



4th INTERNATIONAL MASS SPECTROMETRY SCHOOL Sitges (Barcelona, Spain) – 2019

15th -20th September 2019



4th IMS SCHOOL PROGRAM

SUNDAY, SEPTEMBER 15, 2019

17:00 - 18:00	REGISTRATION	
18:00 - 18:30	WELCOME & PRESENTATION	
18:30 - 19:00	Openin Lecture: Aspects of the History of Mass Spectrometry and One View of its Future	R.G. Cooks (Purdue University, US)
19:00 - 20:00	WELCOME COCKTAIL	

MONDAY, SEPTEMBER 16, 2019

08:30 - 09:30	Mo-1: Introduction to Mass Spectrometry	J.I. García-Alonso (University of Oviedo, Spain)
09:30 - 10:30	Mo-2: Ionization of volatile molecules: EI, CI	G. Giorgi (University of Siena, Italy)
10:30 - 11:00	Coffee break / Posters	
11:00 - 12:00	Mo-3: ESI, APCI, APPI and other atmospheric pressure ionization techniques	F. Fernández (Georgia Institute of Technology, US)
12:00 - 13:00	Mo-4: Matrix-Assited Laser Desorption/Ionization	R. Heeren (University of Maastricht, The Netherlands)
13:00 - 15:00	Lunch	
15:00 - 16:00	Mo-5: Ambient Ionization Mass Spectrometry	G. Cooks (Purdue University, US)
16:00 - 16:30	Coffee break / Posters Sessions	
16:30 - 17:30	Mo-6: Separation Techniques coupled to Mass Spectrometry	J.V. Sancho (Universitat Jaume I, Spain)
17:30 - 19:00	Beer and Science-1:	J.I. García-Alonso (University of Oviedo, Spain) M. Carrascal (IIBB-CSIC)
<p><u>Poster Flash presentations:</u></p> <p>P-58: I. Pessoa (Rio de Janeiro State University, Brazil) A practical approach for <i>in situ</i> analysis of lead isotopes in biological carbonate matrices using "LA-MC-ICP-MS"</p> <p>P-23: J. Fandiño (University of Oviedo, Spain) Pulsed Glow Discharge-Time-Of-Flight MS for the analysis of gaseous samples: Development of an innovative interface for the analysis of volatile organic compounds</p> <p>P-08: J.F. Ayala-Cabrera (University of Barcelona, Spain) Effect of dopants on the atmospheric pressure photoionization of halogenated pollutants for GC-MS determination</p> <p>P-67: D. Romero-Pérez (University of Liverpool, UK) Apta-sensors Paper Spray Mass Spectrometry For Cortisol Detection</p> <p>P-21: D. Fabregat-Safont (University Jaume I) Identification of drugs of abuse in biological fluids by direct analysis using atmospheric solids analysis probe-high resolution mass spectrometry</p> <p>P-54: N. Pardo-Mates (Laboratori Agroalimentari de Cabriels, Spain) Determination of veterinary drug residues by LC-MS/MS using Electrospray and Unispray</p> <p>P-40: A. Lores-Padín (University of Oviedo, Spain) Bioconjugated metal nanoclusters as bimodal labels to determine protein biomarkers in biological samples by LA-ICP-MS and fluorescence</p> <p>P-64: W. Puchala (Institute of Biochemistry and Biophysics Polish Academy of Sciences, Poland) HaDeX - web-server for analysis of data from hydrogen-deuterium exchange-mass spectrometry experiments</p> <p>P-01: R. Abbattista (University of Bari-Aldo Moro, Italy) Investigating keto-enolic tautomerism through H/D exchange and liquid chromatography-Fourier transform mass spectrometry: the case of olive oil secoiridoids</p> <p>P-19: S. Davison (DSTL, UK) Development of High Resolution Mass Spectrometry Database for CWC-related chemicals</p> <p>P-46: F. Martinelli (Laimburg Research Center, Italy) Polyphenols and volatile organic compounds investigation in six different apple varieties by Liquid and Gas Chromatography coupled to Mass Spectrometry</p> <p>P-44: M. Manzi (Centro de Investigaciones en Bionanociencias CIBION-CONICET, Argentina) Mass Spectrometry-based non-targeted lipidomics study for biomarker discovery in clear renal cell carcinoma</p>		

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TUESDAY, SEPTEMBER 17, 2019

08:30 – 09:30	Tu-1: Quadrupole filters and Ion Traps	<i>F. Fernández</i> (Georgia Institute of Technology, US)
09:30 – 10:30	Tu-2: High-resolution MS: FT-ICR, Orbitrap, TOF	<i>G. Giorgi</i> (University of Siena, Italy)
10:30 – 11:00	Coffee break / Posters	
11:00 – 12:00	Tu-3: Tandem Mass Spectrometry: fundamentals and dissociation mechanisms	<i>R.G. Cooks</i> (Purdue University, US)
12:00 – 15:00	Lunch/Beach	
15:00 – 15:40	"Workshop on Ion Mobility Mass Spectrometry"	
	Keynote lecture	
	We-IM-1: Ion Mobility: Where we are and where we are going	<i>F. Fernández</i> (Georgia Institute of Technology, US)
15:40 – 16:10	Companies presentations	
	We-IM-2: Linear Drift Ion Mobility Mass Spectrometry from Fundamentals to Practice: Improving Coverage and Confidence	<i>H. Florance</i> (Agilent Technologies)
16:10 – 16:40	We-IM-3: Ion Mobility-MS to Resolve and Discover Sample Complexity In Small Molecule Analysis	<i>M. McCullagh</i> (Waters)
16:40 – 17:10	We-IM-4: TimsTOF a game changer in ion mobility	<i>F. Marquez</i> (Bruker)
17:10 – 17:30	Coffee break / Posters	
17:30 – 17:35	Poster Flash presentations	
	P-27: Relationship between collision cross-section and structural characteristics for free and conjugated anabolic steroid metabolites	<i>C. Bressan</i> (IMIM, Spain)
17:35 – 17:40	P-08: Portable Ion Mobility Spectrometry to classify Cannabis plant depending on their cannabinoids content	<i>N. Jurado Campos</i> (University of Córdoba, Spain)
17:40 – 18:10	Round Table	<i>F. Fernández</i> (Georgia Institute of Technology, US). <i>Agilent Technologies, Waters, Bruker</i>
18:10 – 19:30	Beer and Science-2:	<i>J.V. Sancho</i> (Universitat Jaume I, Spain) <i>M. Carrascal</i> (IIBB-CSIC)
<p><i>Poster Flash presentations:</i></p> <p>P-45: <i>C. Marques</i> (University of Lisbon, Portugal) Mass Spectrometry contribution to metabolic studies: new insights into Montelukast metabolism</p> <p>P-83: <i>R.S.E. Young</i> (Queensland University of Technology, Australia) Discovering the missing kink: Unsaturation as a sensitive marker for metabolic changes in cancer</p> <p>P-69: <i>E. Sánchez-Jiménez</i> (IRB Barcelona, Spain) Top-down proteomics applied to human CSF</p> <p>P-20: <i>S. Eslava</i> (University of Cadiz, Spain) Endothelial progenitor cell paracrine response to atherosclerotic factors. Quantitative proteomic analysis based on label free approach</p> <p>P-17: <i>C. Contini</i> (University of Cagliari, Italy) Salivary protein profile of patients affected by dementia with lewy bodies: a Top-Down proteomic investigation</p> <p>P-18: <i>S. Cuadras</i> (Fundació IMIM, Spain) Screening of gonadotropin and growth hormone releasing factors by UPLC-MS/MS in doping control</p> <p>P-62: <i>L. Pont</i> (Fundació IMIM, Spain) Immunoaffinity purification of growth hormone-releasing hormones (GHRHs) prior to liquid chromatography mass spectrometry in urine doping controls</p> <p>P-66: <i>G. Riley</i> (University of Witwatersrand, South Africa) The analysis of alcohol biomarkers, using UPLC-MS/MS, to determine recent alcohol consumption in post-mortem vitreous humour samples</p> <p>P-59: <i>M. Picardo</i> (IDAEA-CSIC, Spain) Occurrence of natural biotoxins in Ter river water using a suspect screening method with HPLC-HRMS/MS followed by in-silico tentative identification.</p> <p>P-72: <i>G-L. Schoonraad</i> (University of Pretoria, South Africa) Synthesis and characterization of a novel graphene wool sampler for the determination of organic air pollutants</p> <p>P-09: <i>M.V. Barbieri</i> (IDAEA-CSIC, Spain) Determination of medium to highly polar pesticides residues in sediments by means of pressurized liquid extraction and LC-HESI-MS/MS</p>		

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	P-70: G. Schirinzi (IDAEA-CSIC, Spain) Analysis of polystyrene microplastics and suspected screening of polymers in environmental samples	
WEDNESDAY, SEPTEMBER 18, 2019		
08:30 – 09:30	We-1: Miniaturization in MS	G. Cooks (Purdue University, US)
09:30 – 10:30	We-2: Proteomics and Mass Spectrometry	E. Sábido (University Pompeu Fabra, Spain)
10:30 – 11:00	Coffee break / Posters	
11:00 – 12:00	We-3: Quantitative analysis in Mass Spectrometry. Isotope dilution in Mass Spectrometry	J.I. García-Alonso (University of Oviedo, Spain)
12:00 – 13:00	We-4: Quantitative analysis. Targeted proteomics	E. Sábido (University Pompeu Fabra, Spain)
13:00 – 15:00	Lunch	
	"Workshop on Imaging Mass Spectrometry"	
	Keynote lectures	
15:00 – 15:30	W-IMS-1: Ambient Imaging Mass Spectrometry	G. Cooks (Purdue University, US)
15:30 – 16:00	W-IMS-2: MALDI Imaging Mass Spectrometry	R. Heeren (University of Maastricht, The Netherlands)
	Poster Flash presentations	
16:00 – 16:05	P-72: Bioimaging of specific proteins in ocular tissue by LA-ICP-MS using isotopically-enriched silver nanoclusters as labels	E. Valencia Agudo (University of Oviedo, Spain)
16:05 – 16:10	P-13: Detection of phospholipid change with imaging mass spectrometry during early stage embryogenesis	S. Gitta (University of Pécs, Hungary)
16:10 – 16:40	Round Table	G. Cooks (Purdue University, US) R. Heeren (University of Maastricht, The Netherlands)
20:00 – 24:00	GALA DINNER	

THURSDAY, SEPTEMBER 19, 2019		
09:00 – 10:30	Th-1: Mass Spectrometry informatics 1: proteomics	M. Gay (IRB-Barcelona, Spain)
10:30 – 11:00	Coffee break / Posters	
11:00 – 12:00	Th-2: Native Mass Spectrometry - Protein complex structural analysis	M. Sharon (Weizmann Institute of Science, Israel)
12:00 – 13:00	Th-3: Mass Spectrometry in Forensic analysis	M. Bailey (University of Surrey, UK)
13:00 – 15:30	Lunch/Beach	
15:30 – 16:30	Th-4: Pharmaceuticals and drug discovery	P. Eichhorn (Almirall, Spain)
16:30 – 17:30	Th-5: Mass Spectrometry in Environmental and Food analysis	J.V. Sancho (Universitat Jaume I, Spain)
17:30 – 18:00	Coffee break / Posters	
18:00 – 19:00	Th-6: Metabolomics / Lipidomics	M. Vinaixa (University Rovira i Virgili, Spain)

FRIDAY, SEPTEMBER 20, 2019		
09:00 – 10:00	Fr-1: Mass Spectrometry Informatics 2: metabolomics	M. Vinaixa (University Rovira i Virgili, Spain)
10:00 – 11:00	Fr-2: Protein ligand interactions and structural stability analysis	M. Sharon (Weizmann Institute of Science, Israel)
11:00 – 11:30	Coffee break / Posters	
11:30 – 12:30	Closing Lecture: LC-HRMS and MALDI-TOF Imaging: The Best Choices for Emerging Contaminants Discovery and Proteomic Analysis in Wastewaters	D. Barceló (IDAEA-CSIC, Spain)
12:30 – 13:00	AWARDS AND CLOSING CEREMONY	