantique (Oniris), Laboratoire d'Etudes des Résidus et Contaminants dans les Aliments (LABERCA), INRA UMR 1329, Nantes, France

ThP-152 **Collision cross section as a novel parameter for the characterization of steroids**
M. Hernández-Mesa, B. Le Bizec, F. Monteau, A. M. García-Campaña, G. Dervilly-Pinel
École nationale vétérinaire, agroalimentaire et de l'alimentation de Nantes-Atlantique (Oniris), Laboratoire d'Etudes des Résidus et Contaminants dans les Aliments (LABERCA), INRA UMR 1329, Nantes, France

ThP-153 **Application of CO_2 drift gas in travelling wave ion mobility mass spectrometry for the structural elucidation of environmentally relevant isobaric isomer compounds**
Y. Iinuma, E. Hayakawa, S. Inomata, K. Sato, H. Ren, S. Yue, P. Fu
Okinawa Institute of Science and Technology, Onna, Japan

ThP-154 **Profiles of arrival time distributions in different drift gases as a tool for identification of isomers**
L. Borovcová, J. Ondruchová, V. Havlíček, K. Lemr
Palacký University, Regional Centre of Advanced Technologies and Materials, Department of Analytical Chemistry, Faculty of Science, Olomouc, Czech Republic

ThP-155 **Analysing disease triggering amyloids: combining ESI-IMS and LILBID-MS**
T. Lieblein, R. Zangl, J. Martin, N. Morgner
Goethe-University, Institute for Physical and Theoretical Chemistry, Frankfurt/Main, Germany

ThP-156 **Differential Mobility Separation (DMS)-based separation of bile acid isomers**
D. Merkel, C. Papan, V. Kaever, H. Bähre, J. Dojahn
SCIEX Germany, Application Support, Darmstadt, Germany

ThP-157 **Addition of collision cross sections to searchable libraries: a robust approach to enhance cumulative specificity in screening assays**
R. Mortishire-Smith, M. McCullagh, M. Herman, E. van Hoeck, S. Goscinny
Waters, Wilmslow, United Kingdom

ThP-158 **The use of CCS-enabled libraries for drug metabolism applications**
R. Mortishire-Smith, D. Veyel, B. Krawczyk, J. Vissers
Waters, Wilmslow, United Kingdom

ThP-159 **Separation of intact protein isoforms with differential mobility**
K. Pohl, C. Nortcliffe, F. Sanchez, J. Dojahn, A. Uppal, S. Heidelberger, J. Yves Leblanc
Sciex, Biologics, Darmstadt, Germany

ThP-160 **Ion guide with very strong axial transporting fields**
S. Poteshin, A. Burykina
NRNU MEPHI, Molecular Physics, Moscow, Russian Federation

ThP-161 **Thermal denaturation of proteins by variable-temperature electrospray ionization paired with ion mobility spectrometry-mass spectrometry**
S. Raab, T. El-Baba, D. Woodall, D. Clemmer
Indiana University, Department of Chemistry, Bloomington, USA

ThP-162 **Separation of Isomers with ultra-high-resolution ion mobility spectrometry**
C.-R. Raddatz, A. T. Kirk, S. Zimmermann
Leibniz Universität Hannover, Institute of Electrical Engineering and Measurement Technology, Sensors and Measurement Technology, Hannover, Germany

ThP-163 **Deconvolution of direct infusion TIMS-MS analyses**
P. Sander, S. Meyer
Bruker Daltonics, R&D, Bremen, Germany

ThP-164 **Ion mobility mass spectrometry for profiling and structural characterization of human hippocampus gangliosides**
M. Sarbu, Z. Vukelic´, D. Clemmer, A. D. Zamfir
National Institute for Research and Development in Electrochemistry and Condensed Matter, Department of Condensed Matter, Timisoara, Romania

ThP-165 **A computer code for optimization of Hadamard transform and Fourier transform ion mobility spectrometry experimental conditions**
A. Sarycheva, A. Adamov, S. Poteshin, A. Sysoev
National Research Nuclear University MEPhI, National Research Nuclear University MEPhI, Molecular Physics Department, Moscow, Russian Federation

ThP-166 **FAIMS-MS-IR spectroscopy workflow: a multidimensional platform for the analysis of molecular isoforms**
B. Schindler, I. Compagnon, F. Lépine
Institut Lumière Matière, Université de Lyon, Lyon, France

ThP-167 **Protomer separation, charactarization and ion-molecuele reactions using differential ion mobility**
P. Schorr, D. Volmer
Humboldt University of Berlin, Institute of Chemistry, Berlin, Germany

ThP-168 **Protein analysis using ion mobility MS and in-source ion activation combined with ECD ion fragmentation**
R. Kurulugama, V. Voinov, K. Newton, C. Klein, N. Lopez, G. Stafford, J. Beckman, J. Fjeldsted
Agilent Technologies, R&D, Santa Clara, CA, USA

ThP-169 **Analysis of insulin and insulin analogues from dried blood spots by means of LC-IM-HRMS**
A. Thomas, M. Thevis
German Sport University Cologne, Biochemistry, Cologne, Germany

ThP-170 **5 Hour single shot human proteome analysis using LC-FAIMS-MS/MS**
A. Hebert, S. Prasad, M. Belford, D. Bailey, S. Abbatiello, R. Huguet, G. Mcalister, E. Wouters, J. Dunyach, M. Westphall, J. Coon
University of Wisconsin-Madison, Biotechnology Center, Madison, USA

ThP-171 **Differentiation of Panax ginseng, Panax quinquefolius, and Ginseng products by using differential ion mobility spectrometry coupled with tandem mass spectrometry**
R. Wu, T. W. D. Chan
The Chinese University of Hong Kong, Faculty of Science, Department of Chemistry, Hong Kong

ThP-172 **Ultra-high throughput screening for engineered synthetic biology libraries based on sample chips combined with DESI MS Imaging**
C. Yan, E. Garcia-Ruiz, M. Dunston, K. Hollywood, N. Swainston, A. Jervis, E. Jones, A. Lejeune-Dodge, E. Kempa, Y. Cai, E. Takano, N. Scrutton, S. Flitsch, P. Barran
Manchester Institute of Biotechnology, University of Manchester, Manchester, United Kingdom

ThP-173 **Structural insights into potentially toxic conformations of β-Amyloid (1-42) oligomers**
R. Zangl, J. Martin, T. Lieblein, N. Morgner
Goethe University, Institute of Physical and Theoretical Chemistry, Frankfurt, Germany

ThP-174 **timsToF Pro and PASEF multiplying sequencing speed and sensitivity in mass spectrometry-based proteomics**
A. Brunner, F. Meier, S. Beck, H. Koch, M. Lubeck, N. Goedecke, M. Krause, N. Drechsler, J. Cox, O. Raether, M. Mann
Max Planck Institute of Biochemistry, Department for Proteomics and Signal Transduction, Planegg, Germany

ThP-175 **Cross section of selected extractable and leachable compounds: influence of mobile phase composition**
V. Hanot, R. Feliciano, P. Hu, C. Jones
Baxter, Mass Spectrometry, Braine L'alleud, Belgium

ThP-176 **Lipid and fatty acid isomer analysis using a travelling wave cyclic ion mobility separator**
M. Mccullagh, M. Palmer, G. Isaac, R. Mortishire-Smith, J. Langridge, J. Vissers
Waters Corporation, Wilmslow, United Kingdom

ThPS-S08 - Petroleomics, Hydrocarbons and Biofuels

ThP-177 **Detailed look in SARA fractionation: saturates, not only saturated compounds!**
Z. Farmani, W. Schrader
Max-Planck-Institut für Kohlenforschung, Mass Spectrometry dept., Mülheim a.d. Ruhr, Germany

ThP-178 **Evaluation of degradation degree of lubricating oil by thermal desorption and pyrolysis combined with DART-MS (TDP/DART-MS)**
C. Takei, Y. Otake, K. Yoshizawa
BioChromato, Inc., Application support, Fujisawa, Japan

ThPS-S09 - Materials & Nanomaterials

ThP-179 **Radicals generated by nanoparticles in contact with liquid water using spin trapping and mass spectrometry**
P. A. Clausen, V. Kofoed-Sørensen, A. W. Nørgaard, N. R. Jacobsen, K. A. Jensen
National Research Centre for the Working Environment, New Technologies, Copenhagen Ø, Denmark

ThP-180 **A novel nanocomposite coating based on sol-gel Titania/Hydroxyapatite for solid-phase microextraction coupled to GC-MS**
F. Rahmani, A. Es-Haghi, H. Mohammad-Reza Milani, A. Mollahosseini
Razi Vaccine & Serum Research Institute, Department of Physico Chemistry, Karaj, Iran

ThP-181 **Mass analysis of surface immobilizations of phenol-containing molecules through chemical modifications**
H. Hwang, I. Choi, Y. Kim, W. Yeo
Konkuk University, Department of Bioscience and Biotechnology, Seoul, Republic of Korea

ThP-182 **New binding properties of Pyridine[4]arene capsules studied by IM-MS and IRMPD**
A. Kiesilä, A. Kruve-Viil, C. Schalley, P. Barran, J. Moilanen, E. Kalenius
University of Jyväskylä, Department of Chemistry, Jyväskylä, Finland

ThP-183 **Mass spectrometric analysis of vicinal diol-containing flavonoid molecules via enrichment with boronic acid-functionalized particles**
E. Kim, J. Song, H. Mok, W. Yeo
Konkuk University, Department of bioscience and biotechnology, Seoul, Republic of Korea

ThP-184 **Spectral interferences affecting the nanoparticles determination using sp-ICP-MS**
M. Loula, A. Kana, O. Mestek
University of Chemistry and Technology Prague, Department of Analytical Chemistry, Prague, Czech Republic

ThP-185 **Influence of silica nanoparticles surface charge in MALDI-MS analysis of peptides**
S. Maghari, P. Ghezellou, A. Ghassempour
Shahid Beheshti University, Medicinal Plants and Drugs Research Institute Department: Phytochemistry, Tehran, Iran

ThP-186 **Using LDI-ToF MS for the characterization of covalently functionalized graphene**
M. B. Minameyer, D. Dasler, R. A. Schäfer, J. F. Hitzenberger, F. Hauke, T. Drewello, A. Hirsch
Friedrich-Alexander University (FAU), Physical Chemistry I, Erlangen-Nürnberg, Germany

ThP-187 **The measurement of the oxidation reaction of ferrocenes using LC-MS with ESI**
Y. Okada, M. Tsuchida
Ritsumeikan University, Department of Applied Chemistry, Kusatsu, Japan

ThP-188 **Mass spectrometry-based methods as a tool for monitoring the micro scale chemoenzymatic peptide synthes on solid support**
H. Plóciennik, P. Stefanowicz
University of Wrocław, Faculty of Chemistry, Wrocław, Poland

ThP-189 **LC-MS charecterization of dynamic combinatorial libraries of TASP molecules with novel scaffold**
G. Wolczanski, M. Modzel, P. Stefanowicz, M. Lisowski
University of Wrocław, Faculty of Chemistry, Wroclaw, Poland

ThP-190 **Elemental analysis by Au-nanoparticles enhanced LA-ICP-MS**
F. Mastrorocco, L. C. Giannossa, A. Mangone
Università di Bari, Department of Chemistry, Bari, Italy

ThPS–S10 - Novel food; nanoparticles in food and beverage; future applications

ThP-191 **A new by-product enriched in phenolic compounds, evaluated by UHPLC-HRMS, from olive mill wastewater**
G. Avellone, V. Di Stefano, M. E. Novara, R. Pitonzo
University of Palermo, STEBICEF, Palermo, Italy

ThP-192 **Optimization of espresso coffee extraction with different particle size distribution and analysis through GC-MS and HPLC-VWD**
G. Khamitova, S. Angeloni, G. Caprioli, G. Sagratini, S. Vittori
University of Camerino, Department of Chemistry and Pharmacy, Camerino, Italy

ThP-193 **Studying of phenotypic and physiological influences of abiotic stressors (TiO_2 and excess irradiaiton) on tomato plants**
J. A. Ko
Korea Institute of Toxicology, Future Environment Research Center, Jinju, Republic of Korea

ThPS–S11 - Informatics tools and data analysis

ThP-194 **TAMI Software for the provision of elemental formula from your single quadrupole GC-MS or LC-MS data**
A. Amirav, A. Fialkov, T. Alon
Tel Aviv University, School of Chemistry, Tel Aviv, Israel

ThP-195 **The database for cross-platform mining biomarkers in the brain tumor tissue**
K. Bocharov, A. Sorokin, V. Shurhkhay, I. Popov, E. Zhvansky, A. Potapov, E. Nikolaev
Moscow Institute of Physics and Technology, Laboratory of Ionic and Molecular Physics, Dolgoprudny, Russian Federation

ThP-196 **Combining GC-MS with machine learning for non-invasive cancer and disease diagnostics**
M. Cauchi
University of Limerick, Mathematics & Statistics, Limerick, Ireland

ThP-197 **One small step for Influenza – New mass-based bioinformatics and phylogenetics approach reveals insights into the evolution of the virus**
K. Downard, E. Akand
University of New South Wales, Medicine, Sydney, Australia

ThP-198 **Interoperable and scalable metabolomics data analysis with microservices**
P. Emami Khoonsari, S. Herman, M. Capuccini, M. Carone, A. Larsson, J. Burman, S. Neumann, C. Steinbeck, K. Kultima, O. Spjuth
Uppsala University, Department of Medical Sciences, Clinical Chemistry, Uppsala, Sweden

ThP-199 **Validation of analytical methods for the determination of residues in food: the stumbling block of data processing**
R. Galarini
Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche "Togo Rosati", Center for Method Development and Validation, Perugia, Italy

ThP-200 **Interfacing third party software applications to mass spectrometry data systems**
J. Goshawk, M. Mccullagh, R. Mortishire-Smith
Waters, Scientific Operations, Wilmslow, United Kingdom

ThP-201 **Metabolomic analysis of high density MS data**
A. Luterova, T. Furst, M. Strnad, J. Gruz
Palacky University, LGR, Olomouc, Czech Republic

ThP-202 **A strategy to analyze the spectral datasets of unknown compounds using mass spectral similarity network**
E. Hayakawa
Okinawa Institute of Science and Technology, Okinawa, Japan

ThP-203 **A low pulse current measurement circuit for current monitor system at mass spectrometer**
Z. H. He
Xi'an Jiaotong University, Xi'an, China

ThP-204 **DART imaging for molecular accumulations on the mud surface**
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ThP-205 **High resolution tandem mass spectrometric analysis of natural products**
E. S. Ji, K. H. Kim, G. W. Park, J. S. Yoo, J. Y. Kim
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ThP-206 **Characterising the catabolism of peptides using ion mobility enabled high resolution mass spectrometry with Mass-MetaSite integration for data processing**
J. Kirk, I. Zamora, A. Riera, T. Radchenko, A. Escola, R. Mortishire-Smith, Y. Alelyunas, M. Wrona
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ThP-207 **Semi-quantitative LC/ESI/MS analysis using predictive models of ESI ionization efficiencies**
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ThP-208 **MSIML – An Open-Source program for the visualisation and pixel-by-pixel classification of mass spectrometry imaging datasets**
L. Migas, E. Jones, R. Chapman, S. Pringle, P. Barran
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ThP-209 **Bayesian approach to automatic mass spectrum peak identification in atom probe tomography**
A. Mikhalychev, N. Lappo, A. Ulyanenkov
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ThP-210 **Demystifying match factors in library searching**
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ThP-211 **Towards automated reporting and review of metabolic pathways for large multimodal MSI studies**
T. Murta, A. Dexter, S. A. Thomas, R. T. Steven, C. J. Nikula, E. Elia, A. J. Taylor, T. Fu, A. Al-Afeef, B. Yan, R. Philip, K. N. Robinson, J. Bunch
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ThP-212 **MODplus: towards searching for hundreds of post-transnational modifications in shotgun proteomics**
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ThP-213 **Development and validation of semi-automatic MALDI-HDX sample preparation and data analysis tools**
S. Macintyre, T. Nebl
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ThP-214 **http://ms.cheminfo.org: the ultimate tool for mass spectra processing on-line**
D. Ortiz, L. Menin, L. Patiny
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ThP-215 **Comparison of high- and low-resolution MS data for direct tissue profiling: moving from a laboratory into the clinical practice**
I. Popov, A. Sorokin, E. Zhvansky, V. Eliferov, A. Vorobyev, S. Pekov, V. Shurkhay, A. Potapov, E. Nikolaev
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ThP-216 **Integration of high mass accuracy GC-ToFMS results using EI and FI ionization methods**
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ThP-217 **Beyond the acquisition of FTMS spectra - Data interpretation and visualization of accurate data from complex samples**
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ThP-218 **Automatic identification of metal-bound biomolecules using SNAP-LC, imaging, and 2D-MS**
C. Wootton, M. Willetts, Y. Lam, M. van Agthoven, M. Barrow, P. Sadler, P. O'Connor
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ThP-219 **Bacterial whole cell typing by mass spectra pattern matching with bootstrapping assessment**
Y. Yang, Y. Lin, Z. Chen, T. Gong, P. Yang, H. Girault, B. Liu, L. Qiao
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ThP-220 **Decoy methods for false discovery rate estimation in high mass accuracy peptide spectral library searches**
Z. Zhang, M. Burke, Y. Mirokhin, D. Tchekhovskoi, S. Markey, S. Stein
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ThP-221 **TiSane denoising algorithm for large dense spectra**
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ThP-222 **Validation data processing by Adverse 2.0 free software package: assessment of the analytical requirements of GC-MS method for the determination of 16 PAHs in smoked fish**
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ThP-223 **Unambiguous precursor mass assignment enables accurate and sensitive peptide identification of data-independent acquisition mass spectrometry data**
D. Mun, S. Lee
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ThP-224 **CycloBranch: an open tool for annotation of isotopic fine structures of natural products**
J. Novak, A. Skriba, J. Zapal, M. Kuzma, V. Havlicek
Czech Academy of Sciences, Institute of Microbiology, Prague, Czech Republic

ThPS–S12 - Nutraceutics directions

ThP-225 **Microwave-assisted extraction of olive leaves to obtain phenolic compounds with modulating activity of AMPk**
B. Martin-Garcia, S. Pimentel-Moral, A. M. Gomez-Caravaca, D. Arraez-Roman, A. Muñoz-de-la - peña, A. Segura-Carretero, A. Fernandez-Gutierrez
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ThP-226 **Development of isotope dilution-liquid chromatography/tandem mass spectrometry for the accurate determination of trans- and cis-vitamin K1 isomers in food**
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ThPS–S13 - Cultural heritage and archaeology

ThP-227 **Mass spectrometry analysis of medieval archaeological jewels**
M. Cechová, L. Kucera, P. Bednár
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ThP-228 **Determination of the wine and food traces from archaeological materials by GC/MS methods**
I. Farcas, Z. Moldovan, N. Pop
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ThP-229 **Stable isotope composition of the modern and fossil freshwater gastropods: implications for paleoclimate reconstructions**
A. Macrì, P. Iacumin, D. Usai, V. Linseele, S. Salvatori
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ThP-230 **Mass spectrometry studies of Theriac from "Spezieria di Santa Maria della Scala" (Rome): modern technologies to learn from the past**
L. Mattoli, E. Flamini, M. Burico, V. Mercati, R. Pagiotti, P. M. L. Vázquez de Ágredos, P. Traldi
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ThP-231 **Molecular characterization of the preparative layers of XXIInd Sarchophagus, a mass spectrometry approach**
C. Melchiorre, G. Ntasi, L. Birolo, P. Cennamo, G. Trojsi, G. Fatigati, A. Amoresano, A. Carpentieri
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