

CONFERENCE
PROGRAM

33rd IMMS 2015

Sunday, May 10th, 2015

15:00 – 19:00 *Registration*

19:00 – *Get-together party*

Monday, May 11th, 2015

8:00 – 8:45 *Registration*

Chairman: W. Danikiewicz

8:45 – 9:00 *Opening*

MoOr01 9:00 – 9:20 **M. Claeys, M. S. Shalamzari, R. Vermeylen, F. Blockhuys, T. E. Kleindienst, M. Lewandowski, R. Szmigielski, K. Rudziński, G. Spólnik, W. Danikiewicz and W. Maenhaut**

Characterization of secondary organic aerosol from green leaf volatiles at the molecular level using mass spectrometric approaches

MoOr02 9:20 – 9:40 **R. Szmigielski, P. Wach-Panfilow, G. Spólnik, K. Szmigielska, K. J. Rudziński**

Electrospray tandem mass spectrometry of aqueous-phase isoprene-derived secondary organic aerosols

MoOr03 9:40 – 10:00 **F. L. Bazzó, P. Janzsó, O. Ozohanics, L. Drahos**

Information content of tandem mass spectra

MoOr04 10:00 – 10:20 **A. Maroto, T. Josse, R. Lartia, J. De Winter, P. Gerbaux, A. Memboeuf**

Energy-resolved tandem mass spectrometry for the structural and quantitative analysis of isobaric/isomeric mixtures

10:20 – 11:00 *Coffee break*

Chairman: P. Derrick

MoOr05 11:00 – 11:20 **M. Waliczek, M. Kijewska, M. Rudowska, A. Kluczyk, P. Stefanowicz, Z. Szewczuk**

Peptides labeled with pyridinium salts for sensitive sequencing by electrospray tandem mass spectrometry

MoOr06 11:20 – 11:40 **J. Novák, V. Havlíček**

De novo identification of nonribosomal peptides from accurate product ion mass spectra

33rd IMMS 2015

MoOr07 11:40 – 12:00

L. Mark, Z. Papai, K. Banfai, J. Schmidt

The embryome: molecules in space and time during the early stage development

MoOr08 12:00 – 12:20

M. Kennedy, B. Czerski

Ion mobility mass spectrometry, from research to routine

12:20 – 14:00

Lunch

Chairman: F. De Angelis

MoOr09 14:00 – 14:20

P. J. Derrick, N. J. Demarais, D. Greenwood, A. Radionova

Investigation of protein behaviour on microsecond time-scales using dual-channel nano-electrospray emitters

MoOr10 14:20 – 14:40

G. Grasso

The application of mass spectrometry for the analysis of the cryptic peptides produced by the action of IDE on some of its substrates

MoOr11 14:40 – 15:00

M. Modzel, H. Plóciennik, P. Stefanowicz

A synthesis of new, bi-labelled peptides for quantitative proteomics

15:00 – 16:30

Coffee break and Poster session 1

Chairman: D. Kuck

MoOr12 16:30 – 16:50

J.-C. Tabet, E. Darii, S. Alves, A. Perret

Basicity and acidity influence on the stabilization of the hydrogen bond and salt bridge competitive interactions in anionic arginine/hexose-phosphate complexes

MoOr13 16:50 – 17:10

F. Tisato, V. Peruzzo, M. Porchia, C. Santini, M. Pellei, P. Traldi

ESI-MSⁿ study of the interaction products of a cytotoxic phosphino copper(I) complex with methionine-rich peptides

MoOr14 17:10 – 17:30

W. Szkutnik

Fundamentals and Advances of Orbitrap Mass Spectrometry – applications and current trends in analysis

19:30 –

Grill party

Tuesday, May 12th, 2015

Chairman: K. Vekey

- TuOr01 9:00 – 9:20 **C. Iacobucci, J.-F. Gal, S. Reale, F. De Angelis**
Studying organic reactions mechanism by ESI-MS: the case of the Ugi
and Ugi-Smiles reactions
- TuOr02 9:20 – 9:40 **K. J. Jobst, J. K. Terlouw, T. Luider, N. A. van Huizen,
P. C. Burgers**
Interaction of metal cations with alkylnitriles, alkylamines and
alkylalcohols in the gas-phase: solvation of metal ions
by the hydrocarbon chain
- TuOr03 9:40 – 10:00 **D. Kuck, D. Yang, B. Xia, Y. Jiang, W. Mei**
Fragmentation of protonated 2-(2-phenylethyl)chromones: the diagnostic
role of ion/neutral complexes
- TuOr04 10:00 – 10:20 **B. Repeć, K. Błaziak, W. Danikiewicz**
Gas-phase reactions of methyl thiocyanate and dimethyl disulfide with
carbanions
- 10:20 – 11:00 *Coffee break*

Chairman: P. Traldi

- TuOr05 11:00 – 11:20 **H. Hevér, E. Tóth, O. Ozohanics, A. Telekes, K. Vékey, L. Drahos**
Correcting long-term drifts in HPLC-MS runs
- TuOr06 11:20 – 11:40 **T. Pluháček, K. Lemr, J. Novák, O. Benada, L. Krásný, J. Pól, M.
Volný, M. Strohalm, V. Havlíček**
Imaging mass spectrometry
- TuOr07 11:40 – 12:00 **K. Pawlak, M. Kupiec, W. Jakubczak, M. Matczuk, M. Jarosz**
Mass spectrometry “on the track” of metallodrugs’ metabolism
- TuOr08 12:00 – 12:20 **P. Tarnowski**
Answers for Science. Knowledge for Life.™
- 12:20 – 14:00 *Lunch*

Chairman: V. Havlíček

- TuOr09 14:00 – 14:20 **P. Gerbaux, G. Carroy, V. Lemaux, J. De Winter, J. Cornil**
Supramolecular mass spectrometry: association of MS methods to computational chemistry to access, at a molecular level, systems relevant to host-guest chemistry
- TuOr10 14:20 – 14:40 **I. D. Kellner, T. Drewello**
Influence of single skimmer vs. dual funnel transfer on the appearance of ESI-generated LiCl cluster / β -cyclodextrin inclusion complexes
- TuOr11 14:40 – 15:00 **M. Witt**
Isotopic fine structure – a perfect tool for unambiguous molecular formula elucidation
- 15:00 – 16:30 *Coffee break and Poster session 2*

Chairman: Z. Szewczuk

- TuOr12 16:30 – 16:50 **C. Iacobucci, S. Reale, J-F Gal, F. De Angelis**
Copper(I)-catalyzed azide–alkyne cycloaddition: an ESI-MS(/MS) mechanistic investigation
- TuOr13 16:50 – 17:10 **R.W. Kirschbaum, D. Prenzel, S. Frankenberger, R.R. Tykwinski, T. Drewello**
Gas-phase experiments with polyynes: laser activation and Ag⁺-induced reactivity
- TuOr14 17:10 – 17:30 **E. Fornal**
Application of LC/QTOF in analysis of drugs, drugs candidates and new psychoactive substances

19:30 –

Conference dinner

Wednesday, May 13th, 2015

Chairman: P. Stefanowicz

- WeOr01 9:00 – 9:20 **J. Far, C. Kune, D. Cédric, E. Hanozin, D. Morsa, E. De Pauw**
Probing the liquid to gas phase structural modifications of ions
- WeOr02 9:20 – 9:40 **I. Czerwinska, J. Far, D. Morsa, N. Smargiasso, E. De Pauw**
Ruthenium-arene complexes studied by ion mobility mass spectrometry combined with CID technique
- WeOr03 9:40 – 10:00 **J.F. Hitzengerger, C. Damman, N. Lang, D. Lungerich, G. Bottari, N. Jux, T. Torres, T. Drewello**
Making the invisible visible: formate attachment to divalent metalloporphyrins
- WeOr04 10:00 – 10:20 **M. Zimnicka, M. Koliński, J. L. Sessler**
Gas-phase association modes of monopyrene tweezers through experimental and theoretical approaches
- 10:20 – 11:00 *Coffee break*

Chairman: M. Jarosz

- WeOr05 11:00 – 11:20 **M. Olejnik, L. Radko, B. Korycińska, P. Jedziniak**
Identification of metabolites of polyether antibiotic salinomycin using Q-TOF and hybrid QQQ-linear ion trap
- WeOr06 11:20 – 11:40 **P. Pomastowski, B. Buszewski**
Immobilization of silver onto lactoferrin in light of new antimicrobial application
- WeOr07 11:40 – 12:00 **P. Stalica**
Multi-dimensional chromatographic systems coupled with mass spectrometry

12:00 – 12:20 *Concluding remarks and invitation to the 34th IMMS*

12:20 – 14:00 *Lunch*

15:00 – 18:00 Excursion to the top of the Skrzyczne mountain (up by a chair lift, down either by a chair lift or on foot).

POSTERS

Monday Posters – May 11, 2015

MoPo01	<u>Zrinyi, Z.</u> , Petrovics, D., Rivnyak, A., Tamas, A., Mark, L., Kiss, T., Reglodi, D., Pirger, Z., Maasz, G.	Evolutionarily conserved neuroprotective function of pituitary adenylate cyclase-activating polypeptide (PACAP) in dopamine-based neurodegeneration
MoPo02	<u>B. Jakob</u> , E. Kristóf, K. Csomós, L. Fésüs and É. Csősz	Analysis of the protein crosslink-profile changes during neutrophil extracellular trap formation
MoPo03	Z. Timár, É. Molnár, P. Pádár, E. Beéry, A. Csorba	Generic LC-MS/MS quantification for biowaiver pharmacokinetic transport assays
MoPo04	<u>G. Bartkowiak</u> , K. Tadyszak, S. Jurga, G. Schroeder	Mass spectrometric detection of nitric oxide release from S-nitrosoglutathione and S-nitroso-N-acetyl-DL-penicillamine
MoPo05	<u>A. Godziek</u> , A. Maciejowska, T. Kowalska, E. Talik, M. Sajewicz	HPLC-MS investigation of nano- and microstructures formed from monomeric amino acids phenylglycine and cysteine as a result of oscillatory reaction
MoPo06	<u>A. Maciejowska</u> , A. Godziek, M. Sajewicz, T. Kowalska	Spontaneous oscillatory reaction of protein amino acids in an abiotic system – the LC-MS results
MoPo07	<u>M. Szala</u> , K. Czyż, R. Jędrszczyk, K. Kuna, M. Zawiązalec, T. Paździorek and J. E. Nycz	MS spectra for dyes hydroxyazoquinoline derivatives
MoPo08	<u>A. Nowok</u> , M. Piernik, J.E. Nycz	Synthesis of selected 1,10-phenanthrolines by Skraup reaction; GC-MS investigation
MoPo09	<u>K. Czyż</u> , M. Szala, R. Jędrszczyk, K. Kuna, M. Zawiązalec, T. Paździorek and J. E. Nycz	Synthesis of selected 1,10-phenanthrolines; GC/MS investigation
MoPo10	<u>P. Marczevska</u> , D. Szeremeta, J. Rzepa, M. Sajewicz	GC-MS in analysis of lavender volatile components
MoPo11	<u>D. Szeremeta</u> , P. Marczevska, J. Rzepa, M. Sajewicz	Identification of hexachlorocyclohexane biodegradation products by GC-MS
MoPo12	<u>W. Ostrowski</u> and R. Frański	Formation of curcumin molecular ion under electrospray ionisation conditions in the presence of metal cations
MoPo13	<u>V. Pashynska</u> , S. Stepanian, M. Kosevich, A. Gomory and K. Vekey	Combined model mass spectrometric and quantum chemical study of artemisinin-type agents and aspirin interactions with membrane phospholipids
MoPo14	<u>M. Zimnicka</u>	Probing molecular recognition by mass spectrometry. A case study: examination of properties of noncovalent complexes of selected melanocortin receptor ligands
MoPo15	<u>S. Golba</u> and J. Gabor	MALDI-TOF spectra of conducting polymers

MoPo16	<u>M.Cvijovic</u> , B.Nastasijevic, M.Marceta Kaninski, M.Zivkovic	GC MS and ICP MS determination of restoration formulation used for fireplace clocks
MoPo17	<u>M. Maksymiak</u> , T. Bałakier, J. Jureczak, M. Kowalczyk, G. Adamus	Molecular architecture of novel biodegradable and biocompatible control delivery systems of selected antioxidants established by electrospray ionization multistage mass spectrometry
MoPo18	<u>P.Sendys</u> and W. Danikiewicz	Gas-phase reactions of tert-butyl and cumene peroxide anions with alkyl and allyl halides
MoPo19	<u>K. Macur</u> , P. Czaplewska, I. Behrendt, M. Prądzińska	Characterization of intact anti-human cystatin C antibodies, Cyst10 and Cyst28, using the μ LC-MS/MS TRIPLETOF 5600+ system
MoPo20	<u>M. Piatkowska</u> , P. Jedziniak and J. Żmudzki	Simultaneous determination of ten illegal dyes in animal feed by high performance liquid chromatography coupled with tandem mass spectrometry
MoPo21	M. Antczak and K. Mitrowska	Impact of dwell, pause, scan event, and, loop times on measurement possibilities in multiresidue methods
MoPo22	<u>K. Błaziak</u> and W. Danikiewicz	From proton bonded dimers to absolute proton affinity values (PA) of aromatic carboxylic acids and appropriate phenide anions. Theoretical study based on DFT and multilevel calculations.
MoPo23	<u>A. Lewandowska</u> , K. Macur, P. Czaplewska , S. Ołdziej	Optimisation of the human blood serum fractionation method for the SWATH-MS analysis
MoPo24	<u>M. Roś</u> , M. Pietrowska, P. Widłak	An optimization of the MALDI-TOF analysis method for serum lipidome mass profiling in cancer research
MoPo25	<u>M. Majchrzak</u> , M. Rojkiewicz, A. Mazurkiewicz, R. Celiński, Mieczysław Sajewicz	Novel derivatives of cathinone contained in designer drugs- chromatographic and spectroscopic methods for identification
MoPo26	<u>T. Neugebauer</u> and T. Drewello	Formation and dissociation behaviour of salt-like cluster ions (sodium formate) in ESI-ion trap experiments
MoPo27	<u>V.G. Zobnina</u> , M.V. Kosevich, V.V. Chagovets and O.A. Boryak	Clustering of nitrogen bases with polyethylene glycol: electrospray mass spectrometry and computer experiment
MoPo28	<u>Z. Papai</u> , J. Schmidt, P. Avar, K. Banfai, T. Bakk, L. Mark	Maternal-embryo lipid networking during the early stage embryogenesis
MoPo29	<u>E. Jambor</u> , J. Schmidt, A. Bona, T. Tenyi, L. Mark	New salivary biomarkers of schizophrenia
MoPo30	<u>K. Banfai</u> , T. Jarai, J. Schmidt, L. Mark	Local expression of proteins in the tumor microenvironment of head neck squamous cell carcinoma

MoPo31	<u>G. Kalló</u> , T. Székely, J.A. Mótyán, Sz. Benkó, J. Tózsér and É. Csósz	Relative quantification of the human Nod-like receptor family card domain containing 5 (NLRC5) protein by targeted mass spectrometry approach
MoPo32	<u>M.V. Kosevich</u> , V.S. Shelkovsky, O.A. Boryak, V.G. Zobnina, V.S. Leontiev, V.V. Orlov, V.V. Karachevtsev, O.V. Severinovskaya and V.A. Pokrovskiy	Mass spectrometric search for silver nanoclusters in carbon nanotubes-silver composite
MoPo33	<u>Peter Avar</u>	Cell energetics with HPLC-MS
MoPo34	M. Demeyer, E. Hennebert, G. Caulier, <u>J. De Winter</u> , M. Wisztorski, I. Fournier, I. Eeckhaut, P. Flammang and P. Gerbaux	Molecular diversity and body distribution of saponins in the sea star <i>asterias rubens</i> by mass spectrometry
MoPo35	<u>T. Josse</u> , J. De Winter, P. Dubois, O. Coulembier, A. Memboeuf and P. Gerbaux	A tandem mass spectrometry-based method to assess the architectural purity of synthetic polymers: a case of a cyclic polylactide obtained by click chemistry
MoPo36	<u>A. Troć</u> , M. Zimnicka, M. Koliński, W. Danikiewicz	Analysis of β -lactams by ion mobility – mass spectrometry and theoretical calculations

Tuesday Posters – May 12, 2015

TuPo01	<u>M. Łuczak</u> , Ł. Marczak, M. Stobiecki	Mass spectrometry-based relative quantitation of chronic kidney disease plasma proteins using iTRAQ and label-free strategies
TuPo02	M. Kalinowska-Herok, M. Pietrowska, M. Gawin, M. Chekan, J. Wierzgon, G. Drazek, J. Polanska, A. Polanski, P. Widlak	Molecular characterization of oral squamous cell cancer and adjacent tissues by MALDI-IMS
TuPo03	<u>K. J. Rudzinski</u> , D. Staszek, M. Asztemborska, M. Cieślak, J. Raczko and R. Szmigielski	Troubleshooting sample preparation of <i>dendrolimus pini</i> sex pheromone for ms analysis
TuPo04	<u>D. Staszek</u> , K. J. Rudzinski, M. Asztemborska, M. Cieślak, J. Raczko and R. Szmigielski	Analysis of insect signalling using ion-trap mass spectrometry a case of <i>dendrolimus pini</i>
TuPo05	<u>P. Wach-Panfilow</u> , G. Spólnik, K. J. Rudziński, M. Shalamzari, W. Maenhaut, M. Claeys and R. Szmigielski	Exploration of aqueous organosulfates from isoprene by LC/MS/MS

TuPo06	<u>K. Lech</u>, D. Dąbrowski and M. Jarosz	Identification of tannins by HPLC-UV-VIS-ESI MS in plant dyestuffs
TuPo07	A. Dias, M. Conceição Oliveira	Characterization of Synthetic Dyes with Historical Interest by High Performance Liquid Chromatography Coupled with Diode Array Detector and High Resolution/Tandem Mass Spectrometry (HPLC-DAD-MS/MS)
TuPo08	<u>F. D. Yudin</u> and M. Culea	Accumulation and estimation of heavy metals in water, sediment and fish from Danube River, Romania
TuPo09	<u>K. Syslová</u>, M. Mikoška, J. Vondroušová, M. Haluzík and P. Kačer	Molecular insight into the postoperative state of diabetic patients
TuPo10	J. Vondroušová, K. Syslová, M. Mikoška, H. Tejkalová, J. Horáček, P. Kačer	Method development of monitoring of tryptophan and its metabolites in brain tissue of individuals with immune dysregulation and latent toxoplasmosis
TuPo11	<u>M. Mikoska</u>, K. Syslova, G. Tsenov, P. Kacer	Molecular approach to focal cerebral ischemia
TuPo12	<u>A.M. Iordache</u>, C. Voica, I. E. Geana, S. N. Suvar, R. E. Ionete, M. Culea	Assessment of heavy metals in cosmetic products for health impact
TuPo13	<u>S. Šuvar</u>, E. Horj, D. Florescu, A. Iordache, D. Cocan and M. Culea	Analysis of plasma and meat fatty acids in trout by GC/MS
TuPo14	<u>J. Beinbauer</u>, A. Hanzalová, P. Horčíčka, M. Šebela	Intact spore MALDI-TOF mass spectrometry of puccinia pathogenic fungi
TuPo15	<u>T. Pluháček</u>, M. Petřík, D. Milde and V. Havlíček	Bioimaging of ferriforms of siderophores in lung tissues by LA-ICP-MS
TuPo16	<u>E. Tóth</u>, K. Vékey, O. Ozohanics, I. Dominczyk, P. Widlak, L. Drahos	Changes of protein glycosylation in the course of radiotherapy
TuPo17	<u>D. Luptáková</u>, L. Krásný, I. Juránek and V. Havlíček	Lipid profile changes in hypoxic-ischemic neonatal rat brain identified by imaging mass spectrometry
TuPo18	<u>L. Hartmanová</u>, I. Lorencová, P. Fryčák, H. Chmelíčková, T. Ingr, V. Havlíček and K. Lemr	Lateral resolution of desorption nanoelectrospray
TuPo19	<u>Z. M. Nikolic</u>, B. Nastasijevic, D. Acimovic, T. Brdaric, G. S. Tasic, V. M. Nikolic, M. P. Marceta Kaninski	Determination of pahs content in concrete and mineral oils using UPLC/MS method
TuPo20	<u>A. Puszko</u>, B. Wileńska, A. Misicka	General profile of peptides and lipids in rat kidney

TuPo21	<u>M. Kupiec</u> , K. Pawlak	Characterisation of hydrolysis products of auranofin by ESI-MS
TuPo22	<u>M. Kupiec</u> , K. Pawlak	Probing of auranofin metabolism by single compound EC-MS
TuPo23	<u>M. Kupiec</u> , K. Pawlak	The influence of electrochemical reaction chamber on stability of gold(III) complex
TuPo24	<u>M. Waliczek</u> , M. Kijewska, P. Stefanowicz, Z. Szewczuk	Mass spectrometry as a research tool for analysis of modified peptides containing oxidized threonine
TuPo25	<u>M. Szultka-Mlynska</u> , B. Buszewski	Application of SPME-LC/MS ⁿ for metabolomics drug monitoring in biological samples
TuPo26	<u>H. Płóciennik</u> , M. Modzel, P. Stefanowicz	A new method of oxygen-18 labeling of amino acids or peptides in quantitative proteomics
TuPo27	<u>B. Wileńska</u> , A. Tomczyszyn, A. Szurpnicza and A. Misicka	The influence of platinum(II) ion on fragmentation mechanism of peptides complexed with platinum(II)
TuPo28	<u>P. Świder</u> , K. Mulewski, B. Wileńska, W. Danikiewicz	Radical anions formation in the gas phase addition-elimination reaction of phenide ions with aldehydes
TuPo29	<u>K. Brama</u> and K. Pawlak	Analysis of nicotianamine complexes by means of hilic ESI MS/MS
TuPo30	<u>L. Ceraulo</u> , D. Bongiorno, V. Turco Liveri and S. Indelicato	Ion mobility mass spectrometry of dimethyl ephedrinium bromide (DMEB) supramolecular aggregates
TuPo31	<u>A. Wojakowska</u> , Ł. Marczak, M. Chekan, K. Polanski, P. Widlak, M. Pietrowska	GC/MS profiling of FFPE tissues for screening potential metabolomic biomarkers of different thyroid cancer types
TuPo32	<u>M. Pietrowska</u> , J. Polańska, A. Wojakowska, K. Jelonek, M. Kalinowska-Herok, I. Domińczyk, E. Chawińska, T. Rutkowski, K. Składowski, L. Miszczyk, P. Widlak	Whole body response to radiation in head and neck and prostate cancer patient; the serum proteome comparative analysis
TuPo33	<u>C. Decroo</u> , M. Demeyer, G. Caulier, J. De Winter, P. Flammang, J. Cornil and P. Gerbaux	Ion mobility as a promising tool to definitively access the molecular structure of saponins
TuPo34	<u>G. Spólnik</u> , M. Kania, M. Olejnik, M. Sojka, K. Nestorowicz, A. Sobczak, L. Lipiński, A. Dziembowski, W. Danikiewicz	Differences in soil extraction effectiveness for DDT and its degradants
TuPo35	<u>G. Spólnik</u> , M. Kania, M. Olejnik, M. Sojka, K. Nestorowicz, A. Sobczak, L. Lipiński, A. Dziembowski, W. Danikiewicz	Pesticides degradation: storage in specified condition in opposite to presence in soil