



**2nd Middle Eastern and Mediterranean
Sea Region Countries Mass
Spectrometry - MASSA 2013
Workshop**

SIENA (Italy), June 30 – July 4, 2013

2° Middle Eastern and Mediterranean Sea Region Countries
Mass Spectrometry - MASSA 2013 Workshop

*Società Chimica
Italiana - Divisione di
Spettrometria di
Massa*



*Romanian Society for
Mass Spectrometry*



Romanian Society for
Mass Spectrometry

*Israeli Society for
Mass Spectrometry*



*Sociedade Portuguesa
de Química*



*Hellenic Mass
Spectrometry Society*



*Russian Society for
Mass Spectrometry*



UNIVERSITÀ
DI SIENA 1240

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Scientific Committee

Gianluca Giorgi, Italy *Chairman*

Silvia Catinella, Italy *Chairman*

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The workshop is supported by:

AB Sciex



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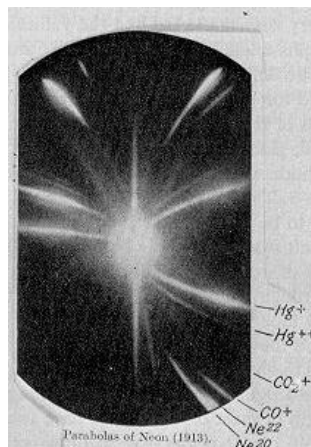
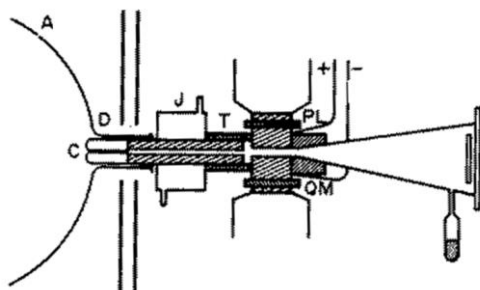


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100 years of mass spectrometry



Joseph John Thomson
Rays of positive electricity
Proceedings of the Royal Society A 89, 1-20 (1913)

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SCIENTIFIC PROGRAMME

Sunday, June 30th

- 17:00 **Registration**
- 19:30 **Welcome cocktail**

Monday, July 1st

- 9:30 **Welcome Addresses**
- Silvia Catinella**
President of the Division of Mass Spectrometry
of the Italian Chemical Society
- Maurizio Taddei**
Director of Department of Biotechnologies, Chemistry &
Pharmacy - University of Siena
- Gianluca Giorgi**
University of Siena
- 9:50 **SCI-DSM Awards Ceremony**
- 10:00 **I Session:**
Chairman: Silvia Catinella
- 10:00 **CLINICAL APPLICATIONS OF CHIP-BASED MASS SPECTROMETRY** MoPlI
Alina D. Zamfir
University of Arad (Romania)
- 10:40 **MASS QUANTIFICATION OF ANANDAMIDE AND RELATED N-ACYLETHANOLAMIDES IN PLASMA FOR CLINICAL INVESTIGATIONS** MoOrI
Ottavia Roberta, Ravelli Alessandro, Gigli Fausto, Ciuffreda Pierangela – University of Milan (Italy)
- 11:00 *Coffee break*

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- 11:30 ***II Session:***
Chairman: Leopoldo Ceraulo
- 11:30 **INVESTIGATIONS OF INTACT VIRUSES, VACCINES AND VIRUS-LIKE-PARTICLES BY MEANS OF NANOSPECIES COMBINED WITH A DIFFERENTIAL MOBILITY AND QqRTOF ANALYZER** **MoPl2**
Guenter Allmaier, Victor Weiss, Jessica Bereszczyk, Marlene Havlik, Martina Marchetti-Deschmann, Matt Kennedy, Albert Heck, Wladyslaw W. Szymanski - Vienna University of Technology, Vienna (Austria)
- 12:10 **METABOLOMIC PROFILING AND IDENTIFICATION OF BIOLOGICALLY ACTIVE COMPOUNDS IN MICROBES** **MoOr2**
Elisa Basso - Bruker Daltonics S.r.l., Macerata, IT
- 12:30 **Oral presentations of posters 1-7** (3 mins each)
- 13:00 ***End of session***
- 13:00 ***Lunch***
- 14:40 ***III Session:***
Chairman: Ornella Curcuruto
- 14:40 **WHAT'S THE FUTURE FOR MASS SPECTROMETRY IN PROTEOMICS?** **MoPl3**
Rob J Beynon - University of Liverpool (UK)
- 15:20 **IDENTIFICATION OF THE IMPURITIES OF A THERAPEUTIC MONOCLONAL ANTIBODY BY LC-MS WITH A COMBINED TOP DOWN AND BOTTOM UP APPROACH** **MoOr3**
Antonio Triolo, Francesca Boscaro, Francesca Romana Dani, Elisa Libralesso, Elena Michelucci, Giuseppe Pieraccini, Gloriano Moneti - Menarini Ricerche Spa, Firenze (Italy)
- 15:40 **Oral presentations of posters 8-15** (3 mins each)
- 16:15 ***Coffee break***

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- 16:45 **IV Session:**
Chairman: Giuseppe Avellone
- 16:45 **USE OF HIGH RESOLUTION MASS SPECTROMETRY
IN DRUG QUANTITATION AND PHARMACO-
KINETIC STUDIES** *MoPl4*
Anthony Tsarbopoulos - University of Athens (Greece)
- 17:25 **ACYLCARNITINES WITH DICARBOXYLIC ACID
RESIDUES AS POSSIBLE EARLY MARKERS FOR
NEURODEGENERATIVE SYNDROMES** *MoOr4*
*Andrea Raffaelli, Riccardo Donzelli, Alessandro Saba, Adriano
Carpita, Gabriele Siciliano* - CNR, Pisa (Italy)
- 17:45 *End of session*
- 20:00 *Social dinner*

Tuesday, July 2nd

Enjoy the Palio

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Wednesday, July 3rd

9:00 **I Session:**

Chairman: Vincenzo Cunsolo

9:00 **FROM SUPERCOMPUTER MODELING TO HIGHEST MASS RESOLUTION IN MASS SPECTROMETRY**

WePI1

Evgeny Nikolaev, Institute For Energy Problems Of Chemical Physics, Moscow (Russian Federation)

9:40 **LC COUPLED TO HIGH RESOLUTION ACCURATE MASS SPECTROMETRY AND GC-MS FOR THE DETERMINATION OF POSSIBLE CONTAMINANTS FROM FOOD CONTACT MATERIALS**

WeOr1

A. Cavazza, C. Bignardi, C. Corradini, P. Salvadeo
University of Parma(Italy)

10:00 **NEW PERSPECTIVES IN STABLE ISOTOPIC MEASUREMENTS WITH HIGH RESOLUTION GAS ISOTOPIC MASS SPECTROMETRY**

WeOr2

Lionnel Mounier - Thermo Fisher Scientific

10:20 *Coffee break*

10:50 **II Session:**

Chairman: Elisa Giocaliere

10:50 **THE BENEFITS OF ACCURATE MASS MEASUREMENTS IN GC/MS ANALYSIS OF ENVIRONMENTAL SAMPLES**

WePI2

A.T. Lebedev, V.B. Artaev, D.M. Mazur, O.V. Polyakova, M.V.Lomonosov - Moscow State University, Moscow (Russian Federation)

11:30 **VALIDATION, UNCERTAINTY AND QUALITY CONTROL OF EXAMINATIONS BY GC-MS: ACTIVE SUBSTANCE IN TEAR GAS WEAPONS**

WeOr3

Ricardo J. N. Bettencourt da Silva, Daniel M. Silveira, M. Filomena G. F. C. Camões, Carlos M. F. Borges, Pedro A. S. Salgueiro - Universidade de Lisboa (Portugal)

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- 11:50 **IDENTIFICATION TREE BASED ON
FRAGMENTATION RULES FOR STRUCTURE
ELUCIDATION OF ORGANOPHOSPHORUS ESTERS
BY ELECTROSPRAY MASS SPECTROMETRY** WeOr4
*Adrián Schwarzenberg, Farid Ichou, Richard B. Cole, Xavier
Machuron-Mandard, Christophe Junot, Denis Lesage, Jean-
Claude Tabet* - UPMC, IPCM/CSOB, Paris (France)
- 12:10 **DETERMINATION OF POLYCYCLIC AROMATIC
HYDROCARBONS IN FOOD USING PRESSURISED
LIQUID EXTRACTION AND MOLECULARLY
IMPRINTED SOLID PHASE EXTRACTION COUPLED
WITH GAS CHROMATOGRAPHY TANDEM MASS
SPECTROMETRY** WeOr5
Fangyan Li, Yai Foong Chew, Sheot Harn Chan - Food Safety
Division, Health Science Authority, Singapore
- 12:30 **USING A NOVEL ION SOURCE AND INNOVATIVE
ION OPTICS TO IMPROVE SENSITIVITY AND
SAMPLE THROUGHPUT IN ANALYSIS OF
CONTAMINANTS** WeOr6
Ariovaldo Bisi - PerkinElmer Europe Southern Region
- 12:50 *End of session*
- 13:00 *Lunch*
- 14:00 **III Session:**
Chairman: Andrea Raffaelli
- 14:00 *Poster session*
- 15:30 **TOWARDS DETECTING 10,000 PROTEINS IN
10 HOURS** WePl3
*Mohammad Pirmoradian Najafabadi, Juan Astorga-Wells,
Thorleif Lavold, Roman A. Zubarev*
Karolinska Institutet, Stockholm (Sweden)
- 16:10 **LIPIDS ANALYSIS USING DIFFERENTIAL ION
MOBILITY** WeOr7
Stefano Fiorina, Larry Campbel, Brigitte Simons
AB SCIEX Srl, Brugherio, Monza Brianza (Italy)

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- 16:30 **IN-CHAIN NEUTRAL HYDROCARBON LOSS FROM CROCINS AND DISTICTION OF POSITIONAL CROCIN ISOMERS DERIVED FROM *CROCUS SATIVUS L.* BY ESI MULTISTAGE MS** WeOr8
Nikolaos Stavros Koulakiotis, Ernst Pittenauer, Günter Allmaier, Anthony Tzarbopoulos - The Goulandris Natural History Museum, Kifissia (Greece)
- 16:50 *Coffee break*
- 17:30 *Division of Mass Spectrometry Meeting*

Thursday, July 4th

- 9:20 **I Session:**
Chairman: Alina Zamfir
- 9:20 **MASS SPECTROMETRY BASED QUANTITATIVE ANALYSIS OF PROTEIN GLYCOSYLATION PATTERN IN THE CONTEXT OF BIOMARKER RESEARCH** ThPl1
Claudia Michael, Sinia Si, Estela Gimenez-Lopez, Andreas Rizzi - University of Vienna (Austria)
- 10:00 **RESURGENCE OF DOUBLE RESONANCE FOR MECHANISTIC INTERPRETATION OF FAST CONSECUTIVE DISSOCIATIONS** ThPl2
Jean-Claude Tabet - CSOB-IPCM, Université Pierre et Marie Curie, Paris (France)
- 10:40 **ELECTROSPRAY DROPLETS AND IONS TRANSFORMATION IN 1ST VACUUM STAGE OF O-TOF MS INTERFACE** ThOr1
Viacheslav I. Kozlovskiy, Vladimir S. Brusov, Ilya V. Soulimenkov, Alexander R. Pikhtelev, Ella V. Shardakova, Michael G. Skoblin - Talrose institute for Energy Problems of Chemical Physics of Russian Academy of Sciences, Chernogolovka (Russia)
- 11:00 *Concluding remarks & Arrivederci !*

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LIST OF POSTER COMMUNICATIONS

- P1 **FABRY DISEASE – RAPID DIAGNOSIS BY CHIP-BASED NANO-ELECTROSPRAY IONIZATION TANDEM MASS SPECTROMETRY**
Sarbu Mirela, Flangea Corina, Mosoarca Cristina, Cozma Claudia, Zamfir Alina D. - University, Arad (Romania)
- P2 **COLISTIN PHARMACOKINETICS IN HUMAN PLASMA BY A NOVEL UPLC-ESI QTOF MS/MS METHODOLOGY**
Dimitrios Anagnostopoulos, Evangelos Gikas, Konstantinos Papanikolaou, Athanassios Skoutelis, George Daikos, Anthony Tsarbopoulos - The Goulandris Natural History Museum, Kifissia, (Greece)
- P3 **PATTERNS OF URINARY METHYLATED CYTOSINE DERIVATIVES IN A SAMPLE OF HEALTHY AND UNHEALTHY PEOPLE**
R. Andreoli, G. De Palma, D. Pignini, P. Mozzoni, M. Goldoni, P. Apostoli, A. Mutti - Italian Workers' Compensation Authority (INAIL), Research Center at the University of Parma (Italy)
- P4 **QTOF TANDEM MS FOR THE ANALYSIS OF DERIVATIZED AND UNDERIVATIZED OLIGOSACCHARIDES**
Roxana M. Ghiulai, Mirela Sarbu, Ioana Sisu, Eugen Sisu, Alina D. Zamfir - University of Medicine and Pharmacy "Victor Babes", Timisoara (Romania)
- P5 **ON THE VARIABILITY OF THE PROTEIN PROFILES OF COW MILK SAMPLES FROM DIFFERENT SOURCES**
Antonella Bertazzo, Giulia Costa, Martina Nanto, Roberta Seraglia, Pietro Traldi - University of Padova (Italy)
- P6 **GAS-PHASE CHARACTERIZATION OF GLYCINE-HISTIDINE CONTAINING PEPTIDE. MASS SPECTROMETRY AND THEORETICAL STUDY OF GHG AND ITS METAL COMPLEXES**
Erika Carla Pierattini, Nicola Messuti, Gianluca Giorgi - University of Siena (Italy)
- P7 **COMMON DRIVING FORCE FOR DISSOCIATIONS OF MULTIPLY-PROTONATED/DEPROTONATED PEPTIDE-DNA COMPLEXES STABILIZED BY SALT BRIDGE INTERACTIONS**
Bessem Brahim, Sandra Alves, Jean-Claude Tabet - CSOB-Institut Parisien de Chimie Moléculaire (UMR 7201- CNRS), Université Pierre et Marie Curie (UPMC), 75005 Paris, France

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- P8 **DEVELOPMENT OF CONFIRMATORY METHOD FOR ANALYSIS OF ANABOLIC STEROIDS IN BOVINE MUSCLE**
M.A. Yunin, P.S. Metalnikov, A.A. Komarov -VGNKI, Moscow (Russia)
- P9 **VENOMIC ANALYSIS OF THE PARASITOID TOXONEURON NIGRICEPS**
Granafei Sara, Bianco Giuliana, Falabella Patrizia, Riviello Lea, Larocca Marilena, Rossano Rocco, Cataldi Tommaso R.I. - Università degli Studi di Bari "Aldo Moro", Bari (Italy)
- P10 **SIMULTANEOUS DETERMINATION OF TRIPHENYLMETHANE DYES IN FISH TISSUE BY ULTRA PERFORMANCE LIQUID CHROMATOGRAPHY HIGH-RESOLUTION TIME-OF-FLIGHT MASS SPECTROMETRY**
Komarov A.A., Sorokin A.A., Metalnikov P.S., Selimov R.N. - VGNKI, Moscow (Russia)
- P11 **ROLE OF AMBIENT HUMIDITY ON THE FORMATION OF MULTICHARGED SPECIES FROM PROTEINS BY SPRAYING ACETONE IN DESI**
A. Warnet, N. Auzeil, J. C. Tabet - CSOB, IPCM CNRS, Université Pierre et Marie Curie, Paris (France)
- P12 **EVALUATION OF THE UNCERTAINTY OF ARSON DETECTION BY MASS SPECTROMETRY ASSISTED WITH MACHINE LEARNING TOOLS**
Pedro A. S. Salgueiro, Carlos M. F. S. Borges, João Aires-de-Sousa, Diogo A. R. S. Latino, Rui P. Fartaria, Ricardo J. N. B. Silva - Laboratório de Polícia Científica da Polícia Judiciária, Lisboa (Portugal)
- P13 **TRACE ANALYSIS OF UV FILTERS IN URBAN WASTEWATER TREATMENT PLANTS BY TANDEM MASS SPECTROMETRY WITH DATA DEPENDENT ACQUISITION**
Emanuele Magi, Marina Di Carro, Luca Bono - University of Genova (Italy)
- P14 **DIRECT PROBE MASS SPECTROMETRY FOR CHARACTERISATION OF ASPHALTENES**
Cristina Flego, Carla Zannoni - ENI R&M, CHIF, S. Donato Milanese (Italy)



PREMIO DSM-SCI PER L'ATTIVITÀ

La Divisione di Spettrometria di Massa della Società Chimica Italiana ha istituito a partire dall'anno 2002 il “**Premio per l'Attività**” che conferisce a personalità o gruppi di persone che nel corso della loro attività di lavoro, studio o ricerca abbiano contribuito alla crescita, promozione e diffusione della Spettrometria di Massa.

Vincitore per l'anno 2013 è il Prof.

Leopoldo Ceraulo

quale solenne riconoscimento per il costante impegno profuso nella diffusione della spettrometria di massa in Italia, nel rafforzamento della sua cultura e in particolare per l'istituzione del primo master universitario di spettrometria di massa in Italia presso l'Università di Palermo.

Vincitori delle precedenti edizioni:

- 2002: C.I.S.M. Università di Firenze - Prof. Gloriano Moneti, Dr. Giuseppe Pieraccini
- 2003: Istituto di Ricerche Farmacologiche “Mario Negri” - Prof. Silvio Garattini
- 2004: Dr. Pietro Traldi, C.N.R. Padova
- 2005: Prof. Giorgio Giacomo Mellerio, Università di Pavia
- 2006: Prof. Gianluca Giorgi, Università di Siena
- 2007: Lab. Spettr. Massa CNR - Pisa – Dr. Sergio Pucci, Dr. Andrea Raffaelli
- 2008: Prof. Francesco De Angelis, Università di L'Aquila

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FELLOWSHIPS FOR YOUNG RESEARCHERS

The Division of Mass Spectrometry of the Italian Chemical Society awarded

10 fellowships

for young researchers, with no permanent position jobs engaged in scientific or educational activities at Universities or other Research Institutes, for attending the 2° Middle Eastern and Mediterranean Sea Region Countries Mass Spectrometry - MASSA 2013 Workshop. The fellowships cover registration fee and reimbursement of expenses.