INTERNATIONAL SCHOOL on

MASS SPECTROMETRY

1st Course

High resolution mass spectrometry

Fundamentals, Advances, and Applications

EMFCSC, Erice (Italy)

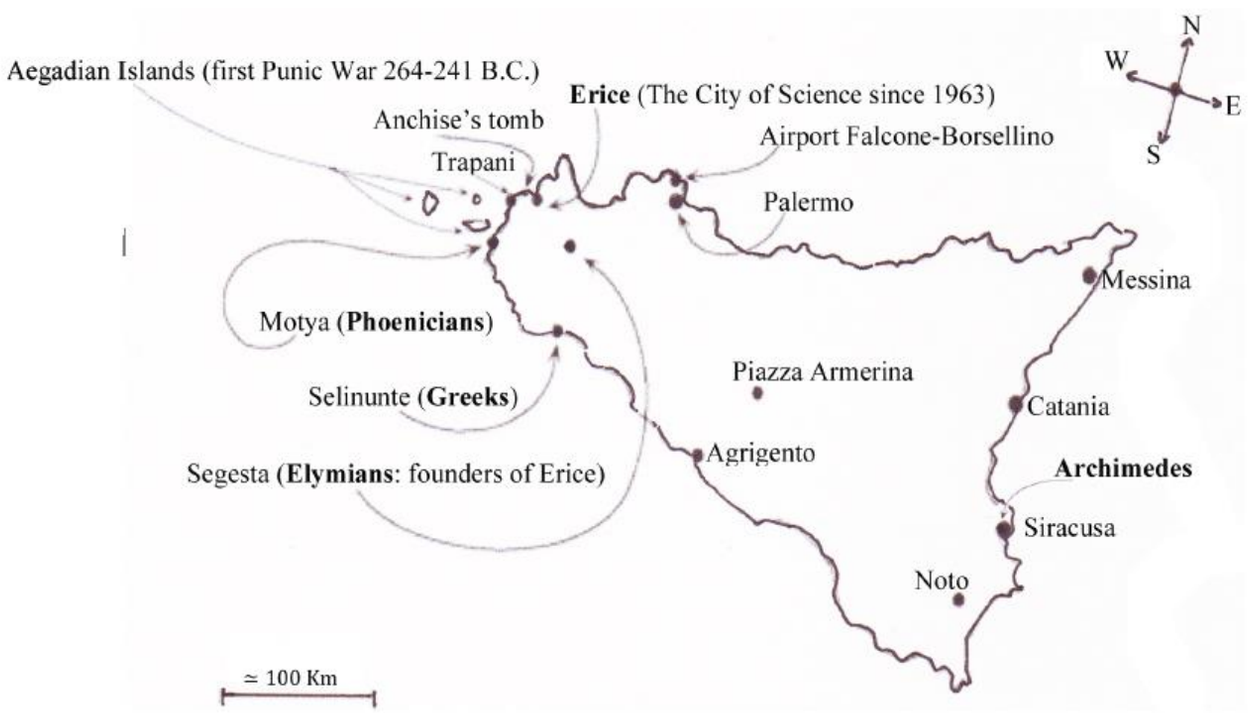
September 25-30, 2022

www.spettrometriadimassa.it/intsms2022

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

«ETTORE MAJORANA» FOUNDATION AND CENTRE FOR SCIENTIFIC CULTURE

A. ZICHICHI – PRESIDENT



Topics

- Mass analyzers: overview & perspectives
- Resolution in mass spectrometry: fundamentals & instrumentation
- TOF, FTMS and other high resolution MS: instrumentation
- Accurate mass measurements
- Data analysis
- HRMS for volatile compound characterizations
- Native mass spectrometry
- High resolution MS in Imaging MS
- Developments in biomolecular analysis
- Complex mixture analysis
- HRMS and petroleomics
- Proteomics and shotgun proteomics
- Metabolomics
- Target & untarget analysis
- Innovation in instrumentation and methodologies

Director

Gianluca Giorgi
University of Siena
Dept. of Biotechnology, Chemistry and Pharmacy
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Tutors

Richard M. Caprioli – Vanderbilt University, Nashville (USA)

Jean-François Focant – University of Liège (Belgium)

Gianluca Giorgi – University of Siena (Italy)

Anton Kaufmann – Official Food Control Authority of the Canton of Zurich (Switzerland)

Joseph A. Loo – UCLA Molecular Biology Institute, Los Angeles (USA)

Evgeny Nikolaev – Skolkovo Institute of Science and Technology, Moscow (Russia)

Peter O'Connor – University of Warwick, Coventry (United Kingdom)

Ljiljana Paša-Tolić – Pacific Northwest National Lab, Richland (USA)

Martial Rey – Institut Pasteur, Paris (France)

Ryan Rodgers – Florida State University, Tallahassee (USA)

Christian Rolando – University of Lille (France)

Simona Scarpella – Waters (Italy)

Yury Tsybin – Spectroswiss, Lausanne (Switzerland)

School program

Sunday, September 25th

12:00 ÷ 5:00 p.m.	Shuttle transfer from the airports in Trapani and Palermo	
6:00 p.m.	Registration	
6:30 p.m.	Welcome address. Presentation of the school	
7:00 p.m.	**Opening lecture:**	
	Mass spectrometry: state of the art and beyond	J. Loo
8:00 p.m.	Welcome party and dinner	

Monday, September 26th

	Analysers, HRMS fundamentals	
8:30 a.m.	**Mass analysers: an overview & perspectives**	C. Rolando
10:00 a.m.	Coffee break	
10:30 a.m.	**Resolution, resolving power, isobaric ions, nominal, monoisotopic and average masses, accurate mass measurements**	P. O'Connor
12:00 p.m.	**From accurate mass to elemental formula**	P. O'Connor
1:00 p.m.	End of session	
1:15 p.m.	Lunch	
	FT-ICR, 2D FT-ICR	
3:00 p.m.	**FT-ICR: fundamentals, phase corrections**	P. O'Connor
4:30 p.m.	Coffee break & **poster session**	
5:30 p.m.	**2D FT-ICR**	C. Rolando
7:00 p.m.	End of session	
8:00 p.m.	Dinner	

Tuesday, September 27th

	Orbitrap - ToF	
8:30 a.m.	**Orbitrap: fundamentals & advances**	Y. Tsybin
10:15 a.m.	Coffee break	
11:00 a.m.	**Time-of-Flight: fundamentals & innovations**	G. Giorgi
12:45 p.m.	End of session	
1:00 p.m.	Lunch	

	FT-ICR – Data processing - Exercises	
3:00 p.m.	**Innovation in FT-ICR**	E. Nikolaev
4:45 p.m.	Coffee break & **poster session**	
5:30 p.m.	**FTMS data processing**	Y. Tsybin
6:30 p.m.	**Exercises**: **FTMS data simulation** (with your laptop!)	Y. Tsybin
7:30 p.m.	End of session	
8:00 p.m.	Dinner	
9:15 p.m.	**Problem solving** … and drinks	

Wednesday, September 28th

	Petroleomics, Imaging MS	
8:30 a.m.	**HRMS and Petroleomics**	R. Rodgers
10:15 a.m.	Coffee break	
11:00 a.m.	**Advanced Imaging Mass Spectrometry: molecular microscopy for biology and medicine**	R. Caprioli
12:45 p.m.	End of session	
1:00 p.m.	Lunch	
	Excursion and gala dinner. Have fun!!	
2:30 p.m.	Excursion to Marsala and Selinunte: guided tour	
8:30 p.m.	Gala dinner	
11:00 p.m.	Go back to Erice	

Thursday, September 29th

	Native MS, Proteomics	
8:30 a.m.	**Native mass spectrometry**	J. Loo
10:15 a.m.	Coffee break & **poster session**	
11:00 a.m.	**Proteomics**	M. Rey
12:45 p.m.	End of session	
1:00 p.m.	Lunch	
	Short orals, GC×GC, ion mobility	
2:45 p.m.	**Short orals by students:**	
OR1 P5	**Fentalogs analysis: from structure elucidation to metabolic pathway identification by means of HPLC-HRMS/MS** *Flaminia Vincenti, Camilla Montesano, Adolfo Gregori, Fabiana Di Rosa, Manuel Sergi, Roberta Curini* Department of Public Health and Infectious Disease, Sapienza University of Rome, Rome (Italy)	
OR2 P8	**GC-MS analysis and synthesis of stable isotope-derivatives of a new 20-keto-steroid S42** *Hui-Chung Wen, Mario Thevis, Mathias Schäfer* Department of Chemistry, University of Cologne, Cologne (Germany)	
OR3 P10	**Biotransformation of phenylarsenic chemical warfare agents in Baltic Sea sediments** *Noora-Kaisa Rantanen, Anna Reunamo, Matti Kjellberg, Olga Rumbin, Hanna Niemikoski, Raisa Turja, Kari Lehtonen, Paula Vanninen* Finnish Institute for Verification of the Chemical Weapons Convention (VERIFIN), Department of Chemistry, University of Helsinki (Finland)	
OR4 P11	**Liquid chromatography coupled with negative chemical ionization tandem mass spectrometry to determine per- and polyfluoroalkyl substances (PFAS)** *Malvika Dutt, Adriana Arigò, Giorgio Famiglini, Pierangela Palma, Achille Cappiello* Dipartimento di Scienze Pure e Applicate (DiSPeA), Università degli Studi di Urbino Carlo Bo, Urbino (Italy)	
OR5 P12	**Development and validation of an µHPLC-HRMS method for the quantification of 21 per-fluoroalkyl substances (PFAS) in maize flour and milk** *C. Schiavone, R. Avolio, S. Squadrone, M. C. Abete, C. Portesi* Politecnico di Torino, Torino (Italy)	

3:40 p.m.	Coffee break		
4:10 p.m.	**Short orals by students (II)**		
OR6 P14	**Characterizing a nutritional intervention through breath metabolomics with secondary electrospray ionization-high resolution mass spectrometry** *Cedric Wüthrich, Miguel de Figueiredo, Kathryn Burton-Pimentel, Guy Vergères, Fabian Wahl, Renato Zenobi, Stamatios Giannoukos* Department of Chemistry and Applied Biosciences, ETHZ, Zurich (Switzerland)		
OR7 P18	**High-resolution-mass-spectrometric determination of phyllobilins in leaves of three medicinal plants and their application forms** *L. M. Gorfer, V. Grigoletto, M. Pramsohler, P. Robatscher, M. Oberhuber* Laimburg Research Centre, Auer (Ora), BZ (Italy)		
OR8 P20	**Hydrogen/Deuterium Exchange mass spectrometry of nucleic acids** *Matthieu Ranz, Eric Largy, Valérie Gabelica, David Monchaud* ARNA Laboratory, Inserm U1212, CNRS UMR 5320, University of Bordeaux, IECB, Bordeaux (France)		
OR9 P24	**Exploring gas-phase MS methodologies for structural elucidation of branched N-Glycan isomers** *Irina Oganesyan, Joanna Hajduk, Julian A. Harrison, Adrien Marchand, Martin F. Czar, Renato Zenobi* Laboratory of Organic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich (Switzerland)		
OR10 P40	**Unravelling amyloid beta plaque pathology associated lipid dynamics in various Alzheimer's disease mouse models** *Junyue Ge, Srinivas Koutarapu, Jörg Hanrieder* Department of Psychiatry and Neurochemistry, Sahlgrenska Academy at the University of Gothenburg (Sweden)		
5:00 p.m.	**GC×GC HRMS**	J.-F. Focant	
6:45 p.m.	**HRMS & ion mobility**	S. Scarpella	
7:15 p.m.	**Award for the best short oral!** **Award for the best poster!**		
7:30 p.m.	End of session		
8:00 p.m.	Dinner		
9:15 p.m.	**Students of the IntSMS 2022 leave their mark!**		

Friday, September 30th

	Single cell, food	
8:30 a.m.	**Single cell metabolomics**	L. Paša-Tolić
10:15 a.m.	Coffee break	
10:45 a.m.	**HRMS and Food**	A. Kaufmann
12:30 p.m.	**Concluding remarks and Arrivederci!**	
1:00 p.m.	Shuttle bus to the airports in Trapani and Palermo	

POSTER COMMUNICATIONS

P1 **Food quality assessment - a case study of tryptophan supplements: release test, targeted and non-targeted studies**

Krzysztof Stępień, Joanna Giebułtowicz

Department of Bioanalysis and Drugs Analysis, Faculty of Pharmacy, Medical University of Warsaw (Poland)

P2 **Main work activities of ICQRF Catania Laboratory**

Sabatino Leonardo

Ministero delle Politiche Agricole Alimentari e ICQRF, Catania (Italy)

P3 **Phyllobilins in fruits during ripening: qualitative analysis in the peels of apples cv. 'Gala' (*Malus* x *domestica* Borkh.) using high-resolution quadrupole-time-of-flight-mass spectrometry**

Luca Vestrucci, Lisa Marie Gorfer, Valentina Grigoletto, Valentina Lazazzara, Angelo Zanella, Peter Robatscher, Matteo Scampicchio, Michael Oberhuber

Faculty of Science and Technology, Free University of Bozen-Bolzano, Bolzano (Italy)

P4 **Oral fluid as a new investigative matrix for the determination of organic gunshot residue exposure**

Flavia Pagano, Flaminia Vincenti, Camilla Montesano, Federico Fanti, Adolfo Gregori, Roberta Curini, Manuel Sergi

Department of Public Health and Infectious Disease, Sapienza University of Rome, Rome (Italy)

P5 **Fentalogs analysis: from structure elucidation to metabolic pathway identification by means of HPLC-HRMS/MS**

Flaminia Vincenti, Camilla Montesano, Adolfo Gregori, Fabiana Di Rosa, Manuel Sergi, Roberta Curini

Department of Public Health and Infectious Disease, Sapienza University of Rome, Rome (Italy)

P6 **Determination of endocannabinoids and related compounds in brain tissues by LC-MS/MS with targeted and semi-untargeted approaches**

Federico Fanti, Flaminia Vincenti, Giulia Imparato, Camilla Montesano, Mauro Maccarrone, Dario Compagnone, Manuel Sergi

Faculty of Bioscience and Technology for Food, Agriculture and Environment, University of Teramo, Teramo (Italy)

P7 **Use of liquid chromatography associated with mass spectrometry (LC-MS/MS) to determine the composition of illegal pharmaceutical products containing anabolic-androgenic steroids**

Agnieszka Kalicka, Krzysztof Stępień, Joanna Giebułtowicz, Zbigniew Fijałek

Department of Bioanalysis and Drug Analysis, Faculty of Pharmacy, Medical University of Warsaw (Poland)

P8 **GC-MS analysis and synthesis of stable isotope-derivatives of a new 20-keto-steroid S42**

Hui-Chung Wen, Mario Thevis, Mathias Schäfer

Department of Chemistry, University of Cologne, Cologne (Germany)

P9 **Octocrylene: from sunscreens to the formation of byproducts during chlorination processes: elucidation of its degradation pathway and ecotoxicity assessment**

A. Medici, A. Siciliano, M. Guida, G. Libralato, G. Luongo, L. Previtera, G. Di Fabio, A. Zarrelli

Department of Chemical Sciences, University of Naples Federico II, Naples (Italy)

P10 **Biotransformation of phenylarsenic chemical warfare agents in Baltic Sea sediments**

Noora-Kaisa Rantanen, Anna Reunamo, Matti Kjellberg, Olga Rumbin, Hanna Niemikoski, Raisa Turja, Kari Lehtonen, Paula Vanninen

Finnish Institute for Verification of the Chemical Weapons Convention (VERIFIN), Department of Chemistry, University of Helsinki (Finland)

P11 **Liquid chromatography coupled with negative chemical ionization tandem mass spectrometry to determine per- and polyfluoroalkyl substances (PFAS)**

Malvika Dutt, Adriana Arigò, Giorgio Famiglini, Pierangela Palma, Achille Cappiello

Dipartimento di Scienze Pure e Applicate (DiSPeA), Università degli Studi di Urbino Carlo Bo, Urbino (Italy)

P12 **Development and validation of an uHPLC-HRMS method for the quantification of 21 per-fluoroalkyl substances (PFAS) in maize flour and milk**

C. Schiavone, R. Avolio, S. Squadrone, M.C. Abete, C. Portesi

Politecnico di Torino, Torino (Italy)

P13 **Anthracene analysis in water by Direct Immersion Solid Phase Microextraction Liquid Chromatography Liquid Electron Ionization Mass Spectrometry (DI-SPME-LC-LEI-MS): a multifactorial approach**

Udodinma Jude Okeke, Giorgio Famiglini, Pierangela Palma, Achille Cappiello

Department of Pure and Applied Sciences, University of Urbino Carlo Bo, Urbino (Italy)

P14 **Characterizing a nutritional intervention through breath metabolomics with secondary electrospray ionization-high resolution mass spectrometry**

Cedric Wüthrich, Miguel de Figueiredo, Kathryn Burton-Pimentel, Guy Vergères, Fabian Wahl, Renato Zenobi, Stamatios Giannoukos

Department of Chemistry and Applied Biosciences, ETHZ, Zurich (Switzerland)

P15 **Target Discovery of the triterpenoid Myrianthic Acid through a Combined Approach**

Alessandra Capuano, Erica Gazzillo, Gilda D'Urso, Vadym Samukha, Maria Giovanna Chini, Maria Valeria D'Auria, Giuseppe Bifulco, Agostino Casapullo

Dipartimento di Farmacia, Università degli Studi di Salerno, Fisciano (Italy)

P16 **From Uv-Vis to mass spectrometry: saffron molecular characterization**

Gennaro Battaglia, Michele Spinelli, Silvia Bisti, Maria Maggi, Angela Amoresano

Dept. of Chemical Sciences, University of Naples Federico II, Naples (Italy)

P17 **In depth LC-ESIMS^n-guided phytochemical analysis of *Thymus daenensis* Celak leaves**

Marzieh Rahmani Samani, Antonietta Cerulli, Milena Masullo, Sonia Piacente

Department of Pharmacy, University of Salerno, Fisciano (SA, Italy)

P18 **High-Resolution-Mass-Spectrometric Determination of Phyllobilins in Leaves of Three Medicinal Plants and their Application Forms**

L. M. Gorfer, V. Grigoletto, M. Pramsohler, P. Robatscher, M. Oberhuber

Laimburg Research Centre, Auer (Ora), BZ (Italy)

P19 **All-ion fragmentation analysis enhances the untargeted profiling of glucosinolates in Brassica microgreens by liquid chromatography and high-resolution mass spectrometry**

Andrea Castellaneta, Ilario Losito, Giovanni Cisternino, Beniamino Leoni, Pietro Santamaria, Cosima Damiana Calvano, Giuliana Bianco, Tommaso R.I. Cataldi

Dipartimento di Chimica, Università degli Studi di Bari Aldo Moro, Bari (Italy)

P20 **Hydrogen/Deuterium Exchange mass spectrometry of nucleic acids**

Matthieu Ranz, Eric Largy, Valérie Gabelica, David Monchaud

ARNA Laboratory, Inserm U1212, CNRS UMR 5320, University of Bordeaux, IECB, Bordeaux (France)

P21 **Native mass spectrometry study of helical ligands targeting non-canonical DNA structures**

Alexander König, Vincent Laffilé, Yann Ferrand, Eric Largy, Valérie Gabelica

Univ. Bordeaux, CNRS, INSERM, ARNA, UMR 5320, U1212, IECB, Bordeaux (France)

P22 **Selective acceptor binding for accurate distance determinations by gas phase transition metal FRET**

D. Svingou, J.B. Metternich, R. Zenobi

Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich (Switzerland)

P23 **ESI-MS and ESI-MS/e-HPLC combination: a tool for the rapid screening of organocatalyzed asymmetric reaction and for the elucidation of reaction mechanisms**

Martina De Angelis, Andrea Sorato, Alessia Ciogli

Dipartimento di Chimica e Tecnologie del Farmaco, Università degli Studi di Roma "La Sapienza", Roma (Italy)

P24 **Exploring gas-phase MS methodologies for structural elucidation of branched N-Glycan isomers**

Irina Oganesyan, Joanna Hajduk, Julian A. Harrison, Adrien Marchand, Martin F. Czar, Renato Zenobi

Laboratory of Organic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich (Switzerland)

P25 **Development and validation of a method for the analysis of antibiotics in bacterial extracts by LC-HRMSn**

Alexia Fataka, Thao Nhi Le, Guillaume Cazals, Mikaïl Berdi, Noémie Fayeulle, Sarah Ployon, Christine Enjalbal

Institut des Biomolécules Max Mousseron - IBMM, Université de Montpellier, Montpellier (France)

P26 **Novel analytical strategies for the characterization of peptide complexes by temperature-controlled cyclic ion mobility mass spectrometry**

P*. Bittner, V. Islami, T. Fiala, H. Wennemers, R. Zenobi*

Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich (Switzerland)

P27 **Carnosine as Cu^{2+}, Mn^{2+} and Zn^{2+} chelating ligand in aqueous solution**

Chiara Abate, Donatella Aiello, Ottavia Giuffrè, Anna Napoli, Claudia Foti

Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali, Università di Messina, Messina (Italy)

P28 **A one-step cross-linking enrichment strategy for mapping membrane protein interactions in human pathogens**

Lucienne Nouchikian, Martial Rey, Guillaume Duménil, Julia Chamot-Rooke

Mass Spectrometry for Biology Unit, Institut Pasteur, Paris (France)

P29 **Molecular characterization of allergenic proteins of fresh legumes and Mung bean isolate protein by high-resolution mass spectrometry (LC-HR/MS)**

Luisa Calcinai, Andrea Faccini, Barbara Prandi, Stefano Sforza, Tullia Tedeschi

Department of Food and Drug, University of Parma, Parma (Italy)

P30 **Chemical topography of metal-associated allergens on non-planar everyday items**

Azar Rezaei, Dhaka Bhandari, Sven Heiles, Siegfried Schindler, Bernhard Spengler

Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Giessen (Germany)

P31 **Structural basis of the pro-coagulant phenotype of prothrombin variant Arg553Trp (p.Arg596Trp - Padua 2) investigated by HDX-MS**

Andrea Pierangelini, Laura Acquasaliente, Anna Pagotto, Daniele Peterle, Paolo Simioni, Vincenzo De Filippis

Department of Pharmaceutical and Pharmacological Sciences, University of Padua, Padua (Italy)

P32 **Study of Post-Translational Modifications (PTMs) with Max Quant software**

Beatrice Aiuto, Simona Cirrincione, Elena Gosso, Laura Cavallarin, Cristina Lamberti, Andrea Mario Rossi, Chiara Portesi, Maria Gabriella Giuffrida

Consiglio Nazionale di Ricerca (CNR) – Istituto delle produzioni alimentari (ISPA) di Torino (Italy)

P33 **Investigation of the proteins of *Leishmania tropica* causing viscerotropism in humans using mass spectrometry**

Merve Beyaz, Melike Dinç, Talat Yalçin, Ahmet Özbilgin, Ibrahim Çavuş

Izmir Institute of Technology, Department of Chemistry (Turkey)

P34 **Probing the stability of the β-hairpin structure of GB1p in the gas phase by combining mass spectrometry coupled to fluorescence spectroscopy, ion mobility spectrometry and molecular dynamics simulations**

Lukas R. Benzenberg, Paul Katzberger, Ri Wu, Jonas B. Metternich, Julian Harrison, Sereina Riniker, Renato Zenobi

Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich (Switzerland)

P35 **Rapid molecular characterization of tumours and their primary tumour cell lines by Rapid Evaporative Ionization Mass Spectrometry**

Adrienn Molnár, Nóra Kucsma, Gabriel Stefan Horkovics-Kovats, Richard Schäffer, Gitta Schlosser, Gergely Szakács, Júlia Balog

ELTE Eötvös Loránd University, Institute of Chemistry, Department of Analytical Chemistry, Budapest (Hungary)

P36 **A proteomic platform unveils the brain glycogen phosphorylase as a potential metabolic target for glioblastoma multiforme**

Giusy Ferraro, Matteo Mozzicafreddo, Roberta Ettari, Lorenzo Corsi, Maria Chiara Monti

Department of Pharmacy, University of Salerno, Fisciano (Italy)

P37 ***N*-acetylaspartate release by glutaminolytic ovarian cancer cells sustains protumoral macrophages**

Alessandra Castegna, Alessio Menga, Maria Favia, Annalisa Campanella

Department of Biosciences, Biotechnologies and Biopharmaceutics, University of Bari, Bari (Italy)

P38 **DESI and/or LA-REIMS? Adjacent automated ambient techniques for the precise identification of cancer tissue**

Gabriel Stefan Horkovics-Kovats, Richard Schaffer, Csaba Hajdu, Gitta Schlosser, Julia Balog

Waters Research Center Kft, Budapest (Hungary)

P39 **Correlative chemical imaging identifies amyloid peptide signatures of neuritic plaques and dystrophy in human sporadic Alzheimer's disease**

Srinivas Koutarapu, Junyue Ge, Durga Jha, Kaj Blennow, Henrik Zetterberg, Tammaryn Lashley, Wojciech Michno, Jörg Hanrieder

Department of Psychiatry and Neurochemistry, Sahlgrenska Academy, University of Gothenburg, Mölndal (Sweden)

P40 **Unravelling amyloid beta plaque pathology associated lipid dynamics in various Alzheimer's disease mouse models**

Junyue Ge, Srinivas Koutarapu, Jörg Hanrieder

Department of Psychiatry and Neurochemistry, Sahlgrenska Academy at the University of Gothenburg (Sweden)

P41 **Development of derivatisation methods to enhance selective detection of certain compound classes**

Ibrahim Alothaim, David G. Watson, Daniel R Gaya

Saudi Food and Drug Authority, Riyadh (Saudi Arabia)

P42 **Identification and discrimination of chelated metals in oil-based paint tubes and dryers explored by ultra-high resolution MALDI FTICR mass spectrometry**

Elena Giaretta, Caterina Bordin, Manal Ridany, Fabrice Bray, Christian Rolando

Université de Lille, CNRS, USR 3290 – MSAP laboratory – Miniaturization for Synthesis Analysis & Proteomics, Lille (France)

POSTER ABSTRACTS