



**ITALIAN CHEMICAL SOCIETY  
DIVISION OF MASS SPECTROMETRY**



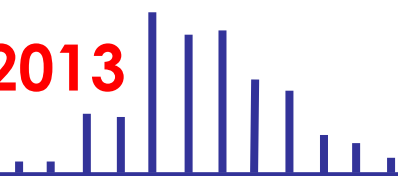
**UNIVERSITÀ  
DI SIENA**  
1240



# **1<sup>st</sup> International Mass Spectrometry School:**

**Advances in identification and structural  
characterization of bioactive molecules**

**Siena (Italy), September 15-20, 2013**



# School program

<b>Sunday, September 15</b>
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16:30	Registration	
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18:00	Opening session	
	Prof. Marcos Eberlin, President IMSF	
	Prof. Graham Cooks	
	Prof. Nico Nibbering	
	Prof. Angelo Riccaboni, Rector of the University of Siena	
	Prof. Alessandra Viviani, Rector delegate for International Relationships, Univ. of Siena	
	Prof. Maurizio Taddei, Director of the Department of Biotechnologies, Chemistry & Pharmacy, Univ. of Siena	
	Dr Silvia Catinella, President of the Division of Mass Spectrometry of the Italian Chemical Society	
	Prof. Gianluca Giorgi	

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18:30	History of mass spectrometry	Gross, Mellerio
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19:15	The future of mass spectrometry	Cooks
		Gross
		Nibbering
		Traldi

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20:30	Welcome cocktail	
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<b>Monday, September 16</b>
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***Ionization techniques: soft methods and new developments***

8:30	Soft ionization techniques: ESI, DESI, APCI. Mechanisms of ion production	Shiea
10:00	Coffee break	
10:30	Matrix-assisted laser desorption ionization	Traldi
12:00	Ambient mass spectrometry	Cooks
13:00	Lunch	

***Ionization techniques for volatile molecules.***

***Analyzers (I): beam instruments***

14:30	Ionization of volatile molecules: electron ionization (EI), chemical ionization (CI). Fragmentation processes, energetics	Nibbering / Kuck
16:00	Coffee break	
16:30	Interpretation of EI-MS and ESI-MS/MS: Fundamentals of most common dissociation reactions of molecular ions and (de)protonated molecules	Eberlin
17:45	Analyzers (I). Beam instruments: sectors, quadrupole, time-of-flight	Reid
19:00	End of session	

**Tuesday, September 17***Analyzers (II). Resolution, accurate mass measurements*

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8:30	Analyzers (II). Ion traps: multipole ion traps, FT-ICR, Orbitrap	Reid
10:30	Coffee break	
11:00	Resolution, accurate mass measurements. Examples and applications	Giorgi
13:00	Lunch	

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*Coupling MS with separation techniques. Tandem mass spectrometry (I)*

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14:30	Coupling MS with GC, GC×GC	Shiea
16:00	Coffee break	
16:30	Coupling MS (HP/UP)LC	Shiea
18:00	Tandem mass spectrometry (MS/MS) and MS <sup>n</sup> : instrumentation and methodologies (I)	Cooks
19:00	End of session	

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<b>Wednesday, September 18</b>
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***Tandem mass spectrometry (II). Fundamentals.  
Interactions of ions with electrons and surfaces***

8:30	Tandem mass spectrometry (MS/MS) and MS <sup>n</sup> : instrumentation and methodologies (II)	Gross
9:30	Fundamentals of decomposition mechanisms of even-electron ions: the role of intermediate ion-neutral complexes	Uggerud
10:30	Coffee break	
11:00	Stereochemistry and chiral recognition	De Angelis
12:00	The interaction of ions with electrons: ECD, ETD	Uggerud
13:00	Lunch	
<b><i>Peptides. MS Imaging</i></b>		
14:30	Prompt/metastable, CID, SID, ExD fragmentations of peptides and ion structures	Gross
16:00	Imaging mass spectrometry: a new view of biology	Caprioli
17:30	End of session	
17:45	<i>Urban trekking</i> in Siena: discover the Gothic magnificence and sneaking corners of the town .....	
20:30	Social dinner !	

<b>Thursday, September 19</b>
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*Ion mobility. Proteins*

8:30	Ion mobility	Ashcroft
9:45	MS and tandem MS in the characterization of proteins and their post-translational modifications	Ashcroft
11:00	Coffee break	

*Do it by yourself !*

11:30	Exercises on MS and MS/MS interpretation, mechanisms, .....	Eberlin, Cooks, Gross
	<b>Award for the best MS solver!</b>	
13:00	Lunch	

*Short orals. Ion spectroscopy*

14:30	Short orals by students	
	<b>Award for the best short oral!</b>	
14:30	Influence of remote charges on radical centres: experimental evidence for non-AUFBAU orbital occupation in gas-phase distonic ions <i>David L. Marshall, Ganna Gryn'ova, Michelle L. Coote, Stephen J. Blanksby</i>	
14:40	Mechanistic studies on an organocatalytic reaction between dialkyl 2-haloethyl-malonates and aromatic enals <i>Alexandra Tsybizova, Jana Roithová, Marek Remeš, Jan Veselý</i>	
14:50	N-methylation of indoles with DCM. ESI-MS interception of a new intermediate <i>Pedro H. Vendramini et al.</i>	
15:00	Mass spectroscopy for understanding gas phase photocatalysis <i>S. B. Sadale</i>	
15:10	Chemical reactivity assessment using reactive paper spray mass spectrometry <i>Xin Yan, Rodinei Augusti, Xin Li, R. Graham Cooks</i>	

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15:20	Pesticides screening in bee using Venturi-Assisted Laser Desorption (VALDI) for ambient ionization mass spectrometry <i>Marcos N. Eberlin, <u>Andrea F. Machado</u>, Marcos F. Franco, Nicolas V. Schwab</i>
15:30	Application of the petroleomics by ESI FT-ICR MS: monitoring of the crude oil and derivatives <i>Eduardo M. Smidt et al.</i>
15:40	Identifying important differences in mass spectra generated by time-of-flight secondary ion mass spectrometry (TOF-SIMS) in a tribochemical study <i>Elize Smit, Werner Jordaan, Stefan de Goede, Egmont R. Rohwer</i>
15:50	Collision induced dissociation of polycyclic aromatic hydrocarbons <i>K. Kulyk, M.H. Stockett, J.D. Alexander, U. Bērziņš, T. Chen, K. Farid, M. Gatchell, A. Johansson, M. Larsson, H.T. Schmidt, H. Zettergren, H. Cederquist</i>
16:00	Coffee break
16:30	Ion spectroscopy <span style="float: right;">Fornarini</span>
18:00	Short orals by students : <b>Award for the best short oral!</b>
18:00	In-chain neutral hydrocarbon loss from crocins and distinction of positional crocin isomers derived from <i>Crocus Sativus</i> L. by ESI multistage MS <i>Nikolaos Stavros Koulakiotis, Ernst Pittenauer, Günter Allmaier, Anthony Tzarbopoulos</i>
18:10	Gas-phase characterization of glycine-histidine containing peptide. mass spectrometry and theoretical study of GHG and its metal complexes <i>Erika Carla Pierattini, Nicola Messuti, Gianluca Giorgi</i>
18:20	Phosphopeptide analysis by microchip electrophoresis electrospray ionization mass spectrometry <i>Elisa Ollikainen, Nina Nordman, Sami Franssila, Tapio Kotiaho, Risto Kostiainen, Tiina Sikanen</i>
18:30	Structural characterization of <i>Mycobacterium Bovis</i> recombinant antigens by MALDI-TOF mass spectrometry <i>Verbisck, N. V.; Souza, I. I.; Kuninari-Nascimento, R.; Matida, E. T.; Ramos, C. A.; Araújo, F. R</i>

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18:40 Mass spectrometry imaging and multivariate data analysis reveal neuroplasticity of mouse-models brain  
*Karolina Škrášková, Gert Eijkel, Johannes Vogt, Myriam Baes, Paul P. Van Veldhoven, Alexey Prokudin, Stephanie de Munter, Ron M.A. Heeren*

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18:50 Proteopectidomic analysis of Bothrops jararaca venom: a breakthrough in snake venomics  
*Carolina Alves Nicolau, André Teixeira da Silva Ferreira, Paulo da Costa Carvalho, Magno Rodrigues Junqueira, Jonas Enrique Aguilar Perales, Ana Gisele da Costa Neves-Ferreira, Richard Hemmi Valente*

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19:00 End of session

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<b>Friday, September 20</b>
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*MS in life sciences and food*

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8:30	MS in diagnosis and clinical biochemistry	la Marca
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9:30	Biomarkers and drug discovery	Pioselli
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10:30	Coffee break	
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11:00	Qualitative drug metabolism	Mortishire-Smith
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12:00	Food authentication and traceability	Sindona
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13:00	Arrivederci!	
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