



SCHOOL AND WORKSHOP PROGRAM

11th July 2022 - SCHOOL

12:30 - 13:30	Registration + welcome cocktail	
13:30 - 13:40	Opening school	Carlos Cordeiro
13:45 - 14:30	Fourier Transform Ion Cyclotron Resonance Mass Spectrometry: Fundamental Concepts	Peter O'Connor
14:30 - 15:15	2D FT-MS	Christian Rolando
15:15 - 16:00	<i>Discussion over coffee</i>	
16:00 - 16:45	Fundamental concepts of Orbitrap	Alexander Makarov
16:45 - 17:30	FTMS proteomics methods for post-translational modifications	Roman Zubarev
17:30 - 18:15	MRMS in the new world of metabolomics	Carlos Cordeiro

12th July 2022 - WORKSHOP

09:30 - 10:00	Registration	
10:00 - 10:15	Opening workshop	Carlos Cordeiro & Luis Carriço
Session 1: FTMS fundamentals and instrumentation		Chair: Alexander Makarov
10:15 - 11:00	Expanding Capabilities of Orbitrap Instrumentation	Alexander Makarov
11:00 - 11:20	<i>Coffee break</i>	
11:20 - 12:05	FT Mass Spectrometer Based on Multielectrode Harmonized Kingdon trap	Evgeny Nikolaev
12:05 - 12:50	Combining Ultraviolet Photodissociation and 2-Dimensional Mass Spectrometry	Peter O'Connor
12:50 - 14:00	<i>Lunch & posters</i>	
14:00 - 14:40	FT Mass spectra simulation: Fundamentals and applications	Yury Tsybin
14:40 - 15:20	FTMS in Cultural Heritage	Christian Rolando

15:20 - 15:50	Vacuum Photoionization on an Orbitrap FTMS Platform: Prototype and Perspectives	Christopher Ruger
15:50 - 16:30	Differential Ion Mobility Spectroscopy of Metabolites	Chiraz El-Saddik
16:30 - 17:00	<i>Coffee break</i>	
Selected oral presentations		
Chair: Christopher Ruger		
17:00 - 17:15	Investigation of Asphaltenes and Asphaltene-related Materials with Thermal Analysis coupled to Fourier Transform Ion Cyclotron Resonance Mass Spectrometry	Anika Neumann
17:15 - 17:30	Linking Asphaltene characterization by LDI(+) FT-ICR MS with its stability behavior	Boniek Gontijo
17:30 - 17:45	Speciation and semi-quantification of nitrogen-containing species in complex mixtures: application to plastic pyrolysis oil	Charlotte Mase
17:45 - 18:00	Chemical characterization of wildfire particulate matter emissions by ESI/APPI FT-ICR MS	Eric Schneider
18:00 - 18:15	Investigating the insoluble organic matter in primitive chondrites using ultra-high-resolution mass spectrometry	Julien Maillard
18:15 - 18:30	Selective characterization of petroporphyrins in shipping fuels and their corresponding emissions using electron-transfer matrix-assisted laser desorption/ionization Fourier transform ion cyclotron resonance mass spectrometry	Maxime Sueur
20:30 - 22:00	<i>Gala Dinner, (supported by Bruker)</i>	

13th July 2022 - WORKSHOP

Session 2: Protein analysis and Proteomics		Chair: Francisco Amado
09:30 - 10:15	Fourier Transform Isotopic Ratio Mass Spectrometry	Roman Zubarev
10:15 - 11:00	Utilization of Fast Photo-Oxidation of Proteins and Top down Mass Spectrometry for structural characterization of proteins	Petr Novak
11:00 - 11:20	<i>Coffee break</i>	
11:20 - 12:05	Structural characterization of major donkey seminal plasma proteins with high-resolution bottom-up/top-down mass spectrometry	Janne Janis
12:05 - 12:50	Current Advances in Deep, Proteome-Wide, MS-based PISA Assay for High Throughput Identification of Drug Targets and Action Mechanisms	Massimiliano Gaetani
12:50 - 14:30	<i>Lunch (supported by Bruker)</i>	
Session 3: MRMS		Chair: Mike Easterling
14:30 - 14:50	Comprehensive top-down analysis of proteins using multi-mode fragmentation on ScimaX MRMS	Alina Theisen
14:50 - 15:30	The Paracell; optimisation and MRMS developments	Christopher Wootton
15:30 - 16:10	New insights in bitumens and lubricants characterization by Fourier transform Mass spectrometry	Carlos Afonso
16:10 - 16:30	<i>Coffee break (supported by Bruker)</i>	
Selected oral presentations		Chair: Maria Elisa Crestoni
16:30 - 16:45	Structural Characterization of Harwood Xylan with Direct-Infusion ESI FT-ICR Mass Spectrometry	Mikko Nikunen
16:45 - 17:00	Noble gas oxide cations in the gas phase - examining Ng+—O energetics (ng = Kr, Xe, Rn) by experiment and theory	Sandrina Oliveira
17:00 - 17:15	Molecular characterization of hydrophobic burned soils by ultra-high resolution mass spectrometry	Nicasio T. Jiménez-Morillo



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17:15 - 17:30	FDS – first instrument independent database for natural organic matter	Alexander Zherebker
17:30 - 17:45	PyC2MC: A Python-Based Framework for Processing Multidimensional High-Resolution Mass Spectrometry Data	Carlos M. Celis-Cornejo
17:45 - 18:00	Our metal brain: amyloid protein aggregation and metal binding	Francesca O. Bellingeri
18:00 - 18:15	Glycoproteomics of glycoengineered simple cells for the identification of bladder cancer molecular targets	André M. N. Silva
18:15 - 18:30	Dark Charge	Callan Littlejohn

14th July 2022 - WORKSHOP

Session 4: FTMS in real life		Chair: Petr Novak
09:30 - 10:15	From ESI analysis to MALDI imaging – studying lipid oxidation on a 7T MALDI FT-ICR instrument	Martina Marchetti-Deschmann
10:15 - 11:00	Salivary proteome of patients with Autoimmune Hepatitis (AIH) and Primary Biliary Cholangitis (PBC): scratching problems and solutions	Francisco Amado
11:00- 11:30	<i>Coffee break</i>	
11:30 - 12:10	LC-HRMS Analysis of Marine Biotoxins in Complex Samples	José Paulo da Silva
12:10 - 12:50	Cation- π Interactions in Ag ⁺ (Benzylamine) Complex Unveiled by IRMPD Spectroscopy and Ion-Molecule Reactions	Maria Elisa Crestoni
12:50 - 14:00	Awards by Refeyn & closing	Carlos Cordeiro & Margarida Santos-Reis
14:00 - 15:00	<i>Farewell cocktail, by Refeyn</i>	