



Società Chimica Italiana

Programma del XXVI Congresso Nazionale della Società Chimica Italiana

Centro Congressi Hotel Ariston
Paestum (SA), 10-14 settembre 2017

- **Programma Generale delle Sessioni Plenarie e Divisionali**

Società Chimica Italiana
Roma, Italia
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PROGRAMMA GENERALE

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Eventi Sociali

Domenica 10 Settembre 2017

		<i>Sala Giunone</i>
20:30-22:30	<i>Party di benvenuto – Welcome party</i>	

Lunedì 11 Settembre 2017

		<i>Terrazze Hotel Ariston</i>
20:00-21:00	<i>Aperitivo serale</i>	

Martedì 12 Settembre 2017

		<i>Sala Giunone</i>
20.30	<i>Cena Cilentana - Typical local dinner</i>	
	<i>“Cerimonia di consegna del Premio SCI-Reaxys” Elsevier</i>	

Mercoledì 13 Settembre 2017

		<i>Sala Giunone</i>
20:30	<i>Cena Sociale – Social Dinner</i>	

Assemblee e Attività Istituzionali

Lunedì 11 Settembre 2017

18:40 – 20:00	<i>Assemblea dei Soci della Divisione di Chimica dell’Ambiente e dei Beni Culturali</i>	<i>Sala Athena</i>
18.30 - 20.00	<i>Assemblea dei Soci della Divisione di Chimica Analitica</i>	<i>Sala Paestum A</i>
18:30 - 20:00	<i>Assemblea dei Soci della Divisione di Elettrochimica</i>	<i>Sala Argiva</i>
18:30-20:00	<i>Assemblea dei Soci della Divisione di Chimica Farmaceutica</i>	<i>Sala Saturno</i>
18:30 - 20:00	<i>Assemblea dei Soci della divisione di Chimica Fisica</i>	<i>Sala Olimpia</i>
14:00 – 15:00	<i>Riunione Gruppo Interdivisionale Catalisi</i> <i>Riunione Comitato Direttivo Divisione Chimica Industriale</i>	<i>Sala Hera</i>
19:00 – 20:00	<i>Assemblea dei Soci della Divisione di Chimica Industriale</i>	<i>Sala Hera</i>
18:45 – 20:00	<i>Assemblea dei Soci della Divisione di Chimica Inorganica</i>	<i>Sala Nettuno</i>
18:30 - 20:00	<i>Assemblea dei Soci della Divisione di Chimica Organica</i>	<i>Sala Giove</i>
19.00– 20.00	<i>Assemblea dei Soci della Divisione di Chimica dei Sistemi Biologici</i>	<i>Sala Diana</i>
18:30 – 20:00	<i>Riunione Consiglio Direttivo e Assemblea dei Soci della Divisione di Didattica</i>	<i>Sala Medusa</i>

Martedì 12 Settembre 2017

11.00-15.00	<i>Riunione Consiglio Centrale SCI</i>	<i>Sala Penelope</i>
18.30-20.00	<i>Assemblea Generale dei Soci della Società Chimica Italiana</i>	<i>Auditorium Giove</i>

Mercoledì 13 Settembre 2017

17:00 – 17:30	<i>Assemblea Gruppo Senior SCI</i>	<i>Sala Diana</i>
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Sessioni Plenarie

Domenica 10 Settembre 2017

<i>Centro Congressi dell'Hotel Ariston - Paestum</i>	
10:00-14:00	<i>Registrazione</i>
<i>Auditorium Giove</i>	
14:30-15:00	<i>Cerimonia di Apertura del XXVI Congresso Nazionale SCI</i>
15:00-15:30	<i>Cerimonia di Conferimento delle Medaglie SCI</i>
<i>Chimica per la tutela dell'ambiente e del patrimonio culturale</i> <i>Chemistry for environmental protection and for preservation of cultural heritage</i>	
<i>Auditorium Giove</i>	
<i>Chairperson: Fabrizio Passarini</i>	
15:30-16:10	GEN PL01 - Martin Scheringer <i>Environmental Chemistry: Quo Vadis?</i>
16:10-16:30	GEN IL01 - Maria Cristina Facchini <i>Marine organic aerosol in Marine Boundary Layer</i>
16:30-16:50	GEN MD01 - Tiezzi SCI Medal Lecture - Nicola Armaroli <i>Light, chemistry and energy: a 20-year journey across sustainable concepts and approaches</i>
16:50-17:20	Coffee Break
<i>Chairperson: Lucia Toniolo</i>	
17:20-18:00	GEN PL02 - Koen Janssens <i>The chemistry of Pigment Degradation: Investigations at different Length Scales</i>
18:00-18:30	GEN MD02 - Cannizzaro SCI Medal Lecture - Gabriele Centi <i>Solar-driven chemistry and solar fuels: the next revolution</i>
18:20-18:40	GEN MD03 - Marotta SCI Medal Lecture - Matteo Guidotti <i>There are no evil molecules. Education and dissemination for a mitigation of "bad" Chemistry</i>
18:40-19:00	GEN MD04 - Marotta SCI Medal Lecture - Domenico Misiti <i>From the Marotta's Institute to Sapienza University passing through Camerino: Sixty years spent working in the field of chemistry</i>
19:00-19:20	GEN MD05 - Illuminati SCI Medal Lecture - Fabio Olmi <i>Far comprendere la chimica per fare amare la chimica-Elogio della didattica</i>

Lunedì 11 Settembre 2017

<i>Sala Paestum B Centro Congressi Hotel Ariston</i>	
14:00-15:00	<i>Sessione Poster 1 (consultare i programmi delle Divisioni)</i>
<i>Auditorium Giove</i>	
21:00-21:30	GEN IL02 Conferenza serale su Etica e Scienza - Enrico Bucci <i>Lies, damned lies: detecting forgeries and manipulations in published scientific images</i>

Martedì 12 Settembre 2017

<i>Sala Paestum B Centro Congressi Hotel Ariston</i>	
14:00-15:00	<i>Sessione Poster 2 (consultare i programmi delle Divisioni)</i>
<i>Auditorium Giove</i>	
<i>Sessione Plenaria-Plenary Session:</i> <i>Chimica per l'economia circolare - Chemistry for circular economy</i>	

Chairperson: Vincenzo Barone	
15:00-15:30	GEN KN01 Vincenzo Balzani <i>From a Linear to a Circular Economy. The Role of Energy</i>
15:30-16:10	GEN PL03 ChemPubSoc Europe Lecture - Ryu Abe <i>Mixed-Anion Semiconductor Photocatalysts for Visible Light Induced Water Splitting</i>
16:10-16:30	GEN MD06 Pisani SCI Medal Lecture - Gianfranco Pacchioni <i>Solid state quantum chemistry: towards the rational design of nano- and photo-catalysts</i>
16:30-17:00	Coffee Break
Chairperson: Alessandro Abboto	
17:00-17:30	GEN KN02 Anders Hagfeldt <i>The Versatility of Mesoscopic Solar Cells</i>
17:30-18:00	GEN KN03 David Peck <i>Critical materials and the circular economy. European actions and opportunities</i>
18:00-18.30	GEN MD07 Natta SCI Medal Lecture - Antonio Facchetti <i>Polymers and Polymeric Composites for Flexible Opto-Electronic Devices</i>

Mercoledì 13 Settembre 2017

Auditorium Giove	
Chimica per la salute - Chemistry for health	
Chairperson: Roberto Fattorusso	
9:00-9:40	GEN PL04 Paola Arimondo <i>Towards the reprogramming of cancer cells with chemical tools targeting DNA methylation</i>
9:40-10:10	GEN KN04 Giuseppe Legname <i>Of Prions and Other Tales</i>
10:10-10:30	GEN MD08 Bertini SCI Medal Lecture - Chiara Gabbiani <i>Exploring the cytotoxic, apoptotic and antitumoral effects of two new gold N-heterocyclic carbene-gold(I) complexes on A2780 human ovarian cancer cells</i>
10:30-11:00	Coffee Break
Chairperson: Francesco Paolucci	
11:00-11:40	GEN PL05 Aldo Roda <i>Advanced instrumentation for the astronaut health monitoring and diagnostics during long-term space exploration</i>
11:40-12:10	GEN KN05 Christian Amatore <i>Seeing, Measuring and Understanding Vesicular Exocytosis of Neurotransmitters with Micro- and Nanoelectrodes</i>
12:10-12:30	GEN MD09 Piria SCI Medal Lecture - Cesare Gennari <i>Tumor Targeting with Integrin Ligand - Drug Conjugates</i>
12:30-13:00	GEN MD10 Avogadro SCI Medal Lecture - Nino Russo <i>Can chemistry replace the scalpel? The case of photodynamic therapy</i>
13:00-14:00	Intervallo Pranzo – Lunch Break
Sala Paestum B Centro Congressi Hotel Ariston	
14:00-15:00	Sessione Poster 3 (consultare i programmi delle Divisioni)

Giovedì 14 Settembre 2017

Auditorium Giove	
Produzione sostenibile e sviluppo economico Sustainable production and economic development	
Chairperson: Vittorio Maglia	

9:00-9.20	<i>Introduction by Chairperson</i>
	<i>Mario Giacomo Levi Award ceremony, a prize of the Division of Industrial Chemistry sponsored by Federchimica in recognition of a public-private joint research project developed at industrial level.</i>
9.20-10:00	GEN PL06 Johannes A. Lercher <i>Lessons from enzymes - On the role of steric constraints and chemical environments for catalysis</i>
10:00-10:30	GEN KN06 Oliver Kappe <i>Organic Synthesis Goes Flow - The Use of Continuous Flow Technology for the Synthesis of Active Pharmaceutical Ingredients</i>
10:30-11:00	Coffee Break
<i>Chairperson: Adriana Saccone</i>	
11:00-11:30	GEN KN07 Paul T. Anastas <i>How will Green Chemistry Influence the Future?</i>
	<i>"Primo Levi Award" ceremony, a prize of the SCI Junior Group</i>
11:30-11.50	GEN IL03 Francesca Ferrazza <i>Overview of the R&D program at Eni</i>
11:50-12:10	GEN MD11 Paternò SCI Medal Lecture by Giorgio Strukul <i>Towards the Greening of Oxidation Reactions</i>
12:10-12:50	GEN PL07 David Cole-Hamilton <i>The catalytic production of chemicals from waste bio-oils</i>
12:50-13:10	<i>Cerimonia di Chiusura – Closing Ceremony</i>

Divisione di Chimica dell'Ambiente e dei Beni Culturali

Lunedì 11 Settembre 2017

<i>Sala Athena</i>	
Sessione ABC+ANA+FIS: La trasversalità della chimica per i Beni Culturali	
Chairperson Lucia Toniolo	
9:00 – 9:25	ABC/ANA/FIS KN01 Rocco Mazzeo <i>Macro Mid-Infrared total reflection (MA-FTIR) mapping for the characterization of outdoor bronze surfaces</i>
9:25 – 9:40	ABC/ANA/FIS OR01 Chiara Berlangieri <i>Formulation and characterization of hydroxypropyl guar based gel-like systems, tailored for the low impact cleaning of works of art surfaces</i>
9:40 – 9:55	ABC/ANA/FIS OR02 Pamela Ferrari <i>Chemical poly ethyl methacrylate (PEMA) organogels for the removal of pressure sensitive tapes (PSTs) from paper artworks</i>
9:55 – 10:10	ABC/ANA/FIS OR03 Nicole Bonelli <i>Surface cleaning of artworks: structure and dynamics of nanostructured fluids confined in a polymeric network</i>
10:10 – 10:25	ABC/ANA/FIS OR04 Giovanna Poggi <i>Nanocomposites for the consolidation and deacidification of cellulose-based artifacts</i>
10:30 – 11:00	Coffee Break
Chairperson Luigia Sabbatini	
11:00 – 11:25	ABC/ANA/FIS KN02 Erika Ribechini <i>GC/MS and HPLC/MS characterization of organic residues from ceramic vessels of Basque whalers of the 16th to 17th century</i>
11:25 – 11:40	ABC/ANA/FIS OR05 Francesca Di Turo <i>FIB-FESEM-EDX study of silver Roman coins: characterization of the core microstructure and corrosion products with a multi-analytical approach</i>
11:40 – 11:55	ABC/ANA/FIS OR06 Antonella Casoli <i>I materiali e la tecnica pittorica di Konrad Witz nel suo capolavoro di Ginevra</i>
11:55 – 12:10	ABC/ANA/FIS OR07 Elettra Barberis <i>Towards the Non-invasive Proteomic Analysis of Cultural Heritage and Archaeological Objects</i>
12:10 – 12:25	ABC/ANA/FIS OR08 Giuseppe Egidio De Benedetto <i>Provenance of Bitumen from different Apulian Bronze Age settlements through a biomarker based approach</i>
12:25 – 12:40	ABC/ANA/FIS OR09 Fantauzzi Marzia <i>From XAES signals to depth-profile reconstruction: the case of copper and copper alloys.</i>
12:40 – 12:55	ABC/ANA/FIS OR10 Marco Orlandi <i>Integrated approach for the chemical characterization of archaeological woods</i>
13:00 – 14:00	Intervallo Pranzo
<i>Sala Paestum B Centro Congressi Hotel Ariston</i>	
14:00-15:00	Sessione Poster I (ABC PO01 – ABC PO13)

<i>Sala Athena</i>	
<i>Sessione Valutazione dell'Impatto Ambientale e rischio chimico</i>	
<i>Chairperson Maurizio Ferretti</i>	
15:00 – 15:10	ABC OR01 Elena Badetti <i>Assessment of nano-TiO₂ colloidal stability in aqueous media by analytical techniques and principal component analysis</i>
15:10 – 15:20	ABC OR02 Beatrice Campanella <i>Thallium speciation in acid mine drainages, surface and tap water: A case study from northern Tuscany, Italy.</i>
15:20 – 15:30	ABC OR03 David Cappelletti <i>Deposition of Airborne Pollutants on Plant Leaves and Role of Plant-Bacteria Interactions in Accumulation and Degradation Processes</i>
15:30 – 15:40	ABC OR04 Federico Dallo <i>Sito di monitoraggio in alta quota nelle Dolomiti Bellunesi (Col Margherita): sistema informatico per la gestione automatizzata dei dati meteo-climatici.</i>
15:40 – 15:50	ABC OR05 Anna Maria Ferrari <i>The Environmental Performance of Natural Defatting Products Used in the Leather Tanning Cycle</i>
15:50 – 16:00	ABC OR06 Luca Ferrero <i>Aerosols along vertical profiles: an overview of ten years of research from Italy to the North Pole</i>
16:00 – 16:10	ABC OR07 Valentina Roviello <i>Radioactivity in Domitia coastal area (Southern Italy): a multidisciplinary approach.</i>
16:10 – 16:20	ABC OR08 Tiziana Siciliano <i>Single particle characterization of particulate matter: Source apportionment</i>
16:20 – 16:30	ABC OR09 Massimiliano Vardè <i>Quanto mercurio nelle acque minerali naturali della Campania?</i>
16:30 – 17:00	Coffee Break
<i>Sessione Tecnologie chimiche per l'ambiente</i>	
<i>Chairperson Antonio Proto</i>	
17:00 – 17:20	ABC KN01 Raffaele Cucciniello <i>A new passive sampler for atmospheric NO_x determination</i>
17:20 – 17:30	ABC OR10 Valentina Caratto <i>Efficiency improvement of the TiO₂ – ZnO NPs photocatalytic coupled system supported on a persistent luminescence material</i>
17:30 – 17:40	ABC OR11 David Chiaramonti <i>Thermal processing alternative of biomass residue for biochar applications</i>
17:40 – 17:50	ABC OR12 Adriano Intiso <i>Catalytic oxidation of trichloroethylene over mayenite: Influence of the preparation method on the catalytic activity.</i>
17:50 – 18:00	ABC OR13 Sante Capasso <i>Clear evidence of the Macromolecular Structure of Humic acids</i>
18:00 – 18:10	ABC OR14 Lara Nobili <i>Accelerated tests to evaluate the combined effect of aggressive saline components of atmospheric particulate matter on corrosion and metal release of weathering steel</i>
18:10 – 18:20	ABC OR15 Caterina Marcoaldi <i>Analysis and detection of emergent contaminants in seawater by passive sampling</i>
18:20 – 18:30	ABC OR16 Giuseppe Mascolo <i>Removal of emerging organic pollutants in wastewater treatment plant effluents by an electrochemical process employing boron-doped diamond electrode</i>

18:30 – 18:40	ABC OR17 Chiara Petroselli <i>Chemical characterization of freshly emitted steel plant fumes by chemical and spectroscopical methods</i>
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Martedì 12 Settembre 2017

<i>Sala Athena</i>	
Sessione Chimica per i Beni Culturali	
Chairperson Erika Ribechini	
9:00 – 9:15	ABC OR18 Isabella Lancellotti <i>Exploitation of agro-residues in designing of silicate materials</i>
9:15 – 9:30	ABC OR19 Cristina Chiavari <i>B-IMPACT: a new project for the development of eco-friendly and non-hazardous outdoor bronze protective coatings</i>
9:30 – 9:45	ABC OR20 Alessandro Ciccola <i>Synthetic pigments, binder and light: a multitechnique study on degradation of contemporary art materials</i>
9:45 – 10:00	ABC OR21 Valeria Comite <i>The assessment of the carbonaceous component in black crusts damaging the stone surfaces of historical monuments</i>
10:00 – 10:15	ABC OR22 Jeannette Lucejko <i>A comprehensive study of the effects induced by brown rot fungi on archaeological waterlogged wood</i>
10:15 – 10:30	ABC OR23 Concetta Pironti <i>Carbon Isotope Ratio in Carbonates and Bicarbonates determined by ¹³C NMR Spectroscopy</i>
10:30 – 11:00	Coffee Break
Sessione Chimica per i Beni Culturali e Valutazione dell'Impatto Ambientale	
Chairperson Antonio Marcomini	
11:00 – 11:15	ABC OR24 Emanuela Perra <i>Characterization and study of the behaviour of acrylic paint films subjected to artificial ageing: the case of Edelwachs acrylic emulsion</i>
11:15 – 11:30	ABC OR25 Chiara Petiti <i>Multianalytical study for the restoration of a gypsum sculpture of Galleria d'Arte Moderna (GAM) of Milan</i>
11:30 – 11:45	ABC OR26 Silvia Prati <i>Fully biodegradable novel bio-based organogels for the cleaning of artworks</i>
11:45 – 12:00	ABC OR27 Simona Raffo <i>Particulate matter and material decay: analysis of dry deposition on horizontal and vertical surfaces exposed through the "Deposition Box" system</i>
12:00 – 12:15	ABC OR28 Giorgia Sciutto <i>A new MA-XRF system and an advanced methodological approach for the elemental characterization of painted surfaces: the exceptional case study of the Cimabue's masterpiece</i>
12:15 – 12:30	ABC OR29 Ilaria Serafini <i>The challenge of orchil dyes: advanced analytical techniques to discriminate the different lichen species</i>
12:30 – 12:45	ABC OR30 Esmeralda Neri <i>Life Cycle Analysis of a pyrolysis process applied to end-of-life tires</i>
12:45 – 13:00	ABC OR31 Mirko Volanti <i>LCA methodology: a case study of the industrial production of terephthalic acid from renewable sources</i>

13:00 – 14:00	Intervallo Pranzo
Sala Paestum B Centro Congressi Hotel Ariston	
14:00-15:00	Sessione Poster 2 (ABC PO014 – ABC PO26)

Mercoledì 13 Settembre 2017

Sala Paestum B	
14:00-15:00	Sessione Poster 3 (ABC PO027 – ABC PO39)

Sala Athena	
ABC + ANA Sessione Processi Chimici nell'Ambiente	
Chairperson Fabrizio Passarini	
15:00 – 15:25	ABC/ANA KN01 Antonio Marcomini <i>An integrated modelling approach to study the impacts of nutrients on coastal aquatic ecosystems in the context of climate change</i>
15:25 – 15:50	ABC/ANA KN02 Davide Vione <i>Photoinduced Processes in Surface Waters: A Photochemical Mapping of Sweden</i>
15:50 – 16:10	ABC/ANA OR01 Luca Carena <i>Application of an electro-activated glassy carbon electrode (GCE) to the analytical monitoring and photochemical studying of acetaminophen</i>
16:10 – 16:30	ABC/ANA OR02 Luca Rivoira <i>Removal and photodegradation of glyphosate herbicide from waters using a mesoporous substrate with adsorbent properties</i>
16:30 – 17:00	Coffee Break
ABC + ANA Sessione Processi Chimici nell'Ambiente	
Chairperson Andrea Gambaro	
17:00 – 17:30	ABC/ANA KN03 Alessandra Genga <i>Elemental carbon, Primary and secondary organic carbon in a coastal site in South Italy.</i>
17:30 – 17:50	ABC/ANA OR03 Sara Padoan <i>Characterization of ionic composition in the submicron fraction of urban aerosol.</i>
18:10 – 18:30	ABC/ANA OR04 Mirko Severi <i>Sea salt sodium record from Talos Dome (East Antarctica) as a potential proxy of the Antarctic past sea ice extent.</i>
18:30 – 18:50	ABC/ANA OR05 Roberto Udisti <i>A six-year record of size distribution and chemical composition of Arctic aerosol. Main results and future bi-polar perspectives.</i>
18:50 – 19:10	ABC/ANA OR06 Janeth Tafur Marinos <i>Effects of biomass, temperature and thermochemical process on PAH concentration in biochar</i>
19:10 – 19:30	ABC/ANA OR07 Ezio Bolzacchini <i>Particulate and gaseous indoor contamination at the Museum of "Last Supper" of Leonardo Da Vinci: results from one year of monitoring activity</i>

Divisione di Chimica Analitica

Lunedì 11 Settembre 2017

<i>Sala Paestum A</i>	
Conferenza Plenaria Chimica Analitica	
Chair: Aldo Roda	
9.00 – 9.15	<i>Apertura Congresso della Divisione Chimica Analitica</i>
9.15 – 10.00	<i>ANA-PL0: <u>Luisa Torsi</u> Printable organic bioelectronics for bioanalytical detections at the physical limit: is this feasible?</i>
10.00 - 10.30	<i>Conferenza Vincitore del Premio Giovane Ricercatore ANA-IN01: Anna Laura Capriotti, Francesca Ferraris, <u>Susy Piovesana</u>, Riccardo Zenezini Chiozzi, Aldo Laganà Development of new polymeric magnetic nanoparticles for phosphopeptide enrichment in shotgun phosphoproteomics</i>
10.30 - 11.00	Coffee Break

Sessione Parallela: Scienza delle Separazioni	
Chair: Maria Careri	
11.00 - 11.30	<i>Finalista premio Levi ANA-IN02: <u>Anna Laura Capriotti</u> A new magnetic graphitized carbon black TiO₂ composite for phosphopeptide selective enrichment in shotgun phosphoproteomics</i>
11.30 - 12.00	<i>ANA-KN01: <u>Sara Bogialli</u>, Paolo Pastore, Luca Lucentini High Resolution mass spectrometry: the re-evolution of the risk assessment and management</i>
12.00 - 12.20	<i>ANA-OR01: <u>Tonino Caruso</u> A validated SIM GC/MS method for the simultaneous determination of linear polyalkylsiloxanes OH-terminated in octamethylcyclotetrasiloxane</i>
12.20 - 12.40	<i>ANA-OR02: <u>Giorgia La Barbera</u>, Giulia Praticò, Göezde Gurdeniz, Maj Britt Schmidt Andersen, Lars Ove Dragsted Identification of urinary biomarkers of meat and dairy products intake by means of UHPLC-QTOF/MS untargeted metabolic profiling</i>
12.40 - 13.00	<i>ANA-OR03: <u>Massimo Del Bubba</u>, Lapo Renai, Claudia Ancillotti, Lorenzo Ciofi, Daniele Rossini, Leonardo Checchini, Maria Concetta Bruzzoniti, Serena Orlandini, Donatella Fibbi, Sandra Furlanetto On-line SPE-LC-MS/MS analysis of wide-range polarity pharmaceutical compounds in aqueous matrices: problems and solutions</i>

<i>Sala Olimpia</i>	
Sessione Parallela Bioanalitica	
Chair: Mara Mirasoli	
11.00 – 11.30	<i>ANA-KN02: <u>Zangheri Martina</u>, Mara Mirasoli, Laura Anfossi, Fabio Di Nardo, Cristina Giovannoli, Massimo Guardigli, Claudio Baggiani, Aldo Roda Biosensors based on chemiluminescent-Lateral Flow Immunoassay: a powerful approach for integrated analytical platforms</i>

11.30 – 11.50	ANA-OR04: <u>Nicola Marchetti</u> , Caterina Bergantin, Annalisa Maietti, Luisa Pasti, Alberto Cavazzini <i>Insights into structure-bioaccessibility relationships of polyphenols in red chicory by HPLC-MS/MS</i>
11.50 – 12.10	ANA-OR05: <u>Marcello Manfredi</u> , Chiara Guglielmetti, Maria Mazza, Sonia Brusadore, Paolo Giuseppe Ubaldi, Luca Magnani, Stefano Gili, Emilio Marengo, Pier Luigi Acutis <i>Shotgun Proteomics for Detecting Seafood Fraud</i>
12.10 – 12.30	ANA-OR06: <u>Matteo Crosera</u> , Marcella Mauro, Elena Baracchini, Massimo Bovenzi, Francesca Larese Filon, Gianpiero AdamiPenelope <i>In vitro meningeal permeation of MnFe₂O₄ Nanoparticles</i>
12.30 – 12.50	ANA-OR07: Camilla Montesano, Gabriele Vannutelli, Federico Fanti, <u>Flaminia Vincenti</u> , Roberta Curini, Adolfo Gregori, Anna Rita Togna, Matteo Marti, Isabella Canazza, Manuel Sergi <i>Identification of MT-45 metabolites: in silico prediction, in vitro incubation with rat hepatocytes and in vivo confirmation</i>

Sala Penelope**Sessione Congiunta: Chimica Analitica - Elettrochimica - Gruppo Sensori****Chair: Aldo Roda**

11.00 - 11.20	ANA/ELE/GS-KN01: <u>Fabiana Arduini</u> , Stefano Cinti, Giorgio Scordo, Renato Massoud, Danila Moscone, Giuseppe Palleschi <i>New Sustainable and cost-effective paper-based electrochemical (bio)sensors</i>
11.20 - 11.50	ANA/ELE/GS- OR01: <u>Erika Scavetta</u> , Federica Mariani, Isacco Gualandi, Domenica Tonelli, Marta Tassarolo, Beatrice Fraboni <i>All PEDOT:PSS electrochemical transistors as a platform for sensing</i>
11.50 - 12.10	ANA/ELE/GS- OR02: <u>Alice Soldà</u> , Marco Giorgio, Pier Giuseppe Pelicci, Nicholas Dale, Francesco Paolucci, Stefania Rapino <i>Development of enzyme-based microsensors for ex vivo analyses</i>
12.10 - 12.30	ANA/ELE/GS-OR03: <u>Ornella Abollino</u> , Andrea Ruo Redda, Francesca Durbiano, Eleonora Conca, Mery Malandrino, Agnese Giacomino <i>Potential and limitations of voltammetric measurements for the characterization of electrode surface</i>
12.30 - 12.50	ANA/ELE/GS- OR04: <u>Laura Fabiani</u> , Giulia Volpe, Elisabetta Delibato, Eleonora Pucci, Silvia Piermarini, Giuseppe Palleschi <i>Development of an electrochemical magneto-immunosensor for the detection of Campylobacter: a preliminary study</i>

Sala Athena**"La Trasversalità della Chimica nei Beni Culturali"****Sessione congiunta: Chimica Analitica -Fisica - Chimica dell'Ambiente e dei Beni Culturali****Chair: Lucia Toniolo**

9.00 – 9.25	ABC/ANA/FIS-KN01: <u>Rocco Mazzeo</u> , Stjin Legrand, Giorgia Sciutto, Silvia Prati, Emilio Catelli, Paolo Oliveri, Koen Janssens <i>Macro Mid-Infrared total reflection (MA-FTIR) mapping for the characterization of outdoor bronze surfaces</i>
9.25 – 9.40	ABC/ANA/FIS-OR01: <u>Rachel Camerini</u> <i>Silica-based composites for the consolidation of earthen materials</i>
9.40 – 9.55	ABC/ANA/FIS-OR02: <u>Pamela Ferrari</u> <i>Chemical poly ethyl methacrylate (PEMA) organogels for the removal of pressure sensitive tapes (PSTs) from paper artworks</i>
9.55 – 10.10	ABC/ANA/FIS-OR03: <u>Nicole Bonelli</u>

	<i>Surface cleaning of artworks: structure and dynamics of nanostructured fluids confined in a polymeric network</i>
10.10 - 10.25	ABC/ANA/FIS-OR04: <u>Giovanna Poggi</u> <i>Nanocomposites for the consolidation and deacidification of cellulose-based artifacts</i>
10.30 - 11.00	Coffee Break
Sessione congiunta: Chimica Analitica -Fisica - Chimica dell'Ambiente e dei Beni Culturali	
Chair: Luigia Sabbatini	
11.00 - 11.25	ABC/ANA/FIS-KN02: <u>Erika Ribechini</u> , Laura Blanco-Zubiaguire, Ilaria Degano, Jacopo La Nasa, Javier García-Iñáñez, Maitane Olivares, Kepa Castro <i>GC/MS and HPLC/MS characterization of organic residues from ceramic vessels of Basque whalers of the 16th to 17th century</i>
11.25 - 11.40	ABC/ANA/FIS-OR05: <u>Francesca Di Turo</u> , Maria Teresa Doménech-Carbò, Noemí Montoya, Caterina De Vito, Fiorenzo Catalli, Gabriele Favero, Antonio Doménech-Carbò <i>FIB-FESEM-EDX study of silver Roman coins: characterization of the core microstructure and corrosion products with a multi-analytical approach</i>
11.40 - 11.55	ABC/ANA/FIS-OR06: <u>Antonella Casoli</u> , Clelia Isca, Stefano Volpin <i>I materiali e la tecnica pittorica di Konrad Witz nel suo capolavoro di Ginevra</i>
11.55 - 12.10	ABC/ANA/FIS-OR07: <u>Elettra Barberis</u> , , Marcello Manfredia, Simone Baiocco, Eleonora Conte, Fabio Gosetti, Elisa Robotti, Pier Giorgio Righetti, Emilio Marengo <i>Towards the Non-invasive Protomic Analysis of Cultural Heritage and Archaeological Objects</i>
12.10 - 12.25	ABC/ANA/FIS-OR08: <u>Giuseppe Egidio De Benedetto</u> , Antonio Pennetta, Daniela Fico <i>Provenance of Bitumen from different Apulian Bronze Age settlements through a biomarker based approach</i>
12.25 - 12.40	ABC/ANA/FIS-OR09: <u>Marzia Fantauzzi</u> , Federica Cocco, Bernhard Elsener, Gabriele Navarra, Antonella Rossi <i>From XAES signals to depth-profile reconstruction: the case of copper and copper alloys</i>
12.40 - 13.00	ABC/ANA/FIS-OR10: <u>Marco Orlandi</u> , Luca Zoia, Anika Salanti, Diego Tamburini, Jeannette Jacqueline Łucejko, Francesca Modugno, Maria Perla Colombini <i>Integrated approach for the chemical characterization of archaeological woods</i>

13.00 - 14.00	Intervallo Pranzo
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Sala Paestum B	
14.00 - 15.00	Sessione Poster 1 (ANA PO01-ANA PO40)

Sala Paestum A	
Sessione Congiunta: Chimica Analitica - Elettrochimica - Gruppo Sensori	
Chair: Salvatore Daniele	
15.00 - 15.30	ANA/ELE/GS-KN02: <u>Andreas Lesch</u> , Milica Jovic, Victor Costa Bassetto, Hubert H. Girault <i>Preparing Nanoparticles on Large Electrodes Using Inkjet Printing and Flash Light Irradiation</i>
15.30 - 15.50	ANA/ELE/GS-OR05: <u>Stefania Rapino</u> , Mirella Trinei, Alice Soldà, Marco Giorgio, Luca Bartolini, Matteo Iurlo, Massimo Marcaccio, Francesco Zerbetto, Pier Giuseppe Pelicci, Francesco Paolucci <i>Rapid, Low-cost and Portable Electrochemical Assay for Heart Injury Diagnosis</i>
15.50 - 16.10	ANA/ELE/GS-OR06: <u>Maria Rita Tomei</u> , Daniela Neagu, Fabiana Arduini, Danila Moscone

	<i>Carbon black modified screen-printed electrodes to detect chlorine dioxide.</i>
16.10 - 16.30	ANA/ELE/GS-OR07: <u>Vincenzo Mazzaracchio</u> , Daniela Neagu, Alessandro Porchetta, Giuseppe Palleschi, Daniela Moscone, Alice Pomponi, Giovanni Faggioni, Florigio Lista, Fabiana Arduini <i>Bacillus anthracis spore detection by using a label free impedimetric aptasensor</i>
16.30 - 17.00	Coffee Break
Sessione Parallela: Ambiente	
Chair: Claudio Minero	
17.00 - 17.30	ANA-KN04: <u>Silvia Becagli</u> , Fabrizio Anello, Carlo Bommarito, Federico Cassola, Giulia Calzolari, Tatiana Di Iorio, Alcide di Sarra, Jose-Luis Gómez-Amo, Franco Lucarelli, Daniela Meloni, Silvia Nava, Giandomenico Pace, Mirko Severi, Damiano Massimiliano Sferlazzo, Rita Traversi, Roberto Udisti <i>Multidisciplinary approach to constrain the ship contribution to the aerosol of the Central Mediterranean Sea</i>
17.30 - 17.50	ANA-OR08: <u>Noemi Colozza</u> , Fabiana Arduini, Danila Moscone, Giuseppe Palleschi <i>A reagent-free paper-based biosensor for the detection of mustard agents</i>
17.50 - 18.10	ANA-OR09: <u>Eleonora Conca</u> , Mery Malandrino, Agnese Giacomino, Andrea Ruo Redda, Sandro Buoso, Marco Grotti, Ornella Abollino, Roberto Udisti <i>Development of a suitable sequential extraction procedure for the assessment of the availability and reactivity of metal species in Arctic PM10 samples</i>
18.10 - 18.30	ANA-OR10: <u>Marianna Rossetti</u> , Alessandro Porchetta, Francesco Ricci, Giuseppe Palleschi <i>DNA-based single step fluorescence detection of Domoic Acid in marine water</i>

Sala Olimpia	
Sessione Parallela: Scienza delle separazioni	
Chair: Alberto Cavazzini	
15.00 – 15.30	ANA-KN05: <u>Paola Donato</u> , Veronica Inferrera, Daniele Giuffrida, Francesco Cacciola, Paola Dugo, Luigi Mondello <i>Supercritical fluid chromatography × reversed-phase liquid chromatography with quadrupole time-of-flight and ion mobility mass spectrometry detection: a proof of concept</i>
15.30 – 15.50	ANA-OR11: <u>Carmela Maria Montone</u> , Anna Laura Capriotti, Chiara Cavaliere, Riccardo Zenezini Chiozzi, Aldo Laganà <i>Development of an analytical strategy for the purification and identification of bioactive peptides from microalgae</i>
15.50 – 16.10	ANA-OR12: <u>Martina Catani</u> , Omar H. Ismail, Simona Felletti, Francesco Gasparri, Alberto Cavazzini <i>Investigation of mass transfer phenomena in new core-shell and sub-2µm fully porous chiral stationary phases for ultrafast high-performance enantioseparations</i>
16.10 – 16.30	ANA-OR13: <u>Valentina Marassi</u> , Barbara Roda, Andrea Zattoni, Sonia Casolari, Pierluigi Reschiglian <i>Integration of separation-based analytical platforms in the development of nanomaterials as bioactive products</i>
16.30 – 17.00	Coffee Break
Sessione Parallela: Equilibri in soluzione e speciazione	
Chair: Concetta De Stefano	
17.00 – 17.20	ANA-OR14: <u>Emilia Furia</u> , Rosangela Elliani, Luana Malacaria, Antonio Tagarelli <i>Coumarin-3-carboxylic acid as ligand: acid-base properties, interactions with Fe³⁺ and characterization of complexes in aqueous solution</i>

17.20 – 17.40	ANA-OR15: <u>Denis Badocco</u> , Valerio Di Marco, Alfonso Venzo, Marco Frascioni, Paolo Pastore <i>Ion pair formation between tertiary aliphatic amines and perchlorate in the biphasic H₂O / CH₂Cl₂ system</i>
17.40 – 18.00	ANA-OR16: Clemente Bretti, <u>Rosalia Maria Cigala</u> , Francesco Crea, Concetta De Stefano, Giuseppe Gattuso, Anna Irto, Gabriele Lando, Demetrio Milea, Silvio Sammartano <i>Acid-base and chelating properties of Gantrez copolymers</i>
18.00 – 18.20	ANA-OR17: <u>Gaetano De Tommaso</u> , Mauro Iuliano, Lucia De Rosa, Luca Domenico D'Andrea, Alessandra Romanelli, Gaetano Malgieri, Carla Isernia <i>Coordination of a bis-histidine oligopeptide with Ga³⁺ ion in aqueous solution</i>

Sala Cassandra**Sessione congiunta: Chimica analitica - Spettrometria di massa****Chair: Tommaso Cataldi**

15.00 – 15.30	ANA/MAS-KN01: <u>Cosima Damiana Calvano</u> , Marco Glaciale, S. Granafei, Anna Maria Sardanelli, Luana Bellanova, Antonella Mastrorocco, Francesco Palmisano, Tommaso R.I Cataldi <i>Advanced mass spectrometric techniques for the untargeted lipidome characterization of fibroblasts in early on-set Parkinson's disease patients</i>
15.30 – 15.50	ANA/MAS-OR01: <u>Simone Nicolardi</u> , Yuri E.M. van der Burgt, Jeroen D.C. Codée, Manfred Wuhrer, Cornelis, H. Hokke, Fabrizio Chiodo <i>Structural characterization of bio-functionalized gold nanoparticles by ultrahigh resolution mass spectrometry</i>
15.50 – 16.10	ANA/MAS-OR02: Lucia Cenci, Graziano Guella, <u>Alessandra Maria Bossi</u> <i>Molecularly imprinted materials coupled to MALDI-TOF Mass Spectrometry for the targeted analysis of peptides and proteins</i>
16.10 – 16.30	ANA/MAS-OR03: <u>Rossana Scarpone</u> , Roberta Rosato, Federico Bacá, Manuel Sergi, Dario Compagnone <i>Unknown and non-target analysis to determine pesticides in fruit and vegetables by means of UHPLC-HRMS (Orbitrap)</i>
16.30 – 17.00	Coffee Break

Sessione Congiunta: Chimica analitica – Spettrometria di Massa**Chair: Paola Montoro**

17.00 – 17.30	ANA/MAS-KN02: <u>Danilo Sciarrone</u> , Antonino Schepis, Luigi Mondello <i>Advanced analytical capabilities exploiting isotope ratio mass spectrometry and quadrupole mass spectrometry coupled to multidimensional gas chromatography</i>
17.30 – 17.50	ANA/MAS-OR04: <u>Andreina Ricci</u> , Paola Cimino, Anna Troiani, Federico Pepi, Stefania Garzoli, Chiara Salvitti and Vincenzo Barone <i>From ascorbic acid to furan molecules: a theoretical and experimental study on the gas phase acid catalyzed degradation of vitamin C</i>
17.50 – 18.10	ANA/MAS-OR05: <u>Veronica Termopoli</u> , Pierangela Palma, Giorgio Famigliani, Maurizio Piergiovanni, Achille Cappiello <i>Liquid-EI (LEI) Atmospheric Pressure Mechanism for the introduction of liquid streams into an unmodified electron ionization source of a mass spectrometer</i>
18.10 – 18.30	ANA/MAS-OR06: <u>Chiara Salvitti</u> , Andreina Ricci, Federico Pepi, Stefania Garzoli, Anna Troiani, Giulia De Petris, Marzio Rosi <i>Selective gas-phase conversion of D-fructose to 5-hydroxymethylfuraldehyde through a base-assisted dehydration</i>

Martedì 12 Settembre 2017

<i>Sala Paestum A</i>	
Sessione Parallela: Sensori	
Chair: Danila Moscone	
9.00 – 9.30	ANA-KN07: <u>Giannetto Marco</u> <i>Nanobiocomposite-based immunosensors for clinically significant biomarkers</i>
9.30 – 9.50	ANA-OR18: <u>Maria Pesavento</u> , Nunzio Cennamo, Luigi Zeni, Simone Marchetti <i>Development of a new platform for chemical sensors based on surface plasmon resonance and molecularly imprinted polymers as receptors</i>
9.50 – 10.10	ANA-OR19: <u>Patrizia Mussini</u> , Serena Arnaboldi, Ivo Franco Buzzi, Mariacristina La Bianca, Gabriella Natale, Silvia Cauteruccio, Emanuela Licandro, Voichita Mihali, Francesco Sannicolò, Simona Rizzo, Armando Gennaro, Abdirisak Ahmed Isse <i>Enantioselective voltammetry on achiral electrodes: a comparison between inherently chiral additives based on different stereogenic element</i>
10.10 – 10.30	ANA-OR20: Paolo Bollella, Dmitry M. Hushpulian, Dónal Leech, Massimo Marcaccio, Gabriele Favero, Franco Mazzei, Lo Gorton, <u>Riccarda Antiochia</u> <i>Hydrogen peroxide sensitive and selective biosensors based on peroxidases from different sources wired by Os-polymer</i>
10.30 – 11.00	Coffee Break
Sessione Parallela: Metodologie Avanzate per la Bioanalitica	
Chair: Emilio Marengo	
11.00 – 11.30	ANA-KN08: <u>Gosetti Fabio</u> <i>Target and non-target LC-MS/MS strategies in environment, food and human health fields</i>
11.30 – 11.50	ANA-OR21: <u>Ilario Losito</u> , Laura Facchini, Tommaso R.I. Cataldi, Francesco Palmisano <i>Seasonal variations of major phospholipids in mussels of sp. Mytilus galloprovincialis: an investigation by hydrophilic interaction liquid chromatography-electrospray ionization Fourier-transform mass spectrometry</i>
11.50 – 12.10	ANA-OR22: <u>Carlo Crescenzi</u> , Giuliana Grasso, Francesco Iadaresta, Erik Holmgren <i>Applications of Porous Graphitic Carbon in liquid chromatography – mass spectrometry</i>
12.10 – 12.30	ANA-OR23: <u>Pasquale Palladino</u> , Maria Grazia Manera, Roberto Rella, Maria Minunni, Simona Scarano <i>Synthetic receptors for Troponin T detection by SPR transduction for acute myocardial infarction diagnosis</i>
12.30 - 12.50	ANA-OR24: <u>Contado Catia</u> <i>Nano- and micro-particles in food and consumer products: the role of the Field Flow Fractionation techniques in their characterization</i>
12.50 – 13.10	ANA-OR25: <u>Daniela Cecconi</u> , Marcello Manfredi, Jessica Brandi, Emilio Marengo <i>Evaluation and comparison of gel-based and gel-free approaches for the in-depth exploration of milk rice proteome</i>

13.00 - 14.00	Intervallo Pranzo
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<i>Sala Olimpia</i>	
Sessione Parallela: Ambiente	
Chair: Carlo Crescenzi	

9.00 – 9.30	ANA-KN09: <u>Marco Grotti</u> , Andrea Bazzano, Francisco Ardini, Kris Latruwe, Frank Vanhaecke <i>New insight into the Pb and Sr isotopic compositions of environmental samples from polar regions via single- and multi-collector inductively coupled plasma mass spectrometry</i>
9.30 – 9.50	ANA-OR26: <u>Francesco Iadaresta</u> , Michele Manniello, Conny Östman, Carlo Crescenzi, Jan Holmbäck, Paola Russo <i>Aromatic Amines in Textile as Potential Threat for Human Health</i>
9.50 – 10.10	ANA-OR27: <u>Attilio Naccarato</u> , Antonella Tassone, Sacha Moretti, Rosangela Elliani, Francesca Sprovieri, Nicola Pirrone, Antonio Tagarelli <i>A greener approach for organophosphate flame retardant determination in airborne particulate matter: microwave-assisted extraction using hydroalcoholic mixture coupled with solid phase microextraction gas chromatography tandem mass spectrometry</i>
10.10 – 10.30	ANA-OR28: <u>Ivan Notardonato</u> , Mario Vincenzo Russo, Pasquale Avino <i>Ultrasound-Vortex-Assisted Liquid-Liquid Micro-Extraction for Simultaneous Determination of Organophosphorus Pesticides and Phthalates in Baby Foods</i>
10.30 – 11.00	Coffee Break

Sessione Parallela: Ambiente

Chair: Gianpiero Adami

11.00 – 11.20	ANA-OR29: <u>Marina Di Carro</u> , Barbara Benedetti, Cristiana Mirasole, Emanuele Magi <i>Calibration of commercial and modified Polar Organic Chemical Integrative Samplers (POCIS) for the analysis of emerging pollutants in waters</i>
11.20 – 11.40	ANA-OR30: <u>Pascale Raffaella</u> , Bianco Giuliana, Caniani Donatella, Masi Salvatore, Buchicchio Alessandro, Caivano Marianna, Ignazio M. Mancini, Mazzone Giuseppina, Tecla Marinelli <i>A new validated gas chromatographic-barrier ionization discharge detector (GC-BID) method for the monitoring of CO₂ and N₂O emissions from settling and disinfection units in wastewater treatment plants (WWTPs)</i>
11.40 – 12.00	ANA-OR31: <u>Sandro Recchia</u> , Carla Tiraboschi, Simone Tumiati, Carlo Dossi, Stefano Poli <i>Development of a prototype analytical apparatus for the quantitative determination of the composition of fluids in synthetic rocks</i>
12.00 – 12.20	ANA-OR32: <u>Andrea Speltini</u> , Francesca Merlo, Matteo Contini, Federica Maraschi, Michela Sturini, Lorenzo Malavasi, Antonella Profumo <i>Solid-phase extraction of trace glucocorticoids from environmental waters on silica-supported humic acids-derived carbons followed by HPLC-ESI-MS</i>
12.20 - 12.40	ANA-OR33: Alessandro Tinti, Lorenza, Corbella, Cristina Colombi, Eleonora Cuccia, Vorne Gianelle, Satoshi Takahama, Stefania Gilardoni, <u>Paola Fermo</u> <i>Aliphatic Amines In Atmospheric Aerosol: Sources And Distribution</i>
12.40 – 13.00	ANA-OR34: <u>Rita Traversi</u> , Silvia Becagli, Laura Caiazzo, Massimo Chiari, Giulia Calzolari, Fabio Giardi, Franco Lucarelli, Angelo Lupi, Mauro Mazzola, Boyan Petkov, Mirko Severi, Vito Vitale, Roberto Udisti <i>Elemental and Organic Carbon contribution to atmospheric aerosol at Ny Ålesund (Svalbard Islands)</i>
13.00 - 14.00	Intervallo Pranzo

Mercoledì 13 Settembre 2017

<i>Sala Paestum B</i>	
14.00 – 15.00	<i>Sessione Poster 3 (ANA PO86-ANA PO134)</i>
<i>Sala Paestum A</i>	
<i>Conferenza Plenaria</i>	
<i>Chair: Giuseppe Palleschi</i>	
15.00 – 15.45	<i>ANA-PL02: Francesco Ricci</i> <i>DNA-based nanodevices for clinical application</i>

<i>Sessione Parallela: Sensori-Elettrochimica</i>	
<i>Chair: Giuseppe Palleschi</i>	
15.50 – 16.10	<i>Finalisti premio Levi</i> <i>ANA-IN03: Alessia Amodio, Abimbola Feyisara Adedeji, Matteo Castronovo, Elisa Franco, Francesco Ricci</i> <i>pH-controlled assembly of DNA tiles</i>
16.10 – 16.30	<i>ANA-OR35: Alessandro Porchetta, Marianna Rossetti, Giuseppe Palleschi, Francesco Ricci</i> <i>Co-localization of DNA-based conformational switches for Single-Step Fluorescence Detection of Antibodies</i>
16.30 – 17.00	Coffee Break
<i>Sessione Parallela: Sensori-Elettrochimica</i>	
<i>Chair: Giovanna Marrazza</i>	
17.00 – 17.30	<i>ANA-KN10: Simona Ranallo, Carl Prévost-Tremblay, Andrea Idili, Alexis Vallée-Bélisle, Francesco Ricci</i> <i>Antibody powered nucleic acid release using a DNA-based nanomachine</i>
17.30 – 17.50	<i>ANA-OR36: Ilaria Palchetti, Francesca Bettazzi, Luigi Falciola, Valentina Pifferi, Anna Testolin, Chiara Ingrosso, Michela Corricelli</i> <i>Colloidal Nanoparticle modified Graphene-based electrochemical platforms for clinical biomarker detection</i>
17.50 – 18.10	<i>ANA-OR37: Donato Calabria, Cristiana Caliceti, Martina Zangheri, Mara Mirasoli, Patrizia Simoni, Aldo Roda</i> <i>Smartphone-based enzymatic biosensor for rapid detection of oxidase substrates using confined multilayer paper reflectometry</i>
18.10 – 18.30	<i>ANA-OR38: Stefano Cinti, Luca Fiore, Renato Massoud, Claudio Cortese, Danila Moscone, Giuseppe Palleschi, Fabiana Arduini</i> <i>A reagentless paper-based screen-printed device to detect chloride ions in serum and sweat</i>
18.30 – 18.50	<i>ANA-OR39: Donatella Coviello, Michela Contursi, Innocenzo Giuseppe Casella</i> <i>PVA/GO/Au: development and characterization of a new electrode material</i>
8.50 – 19.10	<i>ANA-OR40: Paolo Bollella, Daniela A. Stevar, Cristina Tortolini, Lo Gorton, Roland Ludwig, Harry Boer, Anu Koivula, Gabriele Favero, Riccarda Antiochia, Franco Mazzei</i> <i>Glucose/Oxygen Enzymatic Fuel Cell based on a "green" Gold Nanoparticles modified Graphene Screen-printed Electrode for Glucose detection in human saliva</i>
19.10 – 19.30	<i>ANA-OR41: Daniele Zappi, Serena Gabriele, Marta Letizia Antonelli, Claudia Sadun</i> <i>Generation IV ionic liquids and nanomaterials to develop innovative electrochemical biosensing platforms</i>

<i>Sala Olimpia</i>	
<i>Sessione Parallela: Scienza delle Separazioni</i>	
<i>Chair: Achille Cappiello</i>	
15.50 – 16.10	ANA-OR42: <u>Riccardo Zenezini Chiozzi</u> , Francesca Ferraris, Carmela Maria Montone, Susy Piovesana, Aldo Laganà <i>Identification of bioactive peptides derived from cauliflower by-products by multidimensional liquid chromatography and bioinformatics</i>
16.10 – 16.30	ANA-OR43: <u>Simone Marchetti</u> , Maria Pesavento, Rachele Maria Adele Bernini, Domingo Pastran, Daniele Merli, Letizie DeMaria <i>Solid phase extraction of dibenzyl disulphide on a molecularly imprinted polymer</i>
16.30 – 17.00	Coffee Break

<i>Sessione Parallela: Spettroscopia - Chemiometria</i>	
<i>Chair: Giuseppe Spoto</i>	
17.00 – 17.30	ANA-KN11: <u>Ángela I. López-Lorente</u> , Angelo Tricase, Rosaria Anna Picca, Cinzia Di Franco, Maria Chiara Sportelli, Boris Mizaikoff, Christine Kranz, Antonio Valentini, Gerardo Palazzo, <u>Nicola Cioffi</u> <i>What's new and good in the aqueous synthesis of colloidal gold nanoparticles (AuNPs). A critical overview of AuNPs synthetic methods and their analytical applications</i>
17.30 – 17.50	ANA-OR44: <u>Maria Chiara Sportelli</u> , Annalisa Volpe, Margherita Izzi, Maurizio Clemente, Rosaria Anna Picca, Amalia Conte, Matteo Alessandro Del Nobile, Antonio Ancona, Nicola Cioffi <i>Analytical characterization of new composites for food packaging applications</i>
17.50 – 18.10	ANA-OR45: <u>Marco Minella</u> , Claudio Minerò, Matteo Baudino <i>Photocatalytic transformation of C₂Cl₄ in gas phase under UV-irradiated TiO₂</i>
18.10 – 18.30	ANA-OR46: <u>Massimo Innocenti</u> , Francesco Di Benedetto, Emanuele Salvietti, Andrea Giaccherini, Walter Giurlani, Francesco Carlà, Nicola Cioffi, Rosaria A. Picca, Enrico Berretti, Roberto Felice <i>Microscopic and Spectroscopic Analysis with Synchrotron Light of Modified Surfaces of Technological Interest</i>
18.30 – 18.50	ANA-OR47: <u>Alessandra Biancolillo</u> , Remo Bucci, Andrea Magrì, Federico Marini <i>Metodi multi-block per l'analisi degli alimenti</i>
18.50 – 19.10	ANA-OR48: <u>Cristina Malegori</u> , Paolo Oliveri, Maria Alessandra Boggiani, Graziella Pastorini, Monica Casale <i>An innovative NIR hyperspectral imaging approach to pattern cheese ripening</i>
19.10 – 19.30	ANA-OR49: <u>Elisa Robotti</u> , Simona Martinotti, Marcello Manfredi, Daniela Brina, Alessandra Scagliola, Elia Ranzato, Stefano Biffo, Fabio Gosetti, Emilio Marengo <i>Mitochondrial proteome modifications due to eIF6 depletion by UHPLC-QTOF MS/MS with SWATH-MS acquisition</i>

<i>Sala Athena</i>	
<i>Sessione Congiunta: Chimica analitica –Chimica dell'Ambiente e dei Beni Culturali</i>	
<i>Chair: Fabrizio Passarini</i>	
15.00 -15.25	ABC/ANA-KN01 <u>Marco Pesce</u> , <u>Andrea Critto</u> , <u>Silvia Torresana</u> , <u>Monia Santini</u> , <u>Elisa Giubilato</u> , <u>Lisa Pizzol</u> , <u>Paola Mercogliano</u> , <u>Alberto Zirino</u> , <u>Ouyang Wei</u> , <u>Antonio Marcomini</u> <i>An integrated modelling approach to study the impacts of nutrients on coastal aquatic ecosystems in the context of climate change</i>

15.25 - 15.50	ABC/ANA -KN02 <u> Davide Vione</u> , Birgit Koehler, Francesco Barsotti, Marco Minella, Claudio Minero, Lars J. Tranvik, Tomas Landelius <i>Photoinduced Processes in Surface Waters: A Photochemical Mapping of Sweden</i>
15.50 - 16.10	ABC/ANA -OR01 <u> Luca Carena</u> , Silvia Berto, Davide Vione, Federico Valmacco, Matteo Marletti, Agnese Giacomino, Claudia Barolo, Roberto Buscaino, Mery Malandrino <i>Application of an electro-activated glassy carbon electrode (GCE) to the analytical monitoring and photochemical studying of acetaminophen.</i>
16.10 – 16.30	ABC/ANA -OR03 <u> Luca Rivoira</u> , Alessandra Lo Re, Davide Vione, Marco Minella, Marta Appendini, Barbara Onida, Maria Concetta Bruzzoniti <i>Removal and photodegradation of glyphosate herbicide from waters using a mesoporous substrate with adsorbent properties</i>
16.30 – 17.00	Coffee Break

Sessione Congiunta: Chimica analitica –Chimica dell’Ambiente e dei Beni Culturali

Chair: Andrea Gambaro

17.00 – 17:30	ABC/ANA -KN02: <u> Alessandra Genga</u> , Maria Siciliano, Cosimino Malitesta, Tiziana Siciliano, Antonio Proto, Raffaele Cucciniello <i>Primary and secondary carbonaceous species in PM10 and PM2.5 samples</i>
17.30 – 17.50	ABC/ANA -OR04: <u> Sara Padoan</u> , Elena Barbaro, Matteo Feltracco, Roberta Zangrando, Carlo Barbante, Andrea Gambaro <i>Characterization of ionic composition in the submicron fraction of urban aerosol</i>
18.10 – 18.30	ABC/ANA -OR05: <u> Mirko Severi</u> , Silvia Becagli, Laura Caiazzo, Virginia Ciardini, Ester Colizza, Fabio Giardi, Karin Mezgec, Claudio Scarchilli, Barbara Stenni, Elizabeth R. Thomas, Rita Traversi, Roberto Udisti <i>Sea salt sodium record from Talos Dome (East Antarctica) as a potential proxy of the Antarctic past sea ice extent</i>
18.30 – 18.50	ABC/ANA -OR06: <u> Roberto Udisti</u> , Silvia Becagli, Ezio Bolzacchini, Laura Caiazzo, David Cappelletti, Luca Ferrero, Fabio Giardi, Marco Grotti, Angelo Lupi, Mery Malandrino, Mauro Mazzola, Beatrice Moroni, Mirko Severi, Rita Traversi, Vito Vitale <i>A six-year record of size distribution and chemical composition of Arctic aerosol. Main results and future bi-polar perspectives</i>
18.50 – 19.10	ABC/ANA -OR07: <u> Janeth Tafur Marinos</u> , Marco Ginepro, Vincenzo Zelano <i>Effects of biomass, temperature and thermochemical process on PAH concentration in biochar</i>
19.10 – 19.30	ABC/ANA -OR08: <u> Ezio Bolzacchini</u> , Luca Ferrero, Antonio Proto, Concetta Pironti, Raffaele Cucciniello, Oriana Motta, Cristiana Rizzi, Grisa Močnik, Lorenza Dall’Aglia and Chiara Rostagno <i>Particulate and gaseous indoor contamination at the Museum of “Last Supper” of Leonardo Da Vinci: results from one year of monitoring activity</i>

Divisione di Electrochimica

Lunedì 11 Settembre 2017

<i>Hotel Savoy Sala Verdi</i>	
Sessione Electrochimica I	
Chairperson: Musiani-Velardo	
9:00 - 9:15	<i>Saluto Presidente</i>
9:15 - 9:30	ELE OR01: <u>La Mantia</u> , Erinmwingbovo, Koster, Brogioli <i>Dynamic impedance spectroscopy of a Prussian blue derivative thin film</i>
9:30 - 9:45	ELE OR02: <u>Brutti</u> <i>The mixed olivine $\text{Li}(\text{Co}_{1/3}\text{Fe}_{1/3}\text{Mn}_{1/3})\text{PO}_4$ material as positive electrode for lithium batteries</i>
9:45 - 10:00	ELE OR03: <u>Capobianco</u> , Landi, Caruso, Peluso <i>Hole site energies and electronic couplings for hole transport in DNA inferred from electrochemistry and quantum chemical predictions</i>
10:00 - 10:15	ELE OR04: <u>Valenti</u> , Boni, Melchionna, Marcaccio, Rapino, Bonchio, Prato, Fornasiero, Paolucci <i>Co-axial nanostructures for energy conversion: synergic effects between carbon nanotubes and metal oxide</i>
10:15 - 10:30	ELE OR05: <u>Gennaro</u> , Lorandi, Fantin, Isse, Matyjaszewski <i>The use of rotating disk electrode to measure a complete set of kinetic and thermodynamic ATRP parameters</i>
10:30 - 11:00	Coffee Break
<i>Hotel Savoy Sala Verdi</i>	
Sessione Electrochimica II	
Chairperson: Scialdone-Longoni	
11:00 - 11:15	ELE OR06: <u>Di Noto</u> , Negro, Vezzù, Nale, Bang, Bertasi, Pagot, Zlotorowicz, Pace <i>Graphene-based "core-shell" hierarchical nanostructured low-pt electrocatalysts for proton exchange membrane fuel cells</i>
11:15 - 11:30	ELE OR07: <u>Passaponti</u> , Rosi, Salvietti, Castello, Giaccherini, Innocenti <i>Microwave assisted pyrolysis of waste tires: evaluation by rotating ring-disk electrode technique of the catalytic efficiency in O.R.R.</i>
11:30 - 11:45	ELE OR08: <u>Brandiele</u> , Durante, Rizzi, Gennaro <i>New evidences of platinum-yttrium alloyed nanoparticles formation on carbon support and catalytic activity for oxygen reduction reaction</i>
11:45 - 12:00	ELE OR09: <u>Dall'Asta</u> , Buchholz, Ferrara, Changas, Quartarone, Tealdi, Passerini <i>$\text{Na}_{0.44}\text{MnO}_2$ - based cathodes for greener sodium-ion full cells: novel synthesis and electrode processing</i>
12:00 - 12:15	ELE OR10: <u>Zaffora</u> , Di Franco, Di Quarto, Valov, Habazaki, Santamaria <i>Fabrication of Hf-Nb anodic oxides and their use in resistive switching devices</i>
12:15 - 12:30	ELE OR11: <u>Quartarone</u> , Angioni, Millia, Mustarelli, Doria, Temporiti, Mannucci, Corana <i>Photosynthetic microbial fuel cell with polybenzimidazole-type membrane: highly efficient synergy between bacteria and microalgae for simultaneous wastewater removal and biorefinery</i>
12:30 - 12:45	ELE OR12: <u>Lo Vecchio</u> , D'Urso, Aricò, Baglio <i>Nanoclusters based on CoNC and FeNC for oxygen reduction reaction and their applications in direct methanol fuel cell</i>
12:45 - 13:00	ELE OR13: <u>Navarra</u> , Agostini, Lombardo, Matic, Panero <i>Gel polymer electrolytes for high-loading sulfur composite electrodes in Li-batteries</i>
13:00 - 14:00	Intervallo Pranzo

<i>Sala Paestum B</i>	
14:00 – 15:00	<i>Sessione Poster 1 (ELE PO01 – ELE PO24)</i>
<i>Hotel Savoy Sala Verdi</i>	
<i>Sessione Elettrochimica III</i>	
<i>Chairperson: Di Noto</i>	
15:00 - 15:15	ELE OR14: <u>Dini</u> , Bonomo, Scorretti, Di Carlo <i>Study of the influence of the electrolyte on the photoconversion properties of p-type dye-sensitized solar cells</i>
15:15 - 15:30	ELE OR15: <u>Pagot</u> , Bertasi, Vezzù, Nawn, Sun, Nale, Negro, Di Noto <i>EMImCl/(TiCl₄)_{1.4}/(δ-MgCl₂)_x Ionic Liquid Electrolyte for Mg-ion Batteries</i>
15:30 - 15:45	ELE OR16: <u>Tranchida</u> , Pituccio, Di Franco, Di Quarto, Santamaria <i>Growth and characterization of atmospheric and anodic oxide films on weathering steels</i>
15:45 - 16:00	ELE OR17: <u>Lo Faro</u> , Trocino, Zignani, Aricò <i>Syngas production via co-electrolysis of H₂O and CO₂ fed to a Solid Oxide Cell</i>
16:00 - 16:15	ELE OR18: <u>De Bon</u> , Isse, Gennaro <i>Improvements of electrochemically mediated atom transfer radical polymerization of styrene with ionic liquids</i>
16:15 - 16:30	ELE OR19: <u>Colo'</u> , Renault, Bella, Gerbaldi, Brandell <i>An electrolyte study on Na₂BDA anode for Na-based organic batteries</i>
16:30 - 17:00	Coffee Break
<i>Hotel Savoy Sala Verdi</i>	
<i>Sessione Premi</i>	
<i>Chairperson: Durante-Soldà</i>	
17:00 - 17:15	ELE PZ01: <u>Longoni</u> <i>Investigation of sodium-ion battery materials - Premio di Dottorato "Engitec Technologies"</i>
17:15 - 17:30	ELE PZ02: <u>Zampardi</u> <i>In situ analysis of surface and bulk phenomena in lithium-ion batteries by means of scanning electrochemical microscopy - Premio di Dottorato "Fondazione Oronzio e Niccolò De Nora"</i>
17:30 - 17:45	ELE PZ03: <u>Fantin</u> , Lorandi, De Bon, Pan, Matyjaszewski, Gennaro, Isse <i>Electrochemical methods for atom transfer radical polymerization of aqueous and metal free systems - Premio di Dottorato "Fondazione Oronzio e Niccolò De Nora"</i>
17:45 - 18:00	ELE PZ04: <u>Pargoletti</u> , Cappelletti, Vertova, Pifferi <i>Bare and titanium-doped manganese dioxide nanoparticles. Their pivotal role in energetic and sensoristic applications - Premio di Laurea "Bio-Logic SAS"</i>
18:00 - 18:15	ELE PZ05: <u>La Monaca</u> , De Giorgio, Focarete, Fabiani, Zaccaria, Arbizzani <i>Electrospun polymer separators based on PVdF-PEO blends for Li-ion batteries - Premio di Laurea "Photo Analytical s.r.l."</i>
18:15 - 18:30	ELE PZ06: <u>Proietto</u> , Galia, Scialdone <i>Electrochemical conversion of carbon dioxide to formic acid. Study of the effect of the operating parameters - Premio di Laurea "Ametek Scientific Instruments"</i>

Martedì 12 Settembre 2017

<i>Hotel Savoy Sala Vivaldi</i>	
<i>Sessione Congiunta: Chimica Fisica - Elettrochimica - Enerchem</i>	
<i>Chairperson: Minguzzi-Brutti</i>	
9:00 - 9:30	ELE KN01: <u>Ruffo</u> <i>Negative electrode materials for sodium ion batteries</i>
9:30 - 9:45	FIS OR51: <u>Lamberti</u> , Litti, De Bastiani, Sorrentino, Gandini, Meneghetti, Petrozza <i>High-quality, ligands-free, mixed-halide perovskite nanocrystals ink for optoelectronic applications</i>

9:45 - 10:00	ELE OR20: <u>Musiani</u> , Verlatto, Barison, Cimino, Lisi, Mancino, Paolucci <i>Electrochemical preparation of nanostructured CeO₂-Pt catalysts on Fe-Cr-Al alloy foams for the low-temperature combustion of methanol</i>
10:00 - 10:15	FIS OR52: <u>Binetti</u> , Le Donne, Acciarri, Marchionna <i>New earth-abundant thin film solar cells based on Cu₂MnSnS₄</i>
10:15 - 10:30	ELE OR21: <u>Durante</u> , Daniel, Mattiacci, Rizzi, Gennaro <i>Platinum free electrocatalyst based on Fe-Nx moieties supported on mesoporous carbon prepared from polysaccharides for oxygen reduction reaction</i>
10:30 - 11:00	Coffee Break
Hotel Savoy Sala Vivaldi	
Sessione Congiunta: Elettrochimica - Chimica Fisica - Enerchem	
Chairperson: Binetti-Gerbaldi	
11:00 - 11:15	FIS OR53: <u>Mustarelli</u> , Invernizzi, Patrini, Vezzù, Di Noto <i>Polyurethane-based Electrostrictive Nanocomposites as High Strain - Low Frequency Mechanical Energy Harvesters</i>
11:15 - 11:30	FIS OR54: <u>Chiarello</u> , Bernareggi, Pedroni, Magni, Pietralunga, Vassallo, Selli <i>A bilayer WO₃ n-n heterojunction photoanode prepared by RF diode sputtering for improved photoelectrocatalytic water splitting</i>
11:30 - 11:45	ELE OR22: <u>Bella</u> , Colò, Zolin, Pugliese, Stephan, Gerbaldi <i>Lignocellulosic materials for electrochemical energy storage and conversion</i>
11:45 - 12:00	FIS OR55: <u>Brutti</u> , Panero, Paolone, Reale <i>Hydrides as high capacity anodes in lithium cells: An Italian "Futuro in Ricerca di Base FIRB-2010" Project</i>
12:00 - 12:15	ELE OR23: <u>Bertasi</u> , Di Noto <i>Secondary magnesium batteries: an overview on ionic liquid -based electrolytes</i>
12:15 - 12:30	FIS OR56: <u>La Gatta</u> , Milano, Ragni, Agostiano, Farinola, Trotta <i>Bio-hybrid complexes in artificial photosynthesis</i>
12:30 - 12:45	ELE OR24: <u>Minguzzi</u> , Fracchia, Visibile, Naldoni, Malara, Locatelli, Vertova, Ghigna, Rondinini <i>Operando (photo)electrochemical X-ray absorption spectroscopy for water splitting</i>
12:45 - 13:00	FIS OR57: <u>Beneduci</u> , Capodilupo, Corrente, Fabiano, Maltese, Cospito, Ciccarella, Chidichimo, Gigli <i>Electronic coupling in H-shaped tetra-arylamine mixed-valence compounds</i>
13.00 - 14.00	Intervallo Pranzo

Mercoledì 13 Settembre 2017

Hotel Savoy Sala Verdi	
Sessione Elettrochimica IV	
Chairperson: Mussini-Fantini	
15:00 - 15:15	ELE OR25: Di Quarto, Maniscalco, Di Franco, La Mantia, <u>Santamaria</u> <i>Synergistic use of impedance and photoelectrochemical measurements to study the electronic properties of anodic TiO₂</i>
15:15 - 15:30	ELE OR26: <u>Battistel</u> , Reynard, Dennison, Girault <i>Recovery of low grade heat by redox flow battery</i>
15:30 - 15:45	ELE OR27: <u>Lorandi</u> , Michieletto, Fantin, Chmielarz, Isse, Gennaro, Matyjaszewski <i>Boosting aqueous atom transfer radical polymerization of hydrophilic and hydrophobic monomers by means of electrochemistry</i>
15:45 - 16:00	ELE OR28: <u>Chiarotto</u> , Feroci, Pandolfi <i>Voltammetric analysis and chemical reactivity of ionic liquids (ILs) used as "green" reaction media and precursors of efficient catalysts</i>

16:00 - 16:15	ELE OR29: <u>Scialdone</u> , D'Angelo, Vicari, Galia <i>New processes to produce renewable energy: reverse electrodialysis and thermally regenerative ammonia battery</i>
16:15 - 16:30	ELE OR30: <u>Comisso</u> , Armelao, Cattarin, Guerriero, Mattarozzi, Musiani, Rancan, Vázquez-Gómez, Verlatto <i>Preparation of porous oxide layers by oxygen bubble templated anodic deposition followed by galvanic displacement</i>
16:30 - 17:00	Coffee Break
Hotel Savoy Sala Verdi	
Sessione Elettrochimica V	
Chairperson: Santamaria-Zampardi	
17:00 - 17:15	ELE OR31: <u>Mussini</u> , Arnaboldi, Buzzi, Monaco, Sannicolò, Benincori, Apolloni, Penoni, Cirilli <i>Inherently chiral molecular materials with 2,2'- and 3,3'-bisindole atropisomeric cores: interactions between equivalent redox sites, configurational stability and enantioselection ability</i>
17:15 - 17:30	ELE OR32: <u>Macchia</u> , Alberga, Manoli, Mangiatordi, Palazzo, Torsi <i>Organic bioelectronics probing conformational changes in surface confined proteins</i>
17:30 - 17:45	ELE OR33: <u>Di Franco</u> , Seyeux, Zanna, Maurice, Marcus <i>Physicochemical characterization and corrosion behaviour of surface oxide films on bright annealed ferritic stainless steel</i>
17:45 - 18:00	ELE OR34: <u>Zignani</u> , Reis, Saglietti, Oliveira, Trocino, Maisano, Ticianelli, Aricò, Lo Faro <i>La₂NiO₄@Ni core-shell based catalyst as pre-layer for a commercial Solid Oxide Fuel Cell fed with biofuels</i>

Divisione di Chimica Farmaceutica

Lunedì 11 Settembre 2017

Sala Saturno	
Chairpersons: Gabriele Costantino, Fabrizio Giordanetto	
9:00-9:30	FAR KN01 - Fabrizio Giordanetto, D E Shaw Research <i>Fragment-based discovery of AZD2716: a novel, potent secreted phospholipase A2 (sPLA2) inhibitor for the treatment of coronary artery disease</i>
9:30-9:50	FAR OR01 – Tracey Pirali, Università del Piemonte Orientale <i>Discovery of Store-Operated Calcium Entry modulators as an effective treatment for calcium-related rare genetic diseases</i>
9:50-10:10	FAR OR02 – Claudia Spatari, Università della Calabria <i>A new generation of dihydropyridines: photodegradation and photostabilization strategies</i>
10:10-10:30	FAR OR03 – Andrea Carotti, Università di Perugia <i>In Silico Approaches Supporting Pharmaceutical Analysis Enigmas</i>
10:30-11:00	Coffee Break
Chairpersons: Roberto Di Santo, Maria Laura Bolognesi	
11:00-11:30	FAR KN02 – Maria Laura Bolognesi, Università di Bologna <i>Sustainable drug discovery for neglected infectious diseases: the case of cardanol-based anti-trypanosomatid hybrids</i>
11:30-11:50	FAR OR04 – Rolando Cannalire, Università di Perugia <i>2,2-Dioxido-2,1-benzothiazines as new allosteric inhibitors of DENV NS5 RNA-dependent RNA polymerase</i>
11:50-12:10	FAR OR05 – Mattia Mori, Università di Siena – Istituto Italiano di Tecnologia (IIT) <i>Structure-based identification of HIV-1 nucleocapsid protein inhibitors active against wild-type and drug-resistant HIV-1 strains</i>
12:10-12:30	FAR OR06 – Tommaso Felicetti, Università di Perugia <i>Improvement of Staphylococcus aureus NorA efflux pump inhibition by methoxy group introduction on 2-phenylquinoline core</i>
12:30-12:50	FAR OR07 – Iuni Margaret Laura Trist, Università di Parma <i>Blocking PA-PBI Protein-Protein Interaction with the Aid of Molecular Modelling to Counteract Influenza A Virus</i>
13:00-14:00	Intervallo Pranzo – Lunch Break

Sala Paestum B	
14:00-15:00	Sessione Poster 1 (FAR PO01 – FAR PO21)

Sala Saturno	
Chairpersons: Cosimo Altomare, Ersilia De Lorenzi	
15:00-15:30	FAR KN03 – Ersilia De Lorenzi, Università di Pavia <i>Development and chromatographic evaluation of Molecularly Imprinted Polymers for the selective recognition of drugs</i>
15:30-15:50	FAR OR08 – Michele Bianchi, Università del Piemonte Orientale <i>Quantitative in vivo evaluation by LC-ESI-MSn analysis of adenosine 5'-tetrphosphate (Ap4), a nucleotide related to nicotinamide phosphoribosyltransferase activities (NAMPT)</i>
15:50-16:10	FAR OR09 – Matteo Micucci, Università di Bologna <i>Thymus vulgaris L. essential oil in gastrointestinal diseases</i>
16:10-16:30	FAR OR10 – Azzurra Stefanucci, Università di Chieti-Pescara “G. D’Annunzio”

	<i>Structural modification of the β-sheet ARC repressor: design, conformational analysis and binding properties of linear and cyclic ARC mimetics</i>
16:30-17:00	Coffee Break
<i>Chairperson:</i>	
17:00-17:30	FAR MD01 – Claudiu T. Supuran, Università di Firenze (Pratesi DCF Medal)
17:30-17:45	FAR PZ01 – Agostino Bruno, Istituto FIRC di Oncologia Molecolare (DCF Prize)
17:45-18:00	FAR PZ02 – Sergio Valente, Sapienza Università di Roma (DCF Prize)
18:00-18:10	FAR PZ03 – Elisa Azzali, Aptuit Verona (DCF Best PhD Thesis Award)
18:10-18:20	FAR PZ04 – Bruno Cerra, Università di Perugia (DCF Best PhD Thesis Award)
18:30-20:00	<i>Assemblea della Divisione di Chimica Farmaceutica</i>

Martedì 12 Settembre 2017

<i>Sala Saturno</i>	
<i>Chairpersons: Tiziano Bandiera, Maria Menichincheri</i>	
9:00-9:30	FAR KN04 – Maria Menichincheri, Nerviano Medical Sciences <i>Discovery of Entrectinib: a novel and potent inhibitor of ALK, ROS1, and Pan-TRKs kinases active in multiple molecularly defined cancer indications</i>
9:30-9:50	FAR OR11 – Loredana Salerno, Università di Catania <i>Targeting Heme Oxygenase-1 to Overcome Imatinib Resistance in Chronic Myeloid Leukemia</i>
9:50-10:10	FAR OR12 – Marco Lucio Lolli, Università di Torino <i>Potent human dihydroorotate dehydrogenase (hDHODH) inhibitors obtained by scaffold-hopping approaches: from the theoretical design to the in vivo evaluation</i>
10:10-10:30	FAR OR13 – Emanuele Amata, Università di Catania <i>Development of Sigma Receptors Nitric Oxide Photodonor Ligands with Antiproliferative Activity</i>
10:30-11:00	Coffee Break
<i>Chairpersons: Federico Corelli, Rosaria Gitto</i>	
11:00-11:30	FAR KN05 – Rosaria Gitto, Università di Messina <i>Discovery and optimization of isoquinoline-derived inhibitors of human Carbonic Anhydrases (hCAs)</i>
11:30-11:50	FAR OR14 – Giannamaria Annunziato, Università di Parma <i>Discovery of New, Potential Anti-Infecive Compound Based on Carbonic Anhydrase Inhibitors by Rational Target-Focus Repurposing Approach</i>
11:50-12:10	FAR OR15 – Francesco Saccoliti, Sapienza Università di Roma <i>Discovery of Novel Diaryl Sulfide Derivatives as Inhibitors of Trypanothione Reductase Enzyme</i>
12:10-12:30	FAR OR16 – Michele Tonelli, Università di Genova <i>Synthesis of 4,6-diamino-1,2-dihydrotriazines as influenza viruses and respiratory syncytial virus inhibitors targeting the host DHFR</i>
12:30-12:50	FAR OR17 – Carmen Cerchia, Università di Napoli “Federico II” <i>Application of a New Scaffold Concept for the Identification of Analog Series in Commercial Databases</i>
13:00-14:00	Intervallo Pranzo – Lunch Break
<i>Sala Paestum B</i>	
14:00-15:00	<i>Sessione Poster 2 (FAR PO22 – FAR PO48)</i>

Mercoledì 13 Settembre 2017

<i>Sala Paestum B</i>	
14:00-15:00	<i>Sessione Poster 3 (FAR PO49 – FAR PO82)</i>
<i>Sala Saturno</i>	
<i>Chairpersons: Vincenza Andrisano, Paolo Caliceti</i>	
15:00-15:30	FAR KN06 – Paolo Caliceti, Università di Padova <i>New drug delivery nanomachines: visionary concepts or reality</i>
15:30-15:50	FAR OR18 – Marco Paolino, Università di Siena <i>π-Stacked Polymers in Drug Delivery Applications</i>
15:50-16:10	FAR OR19 – Paola Russo, Università di Salerno <i>Clarithromycin dry powders for inhalation: A focus on drug solubility</i>
16:10-16:30	FAR OR20 – Francesco Peri, Università di Milano-Bicocca <i>Synthesis and preclinical evaluation of glycolipid-based TLR4 modulators: new therapeutics for inflammatory and autoimmune diseases</i>
16:30-17:00	Coffee Break
<i>Chairpersons: Gianluca Sbardella, Gilberto Spadoni</i>	
17:00-17:30	FAR KN07 – Gilberto Spadoni, Università di Urbino <i>Strategies to maximize therapeutic opportunities for melatonin derivatives</i>
17:30-17:50	FAR OR21 – Leonardo Pisani, Università di Bari <i>Nitrate-ester prodrugs of dual AChE-MAO B inhibitors as anti-Alzheimer Multitarget Hybrids</i>
17:50-18:10	FAR OR22 – Francesca Spyraakis, Università di Torino <i>Discovering new casein kinase 1d inhibitors with innovative MD-integrated virtual screening</i>
18:10-18:30	FAR OR23 – Letizia Crocetti, Università di Firenze <i>Isoxazol-5(2H)-one: a new scaffold for potent human neutrophil elastase (HNE) inhibitors</i>
18:30-18:50	FAR OR24 – Angelica Mazzolari, Università di Milano <i>Modelling of Glucuronidation Reactions in the MetaQSAR Database: Successful Strategies to Handle Unbalanced Data in Metabolism Prediction</i>

Divisione di Chimica Fisica

Lunedì 11 Settembre 2017

<i>Sala Vivaldi - Hotel Savoy</i>	
Photoactive Materials	
Chairperson: Elena Selli	
9:00 - 9:15	FIS OR01: <u>A. Truppi</u> , F. Petronella, T. Placido, C. Giannini, T. Sibillano, A. Agostiano, M. L. Curri, R. Comparelli <i>TiO₂/Au NRs photocatalysts for photodegradation of water pollutants under UV and visible light</i>
9:15 - 9:30	FIS OR02: <u>F. Ortica</u> , M. Frigoli, A. Zangarelli, D. Pannacci <i>Photochromism of N-phenyl-carbazole benzopyrans</i>
9:30 - 9:45	FIS OR03: <u>A. Panniello</u> , A. E. Di Mauro, E. Fanizza, M. L. Curri, M. Striccoli <i>Hydrophobic carbon dots with intense photoluminescence towards single white emitting materials</i>
New Composite Materials	
Chairperson: Moreno Meneghetti	
9:45 - 10:00	FIS OR04: <u>F. Cesano</u> , S. Cravanzola, F. Gaziano, D. Scarano <i>Graphene-like domains on MoS₂/TiO₂ systems, via acetylene polymerization: in-situ synthesis and characterization</i>
10:00 - 10:15	FIS OR05: <u>C. Ingresso</u> , M. Corricelli, G. V. Bianco, V. Pifferi, P. Guffanti, A. Testolin, F. Bettazzi, F. Petronella, R. Comparelli, A. Agostiano, M. Striccoli, I. Palchetti, L. Falciola, G. Bruno, M. L. Curri <i>Colloidal Nanocrystal Surface Decorated Graphene based Hybrid Materials for Sensors</i>
10:15 - 10:30	FIS OR06: <u>C. Sartorio</u> , V. Campisciano, C. Chiappara, S. Cataldo, M. Gruttadauria, F. Giacalone, B. Pignataro <i>Enhanced power-conversion efficiency in organic solar cells incorporating polymeric compatibilizers</i>
10:30 - 11:00	Coffee Break
Models & Experiments	
Chairperson: Giovanni Marletta	
11:00 - 11:30	FIS KN01: <u>P. Ugliengo</u> , A. Rimola, M. Sodupe M. Fabbiani, G. Martra <i>Amide Bond Formation by Condensation between Unactivated Reagents at Silica Surfaces: Rôle in Prebiotic Chemistry</i>
11:30 - 11:45	FIS OR07: <u>A. Painelli</u> , S. Sanyal, F. Terenziani, S. Pati, C. Sissa <i>Molecular Aggregates: a Fresh Perspective</i>
11:45 - 12:00	FIS OR08: <u>F. Sessa</u> , V. Migliorati, A. Serva, P. D'Angelo <i>On the Zn²⁺ ion speciation in challenging ionic media: a molecular dynamics and X-ray absorption spectroscopy study</i>
Materials for Biotechnological Applications 1	
Chairperson: Patrizia Canton	
12:00 - 12:15	FIS OR09: <u>F. Vischio</u> , N. Depalo, I. Arduino, S. Villa, F. Canepa, E. Fanizza, S. H. Lee, B. C. Lee, R. M. Iacobazzi, V. Laquintana, A. Lapedota, A. Cutrignelli, M. P. Scavo, M. Striccoli, A. Agostiano, M. L. Curri, N. Denora <i>Magnetic Solid Lipid Nanoparticles for Magnetically Targeted Delivery of Sorafenib for Treatment of Hepatocellular Carcinoma</i>
12:15 - 12:30	FIS OR10: <u>A. De Santis</u> , I. R. Krauss, L. Paduano, G. D'Errico <i>Micro-structural characterization of model membranes containing DHA</i>
12:30 - 12:45	FIS OR11: <u>G. Valente</u> , N. Depalo, E. Fanizza, R. M. Iacobazzi, N. Denora, V. Laquintana, L. Zaccaro, A. Del Gatto, I. De Paola, M. Saviano, P. D. Howes, C. Spicer, M. M. Stevens, M. Striccoli, A. Agostiano, L. M. Curri <i>Nanoparticles encapsulation in micellar systems for biomedical applications</i>

12:45 - 13:00	FIS OR12: <u>R. Gelli</u> , L. Mati, F. Ridi, P. Baglioni <i>Effect of cellulose ethers on the formation and properties of magnesium phosphate-based cements for biomedical applications</i>
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13:00 - 14:00	Intervallo Pranzo – Lunch Break
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Sala Paestum B	
14:00 - 15:00	Poster Session 1 (FIS PO01 - FIS PO16)
Molecular and Supramolecular Systems	
Chairperson: Gerardino D'Errico	
15:00 - 15:15	FIS OR13: <u>G. De Filpo</u> , P. Formoso, S. Manfredi, A. I. Mashin, F. P. Nicoletta <i>Bifunctional polymer-dispersed liquid crystals</i>
15:15 - 15:30	FIS OR14: <u>J. Cautela</u> , J. J. Crassous, N. V. Pavel, L. Galantini <i>Supracolloidal association of microgels and supramolecular tubules of bile salt derivatives</i>
15:30 - 15:45	FIS OR15: <u>P. Sassi</u> , B. Gironi, A. Lapini, M. Paolantoni, A. Morresi, P. Foggia <i>The lipid bilayer of model membranes: news from the inside</i>
Physical Studies of Materials and Molecules	
Chairperson: Gianmario Martra	
15:45 - 16:00	FIS OR16: <u>V. Domenici</u> , A. Resetic, J. Milavec, B. Zupancic, B. Zalar <i>Physical-chemical study of a new shape-memory material based on liquid crystalline elastomers</i>
16:00 - 16:15	FIS OR17: <u>G. Cavallaro</u> , V. Bertolino, G. Lazzara, F. Parisi, S. Milioto, M. Gradzielski <i>Hybrid nanostructures based on halloysite nanotubes and sustainable polymers</i>
16:15 - 16:30	FIS OR18: <u>G. Monaco</u> , F. Aquino, R. Zanasi, W. Herrebout, A. Massa <i>Absolute Configuration Assignment of two Hybrid Isoindolinone-phthalide Molecules by Vibrational Circular Dichroism</i>
16:30 - 17:00	Coffee Break
Chemistry of Materials and Surfaces	
Chairperson: Ludovico Valli	
17:00 - 17:15	FIS OR19: <u>E. Groppo</u> , A. Piovano, G. Martino, M. D'Amore, C. Barzan, S. Bordiga <i>Can we speak of "ancillary ligands" also in heterogeneous catalysis? Selected examples in olefin polymerization catalysts</i>
17:15 - 17:30	FIS OR20: <u>E. Fanizza</u> , F. Cascella, A. Panniello, L. Triggiani, N. Depalo, C. Giannini, D. Altamura, A. Agostiano, M. L. Curri, M. Striccoli <i>Synthesis and post preparative shape control of cesium lead bromide colloidal nanocrystals</i>
17:30 - 17:45	FIS OR21: <u>M. L. Saladino</u> , F. Armetta, D. Hreniak, L. Marciniak, W. Stręk, C. Giordano, E. Caponetti <i>Non conventional based Ce:YAG nanocomposites</i>
Materials for Biotechnological Applications 2	
Chairperson: Concetta Giancola	
17:45 - 18:00	FIS OR22: <u>F. Ridi</u> , R. Gelli, L. Gigli, M. Scudero, M. Bonini, P. Baglioni <i>Synthesis and characterization of immunologically relevant calcium and magnesium phosphate amorphous nanostructures and strategies for their stabilisation</i>
18:00 - 18:15	FIS OR23: <u>E. Gatto</u> , R. Lettieri, A. Colella, F. Leonelli, L. Giansanti, L. Stella, M. Venanzi <i>Physico-chemical characterization of smart lipid biointerfaces for the detection of a tumor biomarker</i>
18:15 - 18:30	FIS OR24: <u>I. Miletto</u> , L. Invernizzi, C. Gionco, M. C. Paganini, E. Giamello, L. Marchese, E. Gianotti <i>Luminescent ZrO₂:Ln³⁺@SiO₂ Nanosystems Conjugated with Rose Bengal as Efficient Nanoplatfor for Theranostic Applications</i>

Martedì 12 Settembre 2017

<i>Sala Verdi - Hotel Savoy</i>	
Materials	
Chairpersons: Debora Berti, Gianmarco Martra	
9:00 - 9:15	FIS OR25: <u>A. Girlando</u> , N. Castagnetti, M. Masino <i>Phenomenology of the Neutral-Ionic Valence Instability in Mixed Stack Charge Transfer Crystals</i>
9:15 - 9:30	FIS OR26: <u>M. Fabbiani</u> , G. Tabacchi, E. Fois, G. Martra <i>The effect of temperature in the formic acid - formate system on TiO₂ (101) surfaces</i>
9:30 - 9:45	FIS OR27: <u>M. Tonelli</u> , R. Moscatelli, M. Sebastiani, F. Martini, L. Calucci, M. Geppi, S. Borsacchi, F. Ridi <i>Interaction of phosphate-based additives with MgO/SiO₂ cements</i>
9:45 - 10:00	FIS OR28: <u>L. Triggiani</u> , C. N. Dibenedetto, G. Tartaro, A. Loiodice, T. Sibillano, C. Giannini, G. Bruno, R. Brescia, R. Buonsanti, A. Agostiano, M. Striccoli, E. Fanizza <i>Composition and architecture engineering of colloidal TiO₂ nanocrystals for the enhancement of sunlight conversion ability</i>
10:00 - 10:15	FIS OR29: <u>Y. Miele</u> , A. F. Taylor, T. Bánsági Jr, L. Izzo, F. Rossi <i>Coupling of nonlinear chemical reactions with pH-responsive polymers</i>
10:15 - 10:30	FIS OR30: J. Gubitosa, <u>V. Rizzi</u> , P. Fini, A. Petrella, F. Fanelli, A. Agostiano, M. Perrone, I. Arduino, A. Lopodota, P. Cosma <i>Green synthesis of gold nanoparticles using Punica Granatum Juice for cosmetic applications</i>
10:30 - 11:00	Coffee Break
Materials	
Chairpersons: Alberto Girlando, Gerardo D'Errico	
11:00 - 11:15	FIS OR31: <u>M. Bonini</u> , A. Gabbani, S. Del Buffa, F. Ridi, P. Baglioni, R. Bordes, K. Holmberg <i>Adsorption of Amino Acids and Glutamic Acid-Based Surfactants on Imogolite Clays</i>
11:15 - 11:30	FIS OR32: <u>M. Corno</u> , I. Miletto, E. Gianotti, M. Cossi, L. Marchese <i>Organic-inorganic hybrid materials as heterogenous catalysts for pharma industry</i>
11:30 - 11:45	FIS OR33: <u>L. Ambrosone</u> , G. Bufalo, F. Cuomo, F. Lopez <i>Coupling of sieving and thermogravimetric analyzes for studying the activation energy distribution function of complex reactions</i>
11:45 - 12:00	FIS OR34: <u>M. Baglioni</u> , C. Montis, F. Brandi, T. Guaragnon, I. Meazzini, P. Baglioni, D. Berti <i>Dewetting of acrylic polymeric films induced by water/propylene carbonate/surfactant mixtures - Implications for cultural heritage conservation</i>
12:00 - 12:15	FIS OR35: V. Rizzi, M. A. Ricci, E. Altamura, P. Fini, S. Sortino, A. Fraix, P. Semeraro, L. De Cola, E. A. Prasetyanto, <u>P. Cosma</u> <i>Supramolecular Self-Assembly of Chlorophyll A and Mesoporous Silica Nanoparticles in Water Medium</i>
12:15 - 12:30	FIS OR36: <u>R. Camerini</u> , D. Chelazzi, R. Giorgi, P. Baglioni <i>Silica-based composites for the consolidation of earthen materials</i>
12:30 - 12:45	FIS OR37: <u>B. Di Napoli</u> , P. Conflitti, C. Mazzuca, M. Venanzi, M. De Zotti, F. Formaggio, A. Palleschi <i>Langmuir-Blodgett and MD characterization of peptides at the air/water interface</i>
12:45 - 13:00	FIS OR38: <u>L. Litti</u> , A. Ramundo, V. Amendola, M. Meneghetti <i>Detection and Quantification of Anticancer Drugs with Surface Enhanced Raman Spectroscopy</i>
13:00 - 14:00	Intervallo Pranzo
<i>Sala Paestum B</i>	
14:00 - 15:00	Poster Session 2 (FIS PO17 - FIS PO33)

Mercoledì 13 Settembre 2017

<i>Sala Paestum B</i>	
14:00 - 15:00	<i>Poster Session 3 (FIS PO34 - FIS PO51)</i>
<i>Sala Vivaldi - Hotel Savoy</i>	
Environmental Physical Chemistry	
Chairpersons: Maria Lucia Curri, Riccardo Zanasi	
15:00 - 15:15	FIS OR39: <u>A. Tursi</u> , N. De Vietro, A. Beneduci, F. Chidichimo, F. Fracassi, G. Chidichimo <i>Effective remediation of highly polluted water by petroleum hydrocarbons with functionalized cellulose fiber</i>
15:15 - 15:30	FIS OR40: <u>S. Salvestrini</u> <i>A comparison between the Langmuir rate equation and the pseudo-first and pseudo-second order models for adsorption processes</i>
15:30 - 15:45	FIS OR41: <u>F. Venditti</u> , F. Cuomo, L. Ambrosone, A. Ceglie, G. Cinelli, F. Lopez <i>Microstructured composite for Cr (VI) removal from polluted environment</i>
15:45 - 16:00	FIS OR42: <u>F. Lopez</u> , F. Cuomo, F. Venditti, L. Ambrosone, A. Ceglie <i>Olive mill wastewaters phenol photocatalytic degradation by visible light activated carbon doped titanium</i>
16:00 - 16:15	FIS OR43: <u>P. Semeraro</u> , J. A. Gabaldón, P. Fini, J. A. Pellicer, V. Rizzi, A. Longo, E. Núñez, P. Cosma <i>Removal of an azo textile dye from wastewater using cyclodextrin-epichlorohydrin polymers</i>
16:15 - 16:30	FIS OR44: <u>R. Angelico</u> , C. Colombo, G. Palumbo, G. Ventruti <i>Arsenic Adsorption on Iron Oxides and its Environmental Impact</i>
16:30 - 17:00	Coffee Break
Physical Chemistry of Biological Systems	
Chairpersons: Concetta Giancola, Maria Rosaria Tinè	
17:00 - 17:15	FIS OR45: F. Tadini-Buoninsegni <i>Electrophysiological measurements on a solid supported membrane to investigate the transport activity of sarcoplasmic reticulum Ca^{2+}-ATPase</i>
17:15 - 17:30	FIS OR46: <u>F. Sciubba</u> , M. Delfini, M. E. Di Cocco, F. Ferraris <i>Protein-ligand interaction: a NMR study</i>
17:30 - 17:45	FIS OR47: <u>C. Satriano</u> , P. Di Pietro, N. Caporarello, C. D. Anfuso, G. Lupo, A. Magrì, D. La Mendola <i>Immobilisation of neurotrophin peptides on gold nanoparticles by direct and lipid-mediated interaction: a new multipotential therapeutic nanoplatfom for CNS disorders</i>
17:45 - 18:00	FIS OR48: <u>V. De Leo</u> , F. Milano, R. Comparelli, E. De Giglio, A. Trapani, S. Di Gioia, M. Conese, M. Mattioli-Belmonte, A. Agostiano, L. Catucci <i>Small liposomes for drug delivery</i>
18:00 - 18:15	FIS OR49: <u>G. Arrabito</u> , F. Cavaleri, A. Porchetta, F. Ricci, V. Vetri, M. Leone, B. Pignataro <i>Molecular Confinement in Femtoliter Scale Aqueous Compartments</i>
18:15 - 18:30	FIS OR50: <u>S. Rapino</u> , L. Bartolini, C. Albonetti, A. Soldà, G. Valenti, F. Valle, P. G. Pelicci, F. Paolucci, F. Zerbetto <i>The Influence of Chemical Microenvironment on Living Cell Shape</i>

Joined Sessions
Lunedì 11 Settembre 2017

<i>Sala Athena - Hotel Ariston</i>	
<i>Sessione ABC+ANA+FIS: La trasversalità della chimica per i Beni Culturali</i>	
<i>Chairperson: Lucia Toniolo</i>	
9:00 - 9:25	ABC/ANA/FIS KN01: <u>Rocco Mazzeo</u> <i>Macro Mid-Infrared total reflection (MA-FTIR) mapping for the characterization of outdoor bronze surfaces</i>
9:25 - 9:40	FIS OR65: <u>C. Berlangieri</u> , E. Carretti, G. Poggi, S. Murgia, M. Monduzzi, L. Dei, P. Baglioni <i>Formulation and characterization of hydroxypropyl guar based gel-like systems, tailored for the low impact cleaning of works of art surfaces</i>
9:40 - 9:55	FIS OR66: <u>P. Ferrari</u> , A. Mirabile, M. Trabace, L. Montalbano, R. Giorgi, P. Baglioni <i>Chemical poly ethyl methacrylate (PEMA) organogels for the removal of pressure sensitive tapes (PSTs) from paper artworks</i>
9:55 - 10:10	FIS OR67: <u>N. Bonelli</u> , R. Mastrangelo, C. Montis, P. Tempesti, P. Baglioni <i>Surface Cleaning of Artworks: Structure and Dynamics of Nanostructured Fluids Confined in a Polymeric Network</i>
10:10 - 10:25	FIS OR68: <u>G. Poggi</u> , R. Giorgi, P. Baglioni <i>Nanocomposites for the consolidation and deacidification of cellulose-based artifacts</i>
10:30 - 11:00	Coffee Break
<i>Chairperson: Elisabetta Zendri</i>	
11:00 - 11:25	ABC/ANA/FIS KN02: <u>Erika Ribechini</u> <i>GC/MS and HPLC/MS characterization of organic residues from ceramic vessels of Basque whalers of the 16th to 17th century</i>
11:25 - 11:40	ABC/ANA/FIS OR05: <u>Francesca Di Turo</u> <i>FIB-FESEM-EDX study of silver Roman coins: characterization of the core microstructure and corrosion products with a multi-analytical approach</i>
11:40 - 11:55	ABC/ANA/FIS OR06: <u>Antonella Casoli</u> <i>I materiali e la tecnica pittorica di Konrad Witz nel suo capolavoro di Ginevra</i>
11:55 - 12:10	ABC/ANA/FIS OR07: <u>Elettra Barberis</u> <i>Towards the Non-invasive Proteomic Analysis of Cultural Heritage and Archaeological Objects</i>
12:10 - 12:25	ABC/ANA/FIS OR08: <u>Giuseppe Egidio De Benedetto</u> <i>Provenance of bitumen from different Apulian Bronze Age settlements through a biomarker based approach</i>
12:25 - 12:40	ABC/ANA/FIS OR09: <u>Marzia Fantauzzi</u> <i>From XAES signals to depth-profile reconstruction: the case of copper and copper alloys</i>
12:40 - 12:55	ABC/ANA/FIS OR10: <u>Marco Orlandi</u> <i>Integrated approach for the chemical characterization of archaeological woods</i>
<i>Sala Diana - Hotel Ariston</i>	
<i>Sessione: Sistemi Biologici - Fisica</i>	
<i>Chairpersons: Carla Isernia, Concetta Giancola</i>	
11:00 - 11:50	CSB PL2: <u>Maria Rosaria Tinè</u> <i>Calorimetry and Thermoanalytical Techniques in the Study of Proteins</i>
11:50 - 12:05	FIS OR69: <u>R. Oliva</u> , A. Grimaldi, P. Del Vecchio, V. Cafaro, K. Pane, E. Notomista, L. Petraccone <i>Biophysical studies of membrane perturbation induced by the antimicrobial peptide GK20</i>

12:05 - 12:20	CSB OR3: Alessandro D'Urso <i>Exploiting conformation and structural analysis of endogenous miRNAs to refine gene targeting evaluation</i>
12.20 - 12.35	FIS OR70: <u>A. Del Giudice</u> , C. Dicko, L. Galantini, N. V. Pavel <i>The structural response of Human Serum Albumin to oxidation: a biological buffer to local formation of hypochlorite</i>
12.35 - 12.50	CSB OR4: Jussara Amato <i>Identification and characterization of DNA G-quadruplex interacting proteins</i>

Joined Sessions
Martedì 12 Settembre 2017

<i>Sala Vivaldi - Hotel Savoy</i>	
Sessione Congiunta: Fisica - Elettrochimica - Enerchem	
Chairpersons: Moreno Meneghetti, Alessandro Minguzzi	
9:00 - 9:30	ELE KN01: <u>Riccardo Ruffo</u> <i>Negative Electrode Materials for Sodium Ion Batteries</i>
9:30 - 9:45	FIS OR51: <u>F. Lamberti</u> , L. Litti, M. De Bastiani, R. Sorrentino, M. Gandini, M. Meneghetti, A. Petrozza <i>High-Quality, Ligands-Free, Mixed-Halide Perovskite Nanocrystals Ink for Optoelectronic applications</i>
9:45 - 10:00	ELE OR20: <u>M. Musiani</u> , E. Verlato, S. Barison, S. Cimino, L. Lisi, G. Mancino, F. Paolucci <i>Electrochemical preparation of nanostructured CeO₂-Pt catalysts on Fe-Cr-Al alloy foams for the low-temperature combustion of methanol</i>
10:00 - 10:15	FIS OR52: <u>S. Binetti</u> , A. Le Donne, M. Acciarri, S. Marchionna <i>New Earth-Abundant Thin Film Solar Cells Based on Cu₂MnSnS₄</i>
10:15 - 10:30	ELE OR21: <u>C. Durante</u> , G. Daniel, G. Mattiacci, G. A. Rizzi, A. Gennaro <i>Platinum free Electrocatalyst based on Fe-Nx moieties supported on Mesoporous Carbon prepared from polysaccharides for Oxygen Reduction Reaction</i>
10:30 - 11:00	Coffee Break
Sessione Congiunta: Elettrochimica - Fisica - Enerchem	
Chairpersons: Simona Binetti, Claudio Gerbaldi	
11:00 - 11:15	FIS OR53: <u>P. Mustarelli</u> , F. Invernizzi, M. Patrini, K. Vezzù, V. Di Noto <i>Polyurethane-based Electrostrictive Nanocomposites as High Strain - Low Frequency Mechanical Energy Harvesters</i>
11:15 - 11:30	FIS OR54: <u>G. L. Chiarello</u> , M. Bernareggi, M. Pedroni, M. Magni, S. M. Pietralunga, E. Vassallo, E. Selli <i>A Bilayer WO₃ n-n Heterojunction Photoanode prepared by RF Diode Sputtering for Improved Photoelectrocatalytic Water Splitting</i>
11:30 - 11:45	ELE OR22: <u>F. Bella</u> , F. Colò, L. Zolin, D. Pugliese, A. M. Stephan, C. Gerbaldi <i>Lignocellulosic Materials for Electrochemical Energy Storage and Conversion</i>
11:45 - 12:00	FIS OR55: <u>S. Brutti</u> , S. Panero, A. Paolone, P. Reale <i>Hydrides as High Capacity Anodes in Lithium Cells: An Italian "Futuro in Ricerca di Base FIRB-2010" Project</i>
12:00 - 12:15	ELE OR23: <u>F. Bertasi</u> , V. Di Noto - <i>Secondary Magnesium Batteries: an Overview on Ionic Liquid -based Electrolytes</i>
12:15 - 12:30	FIS OR56: <u>S. La Gatta</u> , F. Milano, R. Ragni, A. Agostiano, G. M. Farinola, M. Trotta <i>Bio-hybrid Complexes in Artificial Photosynthesis</i>
12:30 - 12:45	ELE OR24: <u>A. Minguzzi</u> , M. Fracchia, A. Visibile, A. Naldoni, F. Malara, C. Locatelli, A. Vertova, P. Ghigna, S. Rondinini <i>Operando (photo)electrochemical X-ray absorption spectroscopy for water splitting</i>

12:45 - 13:00	FIS OR57: <u>A. Beneduci</u> , A. L. Capodilupo, G. A. Corrente, E. Fabiano, V. Maltese, S. Cospito, G. Ciccarella, G. Chidichimo, G. Gigli <i>Electronic Coupling in H-Shaped Tetra-Arylamine Mixed-Valence Compounds</i>
13:00 - 14:00	Intervallo Pranzo

Joined Sessions
Mercoledì 13 Settembre 2017

<i>Sala Puccini - Hotel Savoy</i>	
<i>Sessione Congiunta: Fisica - Teorica</i>	
<i>Chairperson: Michele Pavone</i>	
15:00 - 15:40	TEO KN01: <u>C. Cappelli</u> <i>A Fully Polarizable Embedding Model for Molecular Spectroscopy of Aqueous Solutions</i>
15:40 - 16:00	TEO OR01: <u>R. Dovesi</u> , S. Salustro, F. Gentile, Y. Noel <i>Hydrogen defects in diamond. A quantum mechanical approach</i>
16:00 - 16:15	FIS OR58: <u>L. Zamirri</u> , M. Corno, A. Rimola, P. Ugliengo <i>Forsterite surfaces as models of interstellar core dust grains: computational study of carbon monoxide adsorption</i>
16:15 - 16:30	FIS OR59: <u>M. Mattia</u> , D. E. Claudio, D. Luca, P. Cristina, S. Lorenzo <i>Prebiotic Molecules in Interstellar Space: Aminoacetonitrile and C-Cyanomethanimine</i>
16:30 - 17:00	Coffee Break
<i>Chairperson: Ludovico Valli</i>	
17:00 - 17:15	FIS OR60: <u>M. V. La Rocca</u> , L. Izzo, S. Losio, M. Mella <i>Should we introduce pre-equilibria into Markov models for homogeneously catalyzed copolymerization?</i>
17:15 - 17:30	FIS OR61: <u>F. Di Maiolo</u> , C. Pieroni, A. Painelli <i>Intramolecular Energy Transfer in Real Time</i>
17:30 - 17:45	TEO OR02: <u>E. Bodo</u> , A. Le Donne <i>Proton Mobility in Protic Ionic Liquids: New Results from Theoretical Calculations</i>
17:45 - 18:00	TEO OR03: <u>N. Tasinato</u> , L. Spada, C. Puzzarini, V. Barone <i>Computational Tools for the Interpretation of Rotational Spectra within the Virtual Multifrequency Spectrometer</i>
18:00 - 18:15	FIS OR62: <u>A. Mariani</u> , R. Caminiti, L. Gontrani <i>A spotlight on the complex hierarchical structure of some ionic liquid-molecular liquid binary mixtures</i>
18:15 - 18:30	FIS OR63: <u>O. Russina</u> , R. Caminiti <i>Fluorous mesoscopic domains in room temperature ionic liquids</i>
18:30 - 18:45	FIS OR64: <u>E. Fois</u> , R. Arletti, L. Gigli, G. Vezzalini, S. Quartieri, G. Tabacchi <i>Supramolecular Organization of Water-Ethanol Solution in Ferrierite under Pressure</i>

Divisione di Chimica Industriale

Lunedì 11 Settembre 2017

<i>Sala Hera</i>	
<i>Session I - Catalysis and Green Chemistry</i>	
<i>Chairperson Fabrizio Cavani</i>	
9:00 – 9:20	IND-OR01: <u>ElnazBahadori</u> , Matteo Compagnoni, Antonio Tripodi, Laura Prati, Carlo Pirola, GianguidoRamis, Ilenia Rossetti. <i>CO₂ photoreduction at high pressure to both gas and liquid products over titanium dioxide: the effect of unconventional reaction conditions.</i>
9:20 – 9:40	IND-OR02: <u>Giuseppe Bonura</u> , Catia Cannilla, Fabio Costa, Aldo Mezzapica, Francesco Frusteri. <i>How structural and surface properties affect stability of hybrid CuZnZr-zeolite catalysts during DME synthesis via CO₂ hydrogenation.</i>
9:40 – 10:00	IND-OR03: <u>Filippo Bossola</u> , Xavier Isidro Pereira-Hernández, Claudio Evangelisti, Yong Wang, Vladimiro Dal Santo. <i>Investigation of the promoting effect of Mn on a Pt/C catalyst for the steam and aqueous phase reforming of glycerol.</i>
10:00– 10:20	IND-OR04: <u>Emilia Paone</u> , Rosario Pietropaolo, Francesco Mauriello. <i>Selective arene production from aromatic ethers promoted by Pd/Fe₃O₄ catalyst under transfer hydrogenolysis conditions.</i>
10:20 – 10:40	IND-OR05: <u>Riccardo Balzarotti</u> , Matteo Ambrosetti, Gianpiero Groppi, Enrico Tronconi. <i>Investigation of coating deposition and catalytic activation of Periodic Open Cellular Structures (POCS) by spin-coating.</i>
10:40 – 11:00	Coffee Break
<i>Sala Hera</i>	
<i>Session II - New Materials</i>	
<i>Chairperson Rinaldo Psaro</i>	
11:00 – 11:20	IND-OR06: <u>Pier Paolo Proisini</u> , Mariasole Di Carli, Livia Della Seta, Maria Carewska, Ivan Fuso Nerini. <i>Ethylene vinyl acetate: a promising binding material for high power-high energy electrodes with a prolonged cycle life</i>
11:20 – 11:40	IND-OR07: <u>Antonio Abbadessa</u> , Antonio Rescifina, Angelo Nicosia, Andrea A. Scamporrino, Fabiola Spitaleri, Placido G. Mineo. <i>Synthesis and characterization of copolycarbonates having azobenzene units in the main chain as an active group for optical logic gate devices.</i>
11:40 – 12:00	IND-OR08: <u>Vincenzo Villani</u> , Vito Lavallata. <i>Unexpected viscoelasticity of Polydimethylsiloxane liquid blends.</i>
<i>Sala Hera</i>	
<i>Flash Presentation Session 12:00-13:00</i>	
<i>Chairperson Martino Di Serio</i>	
IND-FC01: <u>Francesca Coló</u> , Federico Bella, Jijeesh R. Nair, Claudio Gerbaldi. <i>Polymer electrolytes prepared by industrially compatible processes for renewable energy storage in sodium batteries.</i>	
IND-FC02: <u>Antonio De Luca</u> , Emanuele Piciollo, Claudio Picchi, Alessio Ceccarini, Emanuele Salvietti, Francesco Di Benedetto, Stefano Caporali, Stefano Martinuzzi, Massimo Innocenti. <i>Thin film of black-gold by electrodeposition, for jewellery making.</i>	
IND-FC03: <u>Grazia Leonzio</u> . <i>Study of Fenton reactor in a wastewater treatment plant.</i>	

IND-FC04: <u>Giada Innocenti</u> , Andrea Malmusi, Matteo Della Pasqua, J. Velasquez Ochoa, Fabrizio Cavani. <i>Isoprene production from methanol: an investigation on the reaction mechanism.</i>	
IND-FC05: <u>David Hermann Lamparelli</u> , Antonio Buonerba, Nunzia Galdi, Leone Oliva. <i>Diblock copolymer ethylene-syndiotactic styrene.</i>	
IND-FC06: <u>Federica Leone</u> , Andrea Gignone, Silvia Ronchetti, Roberta Cavalli, Luigi Manna, Mauro Banchemo, Barbara Onida. <i>An organic-solvent-free route to obtain nanostructured zinc oxide-based reservoir of clotrimazole.</i>	
IND-FC07: <u>Marino Malavolti</u> , Antonietta Schirò, Marco Cerra. <i>Cool Roofing, where chemistry indirectly helps environment.</i>	
IND-FC08: <u>Mattia Melloni</u> , Fabrizio Cavani, Anna Maria Raspolli Galletti, Hilda Gomez Bernal, Claudia Antonetti. <i>Integrated catalytic process for biomass hydrolysis: a comparison of different pretreatments and catalysts.</i>	
IND-FC09: <u>Wanda Navarra</u> , Olga Sacco, Vincenzo Vaiano, Diana Sannino, Christophe Daniel, Vincenzo Venditto. <i>Removal of non-degradable organic compounds from water with nanocomposite aerogels.</i>	
IND-FC10: <u>Veronica Pragli</u> , ElnazBahadori, Matteo Compagnoni, GianguidoRamis, Ilenia Rossetti. <i>Heterogeneous photocatalytic processes for the abatement of N-containing pollutants from wastewater.</i>	
IND-FC11: <u>Francesco Puzzo</u> , Giulia Pavarelli, Carlo Lucarelli, Fabrizio Cavani. <i>The upgrading of bio-alcohols: production of added-value chemicals by the gas-phase (oxi)dehydration of 1-butanol over V/P/O catalysts.</i>	
IND-FC12: <u>Antonietta Cozzolino</u> , Paola Rizzo, Gaetano Guerra. <i>Antimicrobial release from s-PS Active Packaging.</i>	
IND-FC13: <u>Antonella Salvini</u> , Arianna Bracciali, Bernardo Grossi, Donatella Giomi, Mario Tredici, Liliana Rodolfi, Massimo D'Ottavio, Luca Meschisi, Alberto Brandi. <i>Biorefinery from the marine microalga Nannochloropsis oceanica.</i>	
IND-FC14: <u>Michela Signoretto</u> , Alberto Olivo, MaelaManzoli, Ilenia Rossetti, Mercedes Maroto-Valer. <i>Lookingat the bigger picture in carbondioxidephotoreduction.</i>	
IND-FC15: <u>Maria Ricciardi</u> , Raffaele Cucciniello, Daniele Cespi, Carmine Capacchione, Ivano Vassura, Fabrizio Passarini, Antonio Proto. <i>Synthesis of monoalkylglyceryl ethers using glycidol as green starting material.</i>	
13:00 – 14:00	Intervallo Pranzo – Lunch Break
<i>Sala Hera</i>	
14:00 – 15:00	Riunione Gruppo Interdivisionale Catalisi Riunione Comitato Direttivo Divisione Chimica Industriale
<i>Sala Paestum B</i>	
14:00 – 15:00	Poster Session (IND FC01 – IND PFC15)
<i>Sala Hera</i>	
Session III - Homogeneous Catalysis	
Chairperson Antonella Salvini	
15:00 – 15:20	IND-OR09: <u>Carlo Bravin</u> , Donato M. Mancino, Giulia Licini, Cristiano Zonta. <i>Molecular recognition and catalysis within confined space.</i>
15:20 – 15:40	IND-OR10: <u>Cristiano Bolchi</u> , Francesco Bavo, Marco Pallavicini. <i>Producing amino acid benzyl esters under ecofriendly conditions and without racemization.</i>
15:40 – 16:00	IND-OR11: <u>Alberto Villa</u> , Ilenia Rossetti, Laura Prati, Aditya Savara. <i>Microkinetic modeling of benzyl alcohol oxidation on Pd and AuPd catalysts.</i>
16:00 – 16:20	IND-OR12: <u>Federica Sabuzi</u> , Pierluca Galloni, Valeria Conte. <i>Sustainable bromination of thymol: synthesis of new biologically active compounds.</i>

16:20 – 16:40	IND-OR13: <u>Marco Zecca</u> , Chiara Dalla Valle, Francesco Frison, Paolo Centomo. <i>New perspectives in the action of halide ions as promoter for the direct synthesis of hydrogen peroxide over palladium catalysts.</i>
16:40 – 17:00	Coffee Break

Sala Hera

Session IV - Catalysis and Materials**Chairperson Paolo Pollesel**

17:00 – 17:20	IND-OR14: <u>Federico Bella</u> , AndersHagfeldt, Michael Grätzel, Claudio Gerbaldi. <i>Current efforts to make perovskite solar cells industrially viable</i>
17:20 – 17:40	IND-OR15: <u>Silvia Bordiga</u> , Elisa Borfecchia, A. Martini, Chiara Negri, Gloria Berlier, Pablo Beato, Kirill A. Lomachenko, Carlo Lamberti, Dimitrios K. Pappas, Michael Martin Dyballa, Stian Svelle, Unni Olsbye. <i>Composition and temperature dependent Cu-speciation in Cu-SSZ-13 catalysts: an in situ XAS and FTIR study.</i>
17:40 – 18:00	IND-OR16: <u>Vito Di Noto</u> , Ketì Vezzù, Enrico Negro, Federico Bertasi, Giuseppe Pace. <i>Conductivity and relaxation phenomena in ion conducting materials by broadband electric spectroscopy.</i>
18:00 – 18:20	IND-OR17: <u>Galliano Simone</u> , Bella Federico, Falco Marisa, Barolo Claudia, Giordano Fabrizio, BoschlooGerrit, Grätzel Michael, HagfeldtAnders, Gerbaldi Claudio, Viscardi Guido. <i>Biosourced polymers for aqueous solar cells: a possible breakthrough towards green photovoltaic commercialization.</i>
18:20 – 18:40	IND-OR18: <u>Olga Sacco</u> , Vincenzo Vaiano, Wanda Navarra, Christophe Daniela, Vincenzo Venditto. <i>Development of N-doped TiO₂ catalyst for the photocatalytic treatment of wastewater in presence of visible light irradiation</i>
18:40 – 19:00	IND-PZ01: <u>Parmaliana Award Lecture by Matteo Monai</u> <i>Nanostructured materials for environmental and energy-related applications</i>
Sala Hera	
19:00 – 20:00	Assemblea dei Soci della Divisione di Chimica Industriale

Martedì 12 Settembre 2017

Sala Hera

Session V - Catalysis and Polymers**Chairperson Vincenzo Venditto**

9:00 – 9:20	IND-OR19: <u>Maria Michela Dell'Anna</u> , Matilda Mali, Giuseppe Romanazzi, Antonino Rizzuti, Cristina Leonelli, Piero Mastroianni. <i>Polymer supported palladium nanoparticles as catalyst for organic reactions in water.</i>
9:20 – 9:40	IND-OR20: <u>Rosa Vitiello</u> , Rosa Turco, Vincenzo Russo, Martino Di Serio, Riccardo Tesser. <i>Bromobutyl rubber synthesis: influence of the reaction temperature on product distribution.</i>
9:40 – 10:00	IND-OR21: <u>Rosita Lapenta</u> , Antonio Buonerba, Assunta De Nisi, Magda Monari, Alfonso Grassi, Stefano Milione, Carmine Capacchione. <i>Stereorigid OSSO-Type group 4 metal complexes in the polymerization of olefins and polar monomers.</i>
10:00 – 10:30	IND-IL01: Invited Lecture by <u>Gaetano Iaquaniello</u> <i>What role will chemistry and chemical engineering play in creating a sustainable and prosperous world</i>
10:30 – 10:50	Coffee Break
Sala Hera	

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Session VI - Materials and Formulations I	
Chairperson Michela Signoretto	
10:50 – 11:20	IND-IL02: Invited Lecture by <u>Amilcare Collina</u> <i>Materials chemistry for sustainable buildings: a review of MAPEI technologies.</i>
11:20 – 11:40	IND-OR22: <u>Elena Ghedini</u> , Michela Signoretto, Alessia Costantin, Alessandria Semenzato, Giuseppina Cerrato. <i>Smart formulations for cosmetic industrial applications.</i>
11:40 – 12:00	IND-OR23: <u>Matteo Guidotti</u> , Rinaldo Psaro, Elisabetta Gargani, Alessandro Caselli, Enrico L. Appiani, C. Cattaneo, Roberto Rappuoli. <i>Inorganically and organically modified mineral clays: a sustainable approach in the control of the olive tree fly pest, Bactrocera oleae.</i>
12:00 – 12:20	IND-OR24: <u>Mirco Nodari</u> , Aldo Longo, Dino Ferri, Andrea Perolo. <i>Modeling approach for applied research: the case-study of PLA synthesis by ring-opening polymerization of lactide</i>
12:20 – 12:40	IND-OR25: <u>Massimo Innocenti</u> , Maurizio Passaponti, Emanuele Salvietti, Stefano Martinuzzi, Emanuele Piciollo, Stefano Mariottini, Luca Rosi, Stefano Caporali, Walter Giurlani, Francesco Di Benedetto. <i>Chemical research in the field of galvanic industries and fashion accessory.</i>
12:40 – 13:00	IND-OR26: <u>Anna Malafronte</u> , Claudio De Rosa, Finizia Auriemma, Carmen Sasso. <i>Manipulating the arrangement of arrays of nanoparticles on solid supports by using self-assembled block copolymers templates.</i>
13:00 – 14:00	Intervallo Pranzo – Lunch Break

Mercoledì 13 Settembre 2017

Sala Paestum B	
14:00 – 15:00	Poster Session (IND PO01 – IND PO13)
Sala Hera	
Sessione VII- MSc and PhD Thesis Awards	
Chairperson Federico Bella	
15:00 – 15:10	IND-PZ02: Best MSc Thesis Award, lecture by <u>Massimo Christian D'Alterio</u> . <i>DFT-D Study of crystal phase transitions in syndiotactic polypropylene</i>
15:10 – 15:20	IND-PZ03: Best MSc Thesis Award, lecture by <u>Cristina Pizzolitto</u> . <i>Development of nanostructured nickel based catalysts for hydrogen production</i>
15:20 – 15:35	IND-PZ04: Best PhD Thesis Award, lecture by <u>Sebastiano Campisi</u> . <i>Novel approaches towards the optimisation of metal nanoparticle based catalysts</i>
15:35 – 15:50	IND-PZ05: Best PhD Thesis Award, lecture by <u>Tommaso Tabanelli</u> . <i>Sustainable catalytic processes for the synthesis and use of organic carbonates</i>
Sala Hera	
Session VIII - Materials and Formulations II	
Chairperson Federico Bella	
15:50 – 16:10	IND-OR27: <u>Giorgio Ferrari</u> . <i>New Sustainable Technology to Recover Returned Concrete.</i>
16:10 – 16:30	IND-OR28: <u>Raffaella Mancuso</u> , Roberta Amuso, Biagio Armentano, Anna R. Cappello, Francesco Galiano, Alberto Figoli, JanHoinkisd, Bartolo Gabriele. <i>Acryloxyalkyltriethylammonium bromides: useful starting materials for the preparation of polymeric membrane coatings with anti-biofouling properties.</i>
16:30 – 16:50	Coffee Break
Sala Hera	
Session IX- Biochemicals	
Chairperson Francesco Pignataro	

16:50 – 17:10	IND-OR29: <u>Paolo Centomo</u> , Chiara Dalla Valle, Federico Rastrelli, Sandro Campestrini, Marco Zecca. <i>Novel ion-exchange catalysts for the esterification of vegetable oil solutions of fatty acids with methanol</i>
17:10 – 17:30	IND-OR30: <u>Domenico Licursi</u> , Claudia Antonetti, Sara Fulignati, Alessandro Corsini, Anna Maria Raspolli Galletti. <i>The hydrothermal conversion of cellulose-rich wastes deriving from the papermaking process to levulinic acid as smart opportunity for their re-use and valorization.</i>
17:30 – 17:50	IND-OR31: <u>Vincenzo Russo</u> , Rosa Vitiello, Rosa Turco, Riccardo Tesser, Martino Di Serio. <i>Levulinic acid esterification kinetics with ethanol in the presence of Amberlyst-15.</i>
17:50 – 18:10	IND-OR32: <u>Nicola Scotti</u> , Federica Zaccheria, Claudio Evangelisti, Rinaldo Psaro, Nicoletta Ravasio. <i>Dehydrogenative coupling promoted by copper catalysts: a way to upgrade bio-alcohols</i>
18:10 – 18:30	IND-OR33: <u>Rosa Turco</u> , Martino Di Serio, Marcella Mazzocca, Vincenzo Russo, Riccardo Tesser, Rosa Vitiello, Donatella Cimini, Chiara Schiraldi. <i>Succinic acid Production from ArundoDonaxhydrolysate for bio-based poly(butylene succinate) synthesis.</i>
18:30 – 18:50	IND-PZ06: Mario Giacomo Levi Award Lecture by <u>Fabrizio Cavani</u> and <u>Mario Novelli</u> <i>n-Butane to Maleic anhydride: an impossible reaction and a catalyst which does miracles</i>
18:50 – 19:10	IND-OR34: <u>Ferruccio Trifirò</u> . <i>The history of the journal “La Chimica e l’Industria”</i>

Divisione Chimica Inorganica

Lunedì 11 Settembre 2017

<i>Sala Nettuno</i>	
<i>Sessione I</i>	
<i>Chairperson Francesco Paolo Fanizzi</i>	
9:00 – 9:45	INO-PL01: <u>J. A. van Bokhoven</u> <i>Action at a distance: observing hydrogen spillover</i>
9:45 – 10:15	INO-KN01: <u>M. Chiesa</u> <i>Exploring and Engineering Spin-states in Solid State and Surface Chemistry</i>
10:15 – 10:30	INO-OR01: T. Kosmala, L. Calvillo, S. Agnoli, <u>G. Granozzi</u> <i>New methods and new catalysts for the oxygen reduction reaction at the cathode of fuel cells: surface science applied to CoO_x/Pd(100) ultrathin films.</i>
<i>Sala Mercurio</i>	
<i>Sessione II</i>	
<i>Chairperson Luigi Monsù Scolaro</i>	
9:45 – 10:15	INO-KN02: <u>M. Ravera</u> <i>Dual-targeting hybrid anticancer platinum(IV) prodrugs for combination therapy.</i>
10:15 – 10:30	INO-OR02: <u>D'Alonso</u> , Linda Leone, Marco Chino, Ornella Maglio, Flavia Nastri, Vincenzo Pavone and Angela Lombardi. <i>Control of enzymatic activity in a Mn-containing synthetic metalloenzyme.</i>
10:30 – 11:00	Coffee Break
<i>Sala Nettuno</i>	
<i>Sessione I</i>	
<i>Chairperson Alberto Albinati</i>	
11:00 – 11:30	INO-KN03: <u>R. Zanoni</u> <i>Highly delocalized stable systems on semiconductor surfaces</i>
11:30 – 11:45	INO-OR03: D. Cherni, N. Moussa, M. F. Ncib, L. Prati, A. Villa <i>Effect of N-doping in the activity of TiO₂ supported catalysts in glycerol oxidation</i>
11:45 – 12:00	INO-OR04: <u>P. Solokha</u> , S. De Negri, A. Saccone <i>Long Period Stacking Ordered phases in the Y-Ni-Mg system: experimental and structural studies</i>
12:00 – 12:15	INO-OR05: <u>M. Benedetti</u> , F. De Castro ^a , F. P. Fanizzi <i>General cooperative effects of single atom ligands on the ⁷³Ge, ¹¹⁹Sn and ²⁰⁷Pb NMR signals of tetrahedral [MX₄] (M = Ge, Sn, Pb; X₄ = combination of Cl, Br, I) coordination compounds</i>
12:15 – 12:30	INO-OR06: <u>F. Barzagli</u> , C. Giorgi, F. Mani, M. Peruzzini <i>CO₂ capture by aqueous Na₂CO₃ combined with the formation of high quality CaCO₃ and the release of pure CO₂ at room conditions</i>
12:30 – 12:45	INO-OR07: <u>M. La Rosa</u> , S. Silvi, G. Jonusauskas, N. D. McClenaghan, A. Credi <i>Long-lived luminescent Quantum Dots as result of Reversible Electronic Energy Transfer</i>
12:45 – 13:00	INO-OR08: <u>G. V. Bianco</u> , M. Grande, L. La Notte, E. Villari, M. M. Giangregorio, M. Losurdo, P. Capezzuto, A. Reale, A. D'Orazio, G. Bruno <i>Grafene Functionalization and Tuning of Transport Properties by Plasma Strategies</i>
<i>Sala Mercurio</i>	
<i>Sessione II</i>	
<i>Chairperson Nazzareno Re</i>	
11:00 – 11:30	INO-KN04: <u>L. Monsù Scolaro</u> <i>On the chirality in porphyrin nanoassemblies.</i>

11:30 – 11:45	INO-OR09: <u>I. Venditti</u> , M. Porchia, F. Tisato, C. Santini, M. Pellei, G. Iucci, C. Battocchio, C. Pietrosanti, G. Testa, I. Fratoddi <i>Drug delivery systems: hydrophilic gold nanoparticles for controlled drug loading and release.</i>
11:45 – 12:00	INO-OR10: <u>L. Conti</u> , A. Bencini, M. G. Fabbrini, C. Gellini, C. Giorgi, G. Pietraprazia, B. Valtancoli <i>Novel strained ruthenium complexes in photodynamic therapy</i>
12:00 – 12:15	INO-OR11: <u>S. Concilio</u> , L. Sessa, A. Massa, S. Piotta, P. Iannelli, R. Diana, B. Panunzi, U. Caruso <i>Fluorescent solvatochromic molecules as probes for lipid bilayers</i>
12:15 – 12:30	INO-OR12: <u>S. Samaritani</u> , D. Belli Dell' Amico, M. Colalillo, L. Labella, F. Marchetti, M. Hyeraci, A. N.García-Argáez, L. Dalla Via <i>Platinum(II) complexes of ligands containing OH functional groups: synthesis, reactivity and antiproliferative properties</i>
12:30 – 12:45	INO-OR13: <u>L. Izzo</u> , M. De Rosa, G. Vigliotta, A. Soriente, V. Capaccio, G. Gorrasi, R. Adami, E. Reverchon, M. Mella <i>Killing bacteria via ion-complexing polymeric materials</i>
12:45 – 13:00	INO-OR14: <u>D. Cirri</u> , T. Marzo, A. Pratesi, L. Messori <i>Novel gold(I) and silver(I) metal complexes as promising antibacterial candidates</i>

Sala Argiva**Sessione Congiunta Chimica Organica - Chimica Inorganica (GICO)****Chairperson Antonella Dalla Cort**

11:30 – 12:00	ORG/INO KN01: <u>Alessandro Caselli</u> <i>Catalytic Applications of Pyridine-Containing Macrocyclic Complexes</i>
12:00 – 12:30	ORG/INO-PZ01: EurJOC Junior Organometallic Chemist Lecture by <u>Valentina Pirovano</u> <i>Gold(I)-catalyzed [4+2] cycloaddition reactions of vinylindoles and allenes</i>
12:30 – 12:45	ORG/INO-OR01: Elia Matteucci, Andrea Baschieri, Cristiana Cesari, Rita Mazzoni, Claudia Bizzarri, <u>Letizia Sambri</u> <i>Functionalized triazolylidenes as versatile mesoionic carbenes: metal complexes for catalysis and luminescent materials</i>
12:45 – 13:00	ORG/INO-OR02: Andrea Squarcina, Martina Zonzin, <u>Mauro Carraro</u> , Marcella Bonchio <i>Copper complexes with biomimetic antioxidant activity</i>

13:00 – 14:00

Intervallo Pranzo -- Lunch Break

Sala Paestum B14:00-15:00 **Sessione Poster I (INO PO01 – INO PO10)****Sala Nettuno****Sessione I****Chairperson Michele Saviano**

15:00 – 15:45	INO-PL02: <u>P. Carloni</u> <i>Multiscale simulation-based structural predictions of metalloproteins of pharmacological relevance</i>
15:45 – 16:15	INO-KN05: <u>L. Zaccaro</u> , A. Del Gatto, L. Russo, B. Farina, A. Liguoro, S. Di Gaetano, D. Capasso, D. Comegna, R. Fattorusso, M. Saviano <i>RGDechi chimeric peptide as new scaffold for gaining insight into structural features of integrins selectivity for theranostics</i>
16:15 – 16:30	INO-OR15: <u>D. La Mendola</u> , G. Pandini, C. Satriano, A. Pietropaolo, I. Naletova, F. Gianì, A. Travalia, V. G. Nicoletti, G. Arena, E. Rizzarelli <i>The inorganic side of neurotrophins: metal coordination and new therapeutic perspectives</i>

Sala Mercurio	
Sessione II	
Chairperson Alceo Macchioni	
15:45 – 16:15	INO-KN06: <u>F. Ragaini</u> <i>Schiff Bases of the BIAN Family: from Symmetrical Biaryl Derivatives to Mixed, Alkyl, Chiral or Reduced Ligands and Heterogeneous Catalysts</i>
16:15 – 16:30	INO-OR16: <u>R. Gobetto</u> , C. Nervi <i>Homogenous and Heterogeneous Transition Metal Catalysts for CO₂ Reduction</i>
16:30 – 17:00	Coffee Break
Sala Nettuno	
Sessione I	
Chairperson Chiara Gabbiani	
17:00 – 17:15	INO-OR17: <u>A. Mariconda</u> , P. Longo, C. Saturnino, R. Lemba, M. S. Sinicropi <i>A new series of Ag and Au carbene complexes with interesting anticancer properties</i>
17:15 – 17:30	INO-OR18: <u>M. I. Nardella</u> , V. Mangini, A. Rosato, F. Arnesano, G. Natile <i>NMR studies on copper transport proteins interacting with silver nanoparticles</i>
17:30 – 17:45	INO-OR19: <u>M. P. Donzello</u> , E. Viola, C. Ercolani <i>New Differently Sized Neutral and Octacationic Porphyrazines. Physicochemical Properties and Potentialities as Anticancer Drugs</i>
17:45 – 18:00	INO-OR20: <u>T. Marzo</u> , D. Cirri, C. Gabbiani, A. Pratesi, T. Gamberi, F. Magherini, A. Guerri, T. Biver, A. Arcangeli, L. Messori <i>Auranofin, Et₃PAuCl and Et₃PAuI exert high in vitro cytotoxic effects toward colorectal cancer cell lines: a comparative chemical, biological and mechanistic study</i>
18:00 – 18:15	INO-OR21: <u>V. Firpo</u> , G. Zambrano, V. Pavone, K. L. Bren, A. Lombardi <i>Hydrogen Evolution Catalyzed by Cobalt Mimochrome VIa</i>
18:15 – 18:30	INO-OR22: <u>E. Gabano</u> , S. Gama, R. Vilar, M. Ravera, D. Osella <i>Bifunctional triamine Pt(II) complexes containing a DNA intercalating moiety</i>
18:30 – 18:45	INO-OR23: <u>L. Leone</u> , M. Chino, O. Maglio, V. Pavone, F. Nastro, A. Lombardi <i>Minimizing the release of reactive intermediates in O₂-dependent oxidation by de novo metalloenzymes</i>
Sala Mercurio	
Sessione II	
Chairperson Roberto Gobetto	
17:00 – 17:15	INO-OR24: <u>C. Capacchione</u> , M. Naddeo, E. Luciano, A. Buonerba, A. Grassi, A. Proto <i>Biosourced Polymers from Stereoregular Polymerization of Monoterpenes in the Presence of Homogeneous Titanium Catalysts.</i>
17:15 – 17:30	INO-OR25: <u>D. Intriari</u> , D. M. Carminati, E. Gallo <i>Sustainable synthesis of aziridines: versatile precursors of fine chemicals</i>
17:30 – 17:45	INO-OR26: <u>G. Manca</u> , A. Ienco, M. Peruzzini, C. Mealli <i>Aspects of the Functionalization of the Phosphorene Surface</i>
17:45 – 18:00	INO-OR27: <u>M. Mazzeo</u> , F. Isnard, M. Lamberti, C. Pellicchia <i>Polyesters from the Alternating Copolymerization of Epoxides and Cyclic Anhydrides</i>
18:00 – 18:15	INO-OR28: <u>L. Fagiolari</u> , G. Patzke, A. Macchioni <i>Water Oxidation catalyzed by Ir(III) and Ru(III)-doped hydrotalcite-like compounds</i>
18:15 – 18:30	INO-OR29: <u>R. Diana</u> , F. Borbone, U. Caruso, S. Concilio, S. Piotta, B. Panunzi, A. Tuzi <i>New Self-Assembling Luminescent Materials from Pyridyl Oxadiazole Zn(II) Complexes</i>
18:30 – 18:45	INO-OR30: <u>C. Garino</u> , G. Volpi, C. Barolo, R. Gobetto, C. Nervi, M. D. Weber, R. D. Costa <i>Luminescent complexes and their bright ligands</i>
Sala Nettuno	
18:45 – 20:00	<i>Assemblea dei Soci della Divisione di Chimica Inorganica</i>

Martedì 12 Settembre 2017

<i>Sala Nettuno</i>	
Sessione I	
Chairperson Maurizio Peruzzini	
9:00 – 9:45	INO-MD01: <u>G. Bertrand</u> <i>Stable carbenes and related species as powerful tools in inorganic chemistry</i> Medaglia Sacconi
9:45 – 10:15	INO-PZ01: <u>G. Ragazzon</u> , S. Silvi, A. Credi <i>Operating Molecular Machines: Thermodynamic and Kinetic Aspects</i> Premio miglior tesi di Dottorato
10:15 – 10:30	INO-IL01: <u>A. J. T. Shore</u> <i>Publishing your research in high impact journals</i>
<i>Sala Puccini (Hotel Savoy)</i>	
Sessione Congiunta Chimica Teorica - Chimica Inorganica	
Chairperson Gianluca Ciancaleoni	
9:00 – 9:40	TEO/INO-KN01: <u>B. Civalieri</u> <i>Ab initio modeling of Metal-Organic Frameworks: from gas adsorption to stimuli responsive properties</i>
9:40 – 10:00	TEO/INO-OR01: <u>A.B. Muñoz-García</u> , M. Pavone <i>Computational design of Sr₂Fe_{1.5}Mo_{0.5}O_{6-δ} (SFMO)-based bifunctional electrodes for proton-conducting solid oxide electrochemical cells</i>
10:00 – 10:20	TEO/INO-OR02: <u>M. Cutini</u> , M. Corno, P. Ugliengo <i>Insight From DFT Simulations On The Collagen/Hydroxyapatite Interface: A Simple Model Based On The Poly-Proline Polymer</i>
10:20 – 10:40	TEO/INO-OR03: <u>L. Falivene</u> , S. Kozlov, L. Cavallo <i>A DFT Rationalization of a Two Metals Strategy to Tune Selectivity in Catalysis</i>
10:30 – 11:00	Coffee Break
<i>Sala Nettuno</i>	
Sessione I	
Chairperson Gaetano Granozzi	
11:00 – 11:30	INO-KN07: <u>D. Armentano</u> , E. Pardo, A. Leyva-Pérez, A. Corma <i>Synthesis and X-ray Snapshots of Ultrasmall Metallic Clusters within Metal-Organic Frameworks for High Performance in Catalysis.</i>
11:30 – 11:45	INO-OR31: <u>M. Perfetti</u> , M. Serri, L Poggini, M Mannini, D Rovai, P Sainctavit, S Heutz, R Sessoli <i>Layer by layer order of molecular thin films detected by Torque Magnetometry</i>
11:45 – 12:00	INO-OR32: <u>F. Tessore</u> , G. Di Carlo, A. Orbelli Biroli, M. Pizzotti <i>Porphyrim-Sensitized Solar Cells: the challenge of photostability</i>
12:00 – 12:15	INO-OR33: <u>M. Melchionna</u> , F. Paolucci, M. Bonchio, F. Vizza, P. Fornasiero, M. Prato <i>Hierarchical materials based on carbon nanostructures as advanced catalysts in energy applications</i>
12:15 – 12:30	INO-OR34: <u>A. Carella</u> , R. Centore, M. Bonomo, D. Dini, A. Di Carlo <i>Pyran based dyes as photosensitizers for p-type dye-sensitized solar cells</i>
12:30 – 12:45	INO-OR35: <u>A. G. Marrani</u> , D. Giacco, R. Zaroni, S. Brutti <i>Unravelling the surface degradation mechanisms in ether electrolyte based Li-O₂ cells</i>
12:45 – 13:00	INO-OR36: <u>I. Fratoddi</u> , I. Venditti, L. Fontana, C. Sibilìa, G. Leahu, A. Belardini, R. Li Voti, C. Battocchio, R. Matassa, G. Familiari <i>Networks based on functionalized noble metal nanoparticles: advanced materials for optical and electronic applications</i>

<i>Sala Mercurio</i>	
<i>Sessione II</i>	
<i>Chairperson Emma Gallo</i>	
11:00 – 11:30	INO-KN08: <u>C. Tubaro</u> , M. Baron <i>Selective syntheses of mononuclear vs dinuclear gold(III) complexes with di(N-heterocyclic carbene) ligands</i>
11:30 – 11:45	INO-OR37: <u>C. Femoni</u> , G. Bussoli, I. Ciabatti, M. Ermini, M. Hayatifar, M. C. Iapalucci, S. Ruggieri, S. Zacchini <i>New examples of interstitial Bismuth atoms in icosahedral rhodium cages</i>
11:45 – 12:00	INO-OR38: <u>M. Atzori</u> , L. Tesi, E. Morra, M. Chiesa, L. Sorace, R. Sessoli <i>Synthetic Strategies Towards Quantum Coherence Time Enhancement in Potential Molecular Spin Qubits</i>
12:00 – 12:15	INO-OR39: <u>F. Grisi</u> , V. Paradiso, C. Costabile, V. Bertolasi <i>Olefin Metathesis Ruthenium Catalysts Bearing Backbone-Substituted Unsymmetrical NHC Ligands</i>
12:15 – 12:30	INO-OR40: L. Armelao, D. Belli Dell'Amico, G. Bottaro, <u>L. Labella</u> , F. Marchetti, S. Samaritani <i>4,4' bipyridine monoxide (bipyMO): a simple heterotopic divergent ligand</i>
12:30 – 12:45	INO-OR41: <u>L. Luconi</u> , G. Tuci, A. Rossin, G. Giambastiani <i>Catalysis by Group IV Amido-Pyridinate Complexes for the Reduction of Carbon Dioxide to Methane</i>
12:45 – 13:00	INO-OR42: M. Monticelli, <u>M. Baron</u> , A. Longhi, C. Tubaro, S. Bellemin-Laponnaz, C. Graiff, M. Rancan, G. Bottaro, L. Armelao <i>Dinuclear d^{10} complexes with nNHC/tzNHC heteroditopic carbene ligands and their luminescence properties</i>
<i>Sala Puccini (Hotel Savoy)</i>	
<i>Sessione Congiunta Chimica Teorica - Chimica Inorganica</i>	
<i>Chairperson Emilia Sicilia</i>	
11:20 – 12:00	TEO/INO-KN02: I. Tolbatov, C. Coletti, A. Marrone, <u>N. Re</u> <i>Insight into the Electrochemical Reduction Mechanism of Pt(IV) Anticancer Complexes</i>
12:00 – 12:20	TEO/INO-OR04: <u>T. Marino</u> , M. Prejanò, P. Piazzetta, N. Russo <i>The role of metal substitution in the metallo-enzymes: A theoretical point of view</i>
12:20 – 12:40	TEO/INO-OR05: <u>G. Ciancaleoni</u> , N. Bartalucci, L. Belpassi, F. Marchetti <i>Back-donation in d^0 Metal Complexes: Does it Exist? The case of Nb(V)</i>
12:40 – 13:00	TEO/INO-OR06: <u>G. Mazzone</u> , C. Regina, N. Russo <i>Combination of Porphyrin and Ruthenium-arene moieties for a Dual Anticancer Function. A Theoretical Investigation</i>
13:00 – 14:00	Intervallo Pranzo

<i>Sala Paestum B</i>	
14:00-15:00	<i>Sessione Poster 2 (INO PO11 – INO PO24)</i>

Mercoledì 13 Settembre 2017

<i>Sala Paestum B</i>	
14:00-15:00	<i>Sessione Poster 3 (INO PO25 – INO PO38)</i>
<i>Sala Nettuno</i>	
<i>Sessione Congiunta</i>	
<i>Chairperson Adriana Saccone</i>	
15:00 – 15:45	INO-PZ02: <u>M. Mannini</u> <i>Titolo della conferenza</i> <i>Premio Nasini</i>

15:45 – 16:30	INO-PZ03: <u>C. Landis</u> <i>Organotransition Metal Complexes, Catalysis, and Industry</i> Premio Chini
16:30 – 17:00	Coffee Break
Sala Nettuno	
Sessione Congiunta Chimica Organica - Chimica Inorganica (GICO)	
Chairperson Fabio Ragaini	
17:00 – 17:30	ORG/INO-KN02: <u>L. Zani</u> <i>Conjugated Organic Compounds for Solar Energy Conversion to Electricity and Fuels</i>
17:30 – 18:00	ORG/INO-PZ02: EurJIC Junior Organometallic Chemist Lecture by <u>M. Bellini</u> <i>Hydrogen and chemicals from renewable alcohols by Organometallic Electro-Reforming (OMER)</i>
18:00 – 18:15	ORG/INO-OR03: <u>W. Baratta</u> , R. Figliolia, S. Baldino, H. Günter Nedden, A. Zanotti-Gerosa <i>Mild N-Alkylation of Amines with Alcohols Catalyzed by Acetate Ruthenium Complexes</i>
18:15 – 18:30	ORG/INO-OR04: <u>R. Mazzoni</u> , C. Cesari, A. Cingolani, V. Zanotti, F. Cavani, F. Puzzo, C. Lucarelli, M. Mella, A. Tagliabue, T. Baker <i>The power of ligand combination in redox active ruthenium and iron complexes</i>
18:30 – 18:45	ORG/INO-OR05: <u>R. Figliolia</u> , S. Baldino, W. Baratta, S. Gibolout, H. Günter Nedden, A. Zanotti-Gerosa <i>Synthesis of New Carbonyl Diphosphane Ruthenium Complexes for Catalytic C-H Bond Activation Reactions</i>
Sala Mercurio	
Sessione II	
Chairperson Alberto Credi	
17:00 – 17:15	INO-OR43: <u>E. Diana</u> , E. Priola, F. Grifasi, R. Gobetto, M. R. Chierotti <i>Symbiotic structural and spectroscopic approach to reticular chemistry: the case study of luminescent Copper(I) cyanide coordination polymers.</i>
17:15 – 17:30	INO-OR44: <u>S. Pragliola</u> , A. Botta, V. Venditto, A. Velardo, R. Liguori, Alfredo Rubino <i>Polymer Stereoregularity Influence on Optical Properties of Carbazole-based Photoconductor Polymers</i>
17:30 – 17:45	INO-OR45: C. Daniel, P. Cortelletti, M. Pedroni, G. Antonio D'Amora, G. Guerra, <u>A. Speghini</u> <i>Upconverting polymeric aerogels</i>
17:45 – 18:00	INO-OR46: <u>C. Crestini</u> , H. Lang, e L. Zongo <i>Coordination Complexes and One Step Assembly of Natural Polyphenols for Versatile Nanocapsule Engineering</i>
18:00 – 18:15	INO-OR47: V. Nicolini, <u>G. Malavasi</u> , L. Menabue, G. Lusvardi, F. Benedetti, S. Valeri, P. Luches <i>Mesoporous bioactive glasses doped with cerium: investigation of catalase and SOD mimetic activities, and bioactivity</i>
18:15 – 18:30	INO-OR48: <u>M. Marchini</u> , A. Luisa, G. Bergamini, N. Demitri, M. Baroncini, P. Ceroni, E. Iengo <i>Tetrahedral Arrays of Metallo-porphyrins</i>
18:30 – 18:45	INO-OR49: <u>M. La Deda</u> , L. Sancey, G. Palermo, R. Termine, A. De Luca, E. I. Szerb, I. Aiello, A. Candreva, L. Ricciardi, M. Ghedini <i>Plasmonics Applied to a Nanotheranostic System: Synthesis, Photophysical Properties and Anticancer Activity of Silica/Gold Nanoparticles</i>

Divisione di Chimica Organica

Lunedì 11 Settembre 2017

<i>Auditorium Giove</i>	
9:00 – 9:30	Opening Remarks and Awards Ceremony
Plenary Session 1	
Chairperson: Cesare Gennari	
9:30-10:00	ORG MD01: Adolfo Quilico Medal Lecture - <u>Raffaele Riccio</u> <i>Changing paradigms in natural product chemistry: from structural elucidation to target identification</i>
10:00-10:30	ORG PZ01: Organic Chemistry for Life Science Award Lecture - <u>Franca Zanardi</u> <i>Playing with Peptidomimetic and Small-Molecule Drug Hybrids to Hit Cancer-Related Biomarkers</i>
10:30-11:00	Coffee Break
<i>Auditorium Giove</i>	
Chairperson: Valeria Conte	
11:00 – 11:30	ORG PZ02: Organic Chemistry for Process Development and Industrial Products Award Lecture - <u>Giorgio Bertolini</u> <i>From few grams to multi Tons of Active Pharmaceutical Ingredients - Some tips</i>
<i>Sala Argiva</i>	
Parallel Session 1A: Organic and Inorganic Chemistry Divisions' Joint Session on Organometallic Chemistry (GICO)	
Chairperson: Antonella Dalla Cort	
11:30 – 12:00	ORG/INO KN01: <u>Alessandro Caselli</u> <i>Catalytic Applications of Pyridine-Containing Macrocyclic Complexes</i>
12:00 – 12:30	ORG/INO PZ01: EurJOC Junior Organometallic Chemist Lecture - <u>Valentina Pirovano</u> <i>Gold(I)-catalyzed [4+2] cycloaddition reactions of vinylindoles and allenes</i>
12:30 – 12:45	ORG/INO OR01: Elia Matteucci, Andrea Baschieri, Cristiana Cesari, Rita Mazzoni, Claudia Bizzarri, <u>Letizia Sambri</u> <i>Functionalized triazolylidenes as versatile mesoionic carbenes: metal complexes for catalysis and luminescent materials</i>
12:45 – 13:00	ORG/INO OR02: Andrea Squarcina, Martina Zonzin, <u>Mauro Carraro</u> , Marcella Bonchio <i>Copper complexes with biomimetic antioxidant activity</i>
<i>Auditorium Giove</i>	
Parallel Session 1B: Enerchem	
Chairperson: Alessandro Abbotto	
11:30 – 11:45	ORG OR01: <u>Giuseppe Sforazzini</u> , Augustina Jozeliunaite, Edvinas Orentas, Daniele Fazzi, Walter Thiel <i>Molecular Engineering of π-Conjugated Systems Towards Light-Responsive Organic Semiconductors</i>
11:45 – 12:00	ORG OR02: <u>Chiara Liliana Boldrini</u> , Norberto Manfredi, Alessandro Abbotto <i>Organic sensitizers for solar fuels from dye-sensitized water splitting</i>
12:00 – 12:15	ORG OR03: <u>Gianluigi Albano</u> , Laura Antonella Aronica, Lorenzo Di Bari <i>Solution and solid-state supramolecular aggregates of new chiral oligothiophenes: synthesis and spectroscopic characterization</i>
12:15 – 12:30	ORG OR04: Francesca Parenti, Mirko Buffagni, <u>Alfonso Zambon</u> , Monica Caselli, Davide Vanossi, Adele Mucci <i>Novel oligothiophenes with reduced HOMO-LUMO band gap for Optoelectronics</i>
12:30 – 12:45	ORG OR05: <u>Alessandra Operamolla</u> <i>Organic and biological materials for organic electronics: adding functionality</i>

12:45 – 13:00	ORG OR06: <u>Roberto Grisorio</u> , Bart Roose, Silvia Colella, Andrea Listorti, Gian Paolo Suranna, Antonio Abate <i>Molecular Tailoring of Hole-Transporting Materials for High-Performing Perovskite Solar Cells</i>
13:00 – 13:15	ORG OR07: <u>Pierluca Galloni</u> , Federica Sabuzi, Barbara Floris, Francesca Valentini, Laura Micheli, Andrea Sartorel, Emanuela Gatto, Giuseppe Palleschi, Valeria Conte <i>KuQuinones as photocatalysts in Light-driven water splitting</i>

13:00 – 14:00	Intervallo Pranzo – Lunch Break
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Sala Paestum B	
14:00 – 15:00	Poster Session 1 (ORG PO01 – ORG PO33)

Sala Argiva	
Parallel Session 2A	
Chairperson: Olga Bortolini	
15:00 – 15:30	ORG PZ03: Methodologies in Organic Chemistry Junior Award Lecture - <u>Giovanni Maestri</u> <i>The chemistry of stable trinuclear all-metal aromatics</i>
15:30 – 16:00	ORG PZ04: Organic Chemistry for Environment, Energy and Nanoscience Junior Award Lecture - <u>Giulia Fiorani</u> <i>Towards Bio-based Organic Carbonates and Polycarbonates via Coupling of Highly Substituted Oxiranes and CO₂</i>
16:00 – 16:15	ORG OR08: <u>Gianluca Salerno</u> , Marco Consumi, Agnese Magnani, Cristina Nativi, Barbara Richichi <i>A quick and facile synthesis of stable, water-soluble CdSe/ZnS quantum dots</i>
16:15 – 16:30	ORG OR09: <u>Francesca Biscaglia</u> , Santina Quarta, Gianmarco Villano, Cristian Turato, Alessandra Biasiolo, Patrizia Pontisso, Moreno Meneghetti, Marina Gobbo <i>PreSI Functionalized Gold Nanostructures for Liver Cancer Cells Targeting and Surface-Enhanced Raman Resonance Scattering Imaging</i>

Auditorium Giove	
Parallel Session 2B	
Chairperson: Giuseppe Musumarra	
15:00 – 15:30	ORG PZ05: Organic Chemistry in Life Science Junior Award Lecture - <u>Laura Russo</u> <i>When glycochemistry meets biomaterials: from design to application of synthetic glyco-tools</i>
15:30 – 16:00	ORG PZ06: Organic Chemistry for Process Development and Industrial Products Junior Award Lecture - <u>Andrea Bonetti</u> , <i>Semisynthetic ways for the preparation of Homoharringtonine: an industrial approach</i>
16:00 – 16:15	ORG OR10: Andrea Rozzi, Saša Korom, Alex Manicardi, Massimiliano Donato Verona, Vincenzo Verdolino, <u>Roberto Corradini</u> <i>Design and Synthesis of polyfunctional PNAs - A Biomolecular Engineering approach</i>
16:15 – 16:30	ORG OR11: <u>Laura Medve</u> , Sonia Serna, Niels Reichardt, Silvia Achilli, Corinne Vivès, Franck Fieschi, Anna Bernardi <i>A Glycomimetic CHIP for microarray Screening of C-type Lectin Receptors</i>
16:30 – 17:00	Coffee Break

Sala Argiva	
Parallel Session 3A	
Chairperson: Maurizio Benaglia	
17:00 – 17:15	ORG OR12: <u>Cristina Prandi</u> , Stefano Nejrotti <i>Gold(I)-catalyzed rearrangement of heterocycles derived 1,3-enynes</i>

17:15 – 17:30	ORG OR13: <u>Francesca Ghirga</u> , Cinzia Ingallina, Federica Aiello, Federica Balzano, Ilaria D'Acquarica, Bruno Botta, Gloria Uccello-Barretta, Deborah Quaglio <i>Snapshot of Ruthenium–Carbene–Resorc[4]arene Complex in an Olefin Metathesis Reaction</i>
17:30 – 17:45	ORG OR14: <u>Mauro Sassi</u> , Sara Mattiello, Myles Rooney, Alessandro Sanzone, Paolo Brazzo, Luca Beverina <i>Efficient Suzuki-Miyaura micellar Cross-Coupling in water, at room temperature and under aerobic atmosphere. Organic materials going green</i>
17:45 – 18:00	ORG OR15: <u>Antonella Leggio</u> , Emilia Lucia Belsito, Alessandra Comandè, Lucia Lo Feudo, Angelo Liguori <i>TiCl₄-Assisted Protocols in Organic Synthesis: the Case of Amides and β-Enaminones</i>
18:00 – 18:15	ORG OR16: <u>Massimo Mella</u> , M. Vincenzo La Rocca, Egle M. Beccalli, Silvia Gazzola, Gianluigi Brogginì <i>Which reaction step controls regio selectivity in CuCl₂-catalyzed cyclization of alkynyl-substituted ureas and carbamates?</i>
18:15 – 18:30	ORG OR17: Raffaella Mancuso, <u>Bartolo Gabriele</u> <i>Divergent Syntheses of (E)-3-Isobenzofuran-1-(3H)-one and (1H)-Isochromen-1-one Derivatives by Palladium-Catalyzed Carbonylation of 2-Alkynylbenzoic Acids</i>
Auditorium Giove	
Parallel Session 3B	
Chairperson: Angela Zampella	
17:00 – 17:15	ORG OR18: <u>Roberto Fiammengo</u> , Hui Cai, Federica Degliangeli, Jia Liu, Christian Pett, Jing Hu, Horst Kunz, Ulrika Westerlind, Menji Lu <i>Eliciting specific humoral and cellular immune response by self-adjuvanting gold nanoparticles carrying tumor-associated MUC1 glycopeptides</i>
17:15 – 17:30	ORG OR19: <u>Alessandro Palmioli</u> , Carlotta Ciaramelli, Michela Spinelli, Gaia De Sanctis, Renata Tisi, Elena Sacco, Cristina Airoidi <i>Natural compounds in cancer prevention: effect of coffee extracts and their main polyphenolic component 5-CQA on oncogenic Ras proteins</i>
17:30 – 17:45	ORG OR20: <u>Filippo Doria</u> , Matteo Nadai, Matteo Scalabrin, Valentina Pirota, Vincenzo Grande, Greta Bergamaschi, Valeria Amendola, Sara N. Richter, Mauro Freccero <i>Synthesis and Binding Properties of a new Selective Scissoring Tool for Quadruplex Nucleic Acids</i>
17:45 – 18:00	ORG OR21: <u>Chiara Pennetta</u> , Alessandro Volonterio <i>Amino- and guanidinoglycoside based vectors for cell transfection</i>
18:00 – 18:15	ORG OR22: <u>Carmen Festa</u> , Simona De Marino, Maria Valeria D'Auria, Angela Zampella, Stefano Fiorucci, Vittorio Limongelli <i>Discovery of a new class of GPBAR1 modulators</i>
18:15 – 18:30	ORG OR23: <u>Silvana Alfei</u> , Gaby Brice Taptue <i>New promising vectors for gene delivery by a step-wise functionalization of a polyester-based non toxic dendrimer with N, N-dimethylglycine, N-methylglycine, lysine and arginine</i>
18:30 - 20:00	Assembly of the Organic Chemistry Division

Martedì 12 Settembre 2017

Sala Argiva	
Parallel Session 4A	
Chairperson: Emanuela Licandro	
9:00 – 9:15	ORG OR24: <u>Nadia Barbero</u> , Sonja Visentin, Claudia Barolo, Roberto Buscaino, Guido Viscardi <i>New polymethine dyes for photodynamic therapy</i>

9:15 – 9:30	ORG OR25: <u>Paola Manini</u> , Carmela Tania Prontera, Valeria Criscuolo, Alessandro Pezzella, Orlando Crescenzi, Michele Pavone, Marco d'Ischia, Maria Grazia Maglione, Paolo Tassini, Carla Minarini <i>From Melanins to OLED Devices: Taking Inspiration from the Black Human Pigments for the Design of Innovative Electroluminescent Materials</i>
9:30 – 9:45	ORG OR26: <u>Lorenzo Guazzelli</u> , Andrea Mezzetta, Stefano Becherini, Cinzia Chiappe <i>Modification of biopolymers in ionic liquids (ILs) media to access added value materials</i>
9:45 – 10:00	ORG OR27: <u>Heiko Lange</u> , Reza Ebrahimi Majdar, Claudia Crestini <i>Towards Integrated Continuous-Flow Fractionation and Functionalisation of Technical Lignins</i>
10:00 – 10:15	ORG OR28: <u>Alice Guarneri</u> , Marco Cesugli, Simone Lotteria, Francesca Vita, Cynthia Ebert, Lucia Gardossi <i>Chemo-enzymatic strategies for the synthesis and functionalization of renewable polymers and composite materials</i>
10:15– 10:30	ORG OR29: <u>Zoia Luca</u> , Anika Salanti, Marco Orlandi <i>Chemical Modifications for the Valorization of Lignin</i>

Sala Mercurio

Parallel Session 4B**Chairperson: Lucio Pellacani**

9:00 – 9:15	ORG OR30: <u>Luca Banfi</u> , Lisa Moni, Renata Riva, Andrea Basso, Andrea Bozzano, Daniele Cartagenova, Chiara Lambruschini, Elisa Martino, Marta Nola, Gabriella Vitali Forconesi <i>Multicomponent reactions on biocatalytically produced substrates</i>
9:15 – 9:30	ORG OR31: <u>Andrea Gualandi</u> , Daniele Mazarella, Aitor Ortega Martínéz, Luca Mengozzi, Fabio Calcinelli, Elia Matteucci, Filippo Monti, Nicola Armaroli, Letizia Sambri, Pier Giorgio Cozzi <i>Photocatalytic Radical Alkylation of Electrophilic Olefins by Benzylic and Alkyl Zinc-Sulfonates</i>
9:30 – 9:45	ORG OR32: <u>Polyssena Renzi</u> , Johnny Hioe, Ruth M. Gschwind <i>Decrypting Transition States by Light (DTS-hv) in Brønsted Acid Catalysis</i>
9:45 – 10:00	ORG OR33: <u>Osvaldo Lanzalunga</u> <i>Structural and Medium Effects in the Hydrogen Atom Transfer Processes Promoted by Short-Lived Aminoxyl Radicals</i>
10:00 – 10:15	ORG OR34: <u>Marco Paolino</u> , Stefania Fusi, Andrea Cappelli, Michael Filatov, Jérémie Léonard, Massimo Olivucci <i>An Ultrafast Molecular Photoswitch Bio-inspired by Green Fluorescent Protein Fluorophore</i>
10:15– 10:30	ORG OR35: Fabio Bellina, Nicola Guazzelli, <u>Marco Lessi</u> , Chiara Manzini, Giulia Marianetti, Luca A. Perego, Cristoforo Pezzetta, Andrea Pucci, Daniele Vergara <i>Highly selective arylation protocols to prepare bioactive and fluorescent imidazole-based compounds</i>

Auditorium Giove

Parallel Session 4C: Biotechnology**Chairperson: Francesco Nicotra**

9:00 – 9:15	ORG OR36: <u>Elena Lenci</u> , Alessio Rossi, Gloria Menchi, Andrea Trabocchi <i>Short Build/Couple/Pair Approaches for the Synthesis of Novel Glyco- and Peptidomimetic Scaffolds</i>
9:15 – 9:30	ORG OR37: <u>Roberta Teta</u> , Viggo Thor Marteinsson, René Groben, Marie-Lise Bourguet-Kondracki, Valeria Costantino, Alfonso Mangoni <i>A New Antibacterial Cyclic Peptide from Hot Springs</i>

9:30 – 9:45	ORG OR38: <u>Francesca Leonelli</u> , Angela La Bella, Luisa Maria Migneco, Rinaldo Marini Bettolo <i>Recent advances in the synthesis of stemarane diterpenoids</i>
9:45 – 10:00	ORG OR39: <u>Veronica Esposito</u> , Antonella Virgilio, Annapina Russo, Teresa Amato, Giulia Russo, Michela Varra, Luciano Mayol, Aldo Galeone <i>Easy chemical modifications to explore the 'Janus face' of TBA: anticoagulant vs antiproliferative properties</i>
10:00 – 10:15	ORG OR40: <u>Maria Luisa Di Gioia</u> , Monica Nardi, Manuela Oliverio, Antonio Procopio, Rosina Paonessa, Giovanni Sindona <i>The greening of protection/deprotection strategies in peptide synthesis</i>
10:15 – 10:30	ORG OR41: <u>Cosimo Gianluca Fortuna</u> , Carmela Bonaccorso, Vincenza Barresi, Cristina Satriano, Irina Naletova <i>Design, synthesis of new heterocyclic compounds and their biological activity against MCF-7 cell line</i>
10:30 – 11:00	Coffee Break
Plenary Session 2	
Chairpersons: Luca Banfi, Cinzia Chiappe and Domenico Misiti	
11:00 – 11:30	ORG MD02: Angelo Mangini Medal Lecture - <u>Maurizio Taddei</u> <i>From ADDA to Antibody Drug Conjugates. Some Examples of Target Oriented Syntheses, a Blessing and a Curse for a Chemist</i>
11:30 – 12:00	ORG MD03: Giacomo Ciamician Medal Lecture - <u>Davide Ravelli</u> <i>Photocatalytic Hydrogen Atom Transfer (HAT) in Organic Synthesis</i>
12:00 – 12:30	ORG PZ07: Methodologies in Organic Chemistry Award Lecture - <u>Massimo Bietti</u> , <i>Tuning Reactivity and Selectivity in Hydrogen Atom Transfer from Aliphatic C–H Bonds</i>
12:30 – 13:00	ORG PZ08: Organic Chemistry for Environment, Energy and Nanoscience Award Lecture - <u>Mauro Comes Franchini</u> <i>Organic coating of Metallic nanoparticles: theranostic applications in nanomedicine</i>
13:00 – 13:10	REAXYS-MYCS: <u>Carlos Rodriguez Del Rio (Elsevier)</u> <i>Oceans of data for informed decisions in chemistry. The shortest path from the question to insight</i>

13:00 – 14:00	Intervallo Pranzo – Lunch Break
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Sala Paestum B	
14:00 – 15:00	Poster Session 2 (ORG PO34 – ORG PO72)

Mercoledì 13 Settembre 2017

Sala Paestum B	
14:00 – 15:00	Poster Session 3 (ORG PO73 – ORG PO104)
Auditorium Giove	
Plenary Session 3	
Chairperson: Alberto Brandi	
15:00 – 15:30	ORG MD04: Piero Pino Medal Lecture - <u>Enrico Dalcanale</u> <i>The evolution of cavitand-based supramolecular polymers: from self-assembly to self-diagnostics</i>
Auditorium Giove	
Parallel Session 5A: Organic Chemistry in Industry	
Chairperson: Paolo Scrimin	
15:30 – 15:45	ORG OR42: <u>Luciano Lattuada</u> , Lorena Beltrami, Enrico Cappelletti, Aurelia Ferrigato, Giovanni Battista Giovenzana, Loredana Sini <i>Synthesis and application of bifunctional chelating agents based on AAZTA scaffold</i>

15:45 – 16:00	ORG OR43: <u>Simone Mantegazza</u> , Gabriele Razzetti, Emanuele Attolino, Chiara Vladiskovic <i>QU-IBX and B3-IBX: safe IBX adducts for periodinane oxidation reactions</i>
16:00 – 16:15	ORG OR44: <u>Aurelio Bonasera</u> , Sebastian Fredrich, Virginia Valderrey, Stefan Hecht <i>Light-Activated Amine Detection via Innovative Diarylethene Probes</i>
16:15 – 16:30	ORG OR45: <u>Alessandro Agosti</u> , Giorgio Bertolini, Giacomo Bruno, Christian Lautz, Thomas Glarner, Walter Deichtmann <i>Handling Hydrogen Peroxide On Large Scale: Synthesis of 5-bromo-2-nitropyridine</i>
Sala Argiva	
Parallel Session 5B: Green Chemistry - Sustainable Chemistry	
Chairperson: Marco d'Ischia	
15:30 – 15:45	ORG OR46: <u>Matteo Tiecco</u> , Raimondo Germani <i>Zwitterionic Deep Eutectic Solvents as Effective Alternatives to Organic Solvents and to Ionic Liquids</i>
15:45 – 16:00	ORG OR47: <u>Serena Gabrielli</u> , Enrico Marcantoni, Roberto Ballini, Susanna Sampaolesi, Elena Chiurchiù, Alessandro Palmieri <i>Innovative Two-Step Synthesis of Polysubstituted 6-NitroIndoles</i>
16:00 – 16:15	ORG OR48: <u>Marco Chiarini</u> , Giorgio Cerichelli <i>NMR study of mixed micelles: zwitterionic – cationic surfactant systems</i>
16:15 – 16:30	ORG OR49: <u>Salvatore Marullo</u> , Francesca D'Anna, Rossella Arrigo, Nadka Tzankova Dintcheva, Renato Noto, Carla Rizzo <i>Diimidazolium-based supramolecular ionogels for dye removal from wastewaters</i>
16:30 – 17:00	Coffee Break
Sala Nettuno	
Parallel Session 6A: Inorganic and Organic Chemistry Divisions' Joint Session on Organometallic Chemistry (GICO)	
Chairperson: Fabio Ragaini	
17:00 – 17:30	ORG/INO KN02: <u>Lorenzo Zani</u> <i>Conjugated Organic Compounds for Solar Energy Conversion to Electricity and Fuels</i>
17:30 – 18:00	ORG/INO PZ02: EurJIC Junior Organometallic Chemist Lecture - <u>Marco Bellini</u> <i>Hydrogen and chemicals from renewable alcohols by Organometallic Electro-Reforming (OMER)</i>
18:00 – 18:15	ORG/INO OR03: <u>Walter Baratta</u> , Rosario Figliolia, Salvatore Baldino, Hans Günter Nedden, Antonio Zanotti-Gerosa <i>Mild N-Alkylation of Amines with Alcohols Catalyzed by Acetate Ruthenium Complexes</i>
18:15 – 18:30	ORG/INO OR04: <u>Rita Mazzoni</u> , Cristiana Cesari, Andrea Cingolani, Valerio Zanotti, Fabrizio Cavani, Francesco Puzzo, Carlo Lucarelli, Massimo Mella, Andrea Tagliabue, Tom Baker <i>The power of ligand combination in redox active ruthenium and iron complexes</i>
18:30 – 18:45	ORG/INO OR05: <u>Rosario Figliolia</u> , Salvatore Baldino, Walter Baratta, Steven Gibolout, Hans Günter Nedden, Antonio Zanotti-Gerosa <i>Synthesis of New Carbonyl Diphosphane Ruthenium Complexes for Catalytic C-H Bond Activation Reactions</i>
Auditorium Giove	
Parallel Session 6B	
Chairperson: Giulia Licini	
17:00 – 17:15	ORG OR50: <u>Laura Goracci</u> , Martina Ceccarelli, Björn Wagner, Rubén Alvarez-Sanchez, Gabriele Cruciani <i>Assessment of drug-induced phospholipidosis risk based on distribution coefficient in brain polar lipids</i>

17:15 – 17:30	ORG OR51: Assunta Giordano, Giovanni Forte, Fabrizio Dal Piaz, Federica del Gaudio, Nunziatina De Tommasi, Patrizia Gazzero, Raffaele Riccio, Giuseppe Bifulco, <u>Simone Di Micco</u> <i>Identification of new ErbB4 inhibitors by inverse virtual screening</i>
17:30 – 17:45	ORG OR52: <u>Gianluigi Lauro</u> , Stefania Terracciano, Ines Bruno, Raffaele Riccio, Vincenza Cantone, Oliver Werz, Andreas Koeberle, Michele Manfra, Paolo Tortorella, Pietro Campiglia, Giuseppe Bifulco <i>Recent advances in the discovery of novel microsomal prostaglandin E₂ synthase-1 (mPGES-1) inhibitors</i>
17:45 – 18:00	ORG OR53: <u>Vittoria Graziani</u> , Valentina Belli, Monica Scognamiglio, Brigida D'Abrosca, Angela Chambery, Severina Pacifico, Simona Piccolella, Teresa Troiani, Nicoletta Potenza, Antonio Fiorentino <i>Cytotoxic secondary metabolites from Mediterranean Fabaceae species display antiproliferative activity against colon cancer cell lines</i>
18:00 – 18:15	ORG OR54: <u>Sara Piantini</u> , Stefano Menichetti, Luisa Bracci, Chiara Falciani, Jlenia Brunetti <i>Synthesis of new peptide-drug conjugates for targeted cancer diagnosis and therapy</i>
18:15 – 18:30	ORG OR55: <u>Salvatore Vincenzo Giofrè</u> , Roberto Romeo, Consuelo Celesti, Maria Assunta Chiacchio <i>Synthesis and Biological Evaluation of Some Pyrimidin-2,4-diones as Novel Non-Nucleoside Reverse Transcriptase Inhibitors</i>
18:30 – 18:45	ORG OR56: <u>Elena Petricci</u> , Fabrizio Manetti, Elena Cini, Roberta Santini, Barbara Stecca, Giuseppe Giannini <i>Synthesis and decoration of small molecules targeting the Hedgehog Signaling Pathway</i>
18:45 – 19:00	ORG OR57: <u>Francesco Sansone</u> , Stefania E. Sestito, Fabio A. Facchini, Iaria Morbioli, Jean-Marc Billod, Sonsoles Martin-Santamaria, Alessandro Casnati, Francesco Peri <i>Amphiphilic Guanidinocalixarenes Inhibit Lipopolysaccharide- and Lectin-stimulated Toll-like Receptor 4 Signaling</i>
Sala Argiva	
Parallel Session 6C	
Chairperson: Vito Capriati	
17:00 – 17:15	ORG OR58: <u>Silvia Cauteruccio</u> , Davide Dova, Clara Baldoli, Roberta Franzini, Claudio Villani, Emanuela Licandro <i>Synthesis and stereochemical properties of axially chiral benzo[1,2-b:4,3-b']dithiophene derivatives</i>
17:15 – 17:30	ORG OR59: <u>Margherita De Rosa</u> , Pellegrino La Manna, Carmen Talotta, Carmine Gaeta, Annunziata Soriente, Antonio Rescifina, Giuseppe Floresta, Placido Neri <i>Bioinspired organocatalysis of C-C bond-forming reactions</i>
17:30 – 17:45	ORG OR60: Marina Sicignano, Rosaria Schettini, Antonella Dentoni Litta, Francesco De Riccardis, Irene Izzo, <u>Giorgio Della Sala</u> <i>Highly diastereoselective synthesis of γ-butenolides and phthalides by Michael addition catalyzed by crown ethers</i>
17:45 – 18:00	ORG OR61: <u>Carla Sappino</u> , Paolo Bovicelli, Federica Di Pietro, Giuliana Righi, Marzia Oneto, Ludovica Primitivo, Lorenza Suber <i>Design of a new chiral nanosupported catalyst for asymmetric reactions</i>
18:00 – 18:15	ORG OR62: Vincenzo Algieri, <u>Antonio De Nino</u> , Loredana Maiuolo, Beatrice Russo, Pedro Merino <i>Asymmetric 1,3-dipolar cycloadditions catalyzed by a new imidazolidinone organocatalyst</i>
18:15 – 18:30	ORG OR63: <u>Susanna Sampaolesi</u> , Federico Vittorio Rossi, Alessandro Palmieri, Pietro Allegrini <i>A new highly efficient strategy to prepare racemic Anatabine</i>

18:30 – 18:45	ORG OR64: Carlo Bravin, Elena Badetti, Giulia Licini, <u>Cristiano Zonta</u> <i>Molecular Events within Confined Spaces</i>
18:45 – 19:00	ORG OR65: <u>Carlo F. Morelli</u> , Fabio Romagnuolo, Gabriele A. Franza, Cinzia Calvio, Giovanna Speranza <i>Synthetic application of bacterial γ-glutamyltransferases (GGTs)</i>

Divisione di Chimica dei Sistemi Biologici

Lunedì 11 Settembre 2017

Sala Diana

Sessione della Divisione di Chimica dei Sistemi Biologici**Chairpersons R. Purrello, S. Ciurli**

9.00 – 9.50	CSB PL01: <u>M. J. Maroney</u> , J.O. Campeciño, C.E. Carr, H.Q. Hu, H.T. Huang, Musiani F. and S. Ciurli <i>Bioinorganic chemistry from metals to enzymes: A nickel tour.</i>
9.50 – 10.10	CSB OR01: <u>L. Mazzei</u> , F. Musiani, G. Lente, M. Palombo, M. Cianci, S. Benini and S. Ciurli. <i>Biochemical and structural studies on the inhibition of urease, a nickel-dependent virulence factor.</i>
10.10 – 10.30	CSB OR02: <u>C. Pozzi</u> , S. Ciambellotti, C. Bernacchioni, F. Di Pisa, P. Turano and S. Mangani. <i>Structural and mechanistic insights into iron processing and biomineralization by vertebrate ferritins</i>
10.30 – 11.00	Coffee Break
Sessione congiunta con la Divisione di Chimica Fisica dedicata al Prof. Guido Barone	
Chairpersons C. Isernia, C. Giancola	
11.00 – 11.50	CSB PL02: M.R. Tiné. <i>Calorimetry and Thermoanalytical Techniques in the Study of Proteins.</i>
11.50 – 12.05	Divisione di Chimica Fisica: <u>R. Oliva</u> . <i>Biophysical studies of membrane perturbation induced by the antimicrobial peptide GKY20</i>
12.05 – 12.20	CSB OR03: <u>A. D'Urso</u> , C.M.A. Gangemi, S. Alaimo, A. Pulvirenti, A. Ferro and R. Purrello. <i>Exploiting conformation and structural analysis of endogenous miRNAs to refine gene targeting evaluation.</i>
12.20 – 12.35	Divisione di Chimica Fisica: <u>A. Del Giudice</u> . <i>The structural response of Human Serum Albumin to oxidation: a biological buffer to local formation of hypochlorite.</i>
12.35 – 12.50	CSB OR04: <u>J. Amato</u> . <i>Identification and characterization of DNA G-quadruplex interacting proteins.</i>

13.00 - 14.00

Intervallo Pranzo

Sala Diana

Sessione della Divisione di Chimica dei Sistemi Biologici**Chairpersons M.J. Maroney, A. Rosato**

15.00 – 15.50	CSB PL03: R. Fattorusso. <i>Protein folding pathways investigated by NMR spectroscopy.</i>
15.50 – 16.10	CSB OR05: <u>D. Marasco</u> , E. Novellino and S. La Manna. <i>Insights in self-recognition, misfolding and mislocalization mechanisms of Nucleophosmin 1 in Acute Myeloid Leukemia.</i>
16.10 – 16.30	CSB OR06: <u>L. Russo</u> , K. Giller, E. Pfitzner, C. Griesinger and Stefan Becker. <i>The molecular recognition mechanism of the coactivator NCoA-1 by STAT6.</i>
16.30 – 17.00	Coffee Break
Sessione della Divisione di Chimica dei Sistemi Biologici	
Chairpersons G. Fossati, A. D'Urso	

17.00 – 17.30	Premio Divisione di Chimica dei Sistemi Biologici- Italfarmaco CSB PL04: S. Sattin <i>Towards unconventional therapeutic approaches.</i>
17.30 – 17.45	CSB OR07: <u>M. Prejanò</u> , T. Marino, and N. Russo. <i>How can work methanol dehydrogenase from <i>Methylacidiphilum fumariolicum</i> with the alien Ce(III) ion in the active center? A theoretical study.</i>
17.45 – 18.00	CSB OR08: <u>V. Maggi</u> , F. Bianchini, A. Sartori and R. Fiammengo. <i>Aminoproline-RGD functionalized gold nanoparticles for targeting of integrins involved in tumor angiogenesis.</i>
18.00– 18.15	CSB OR09: <u>V. Oliveri</u> , S. Zimbone, M. L. Giuffrida, F. M. Tomasello, F. Bellia, G. Vecchio. <i>Functionalized cyclodextrins as modulators of Aβ cytotoxicity.</i>
18.15– 18.30	CSB OR10: <u>A. Bortot</u> , F. Munari, S. Zanzoni, M. D’Onofrio, D. Fushman and M. Assfalg. <i>Specific secondary interactions between ubiquitin and UBA observed in cell-mimicking crowded solution.</i>
18.30– 18.45	CSB OR11: <u>M. Gaeta</u> , R. Randazzo, D. A. Cristaldi, A. D’Urso, R. Purrello and M. E. Fragalà. <i>ZnTPPS demetallation: role of polyelectrolytes on aggregation after protonation in acid.</i>
18.45– 19.00	CSB OR12: <u>F. Arcudi</u> and M. Prato. <i>Synthesis, Separation and Characterization of Small and Highly Fluorescent Nitrogen-Doped Carbon NanoDots.</i>
Sala Diana	
19.00– 20.00	<i>Assemblea dei Soci della Divisione di Chimica dei Sistemi Biologici</i>

Martedì 11 Settembre 2017

Sala Diana	
Sessione congiunta con il gruppo Interdivisionale di Biotecnologie	
Chairpersons L. Cipolla, M. Coletta	
9.00 – 9.50	CSB PL05: D. Montesarchio. <i>Multifunctional nanosystems for theranostics.</i>
9.50 – 10.10	CSB OR13: <u>M. Gobbo</u> , F. Biscaglia, S. Rajendran, C. Benna, G. Bocchinfuso, P. Conflitti, L. Litti, R. Sommaggio, D. Nitti, A. Rosato, A. Palleschi, S. Mocellin and M. Meneghetti. <i>Peptide Targeted Gold Nanostructures for high effective SERRS Imaging of Colorectal Cancer Cells.</i>
10.10 – 10.30	Divisione di Chimica Organica: <u>G. Oliviero</u> , M. Marzano, A.P. Falanga, S. D’Errico, G. Piccialli, N. Borbone. <i>Higher order G-quadruplex-based aptamers from tetra-end-linked oligonucleotides with in vitro anti-HIV activity</i>
10.30 – 11.00	Coffee Break
Sessione della Divisione di Chimica dei Sistemi Biologici	
Chairpersons M. Assfalg, R. Fattorusso	
11.00 – 11.50	CSB PL06: S. C. Baffoni. <i>Unravelling the molecular mechanisms of iron-sulfur protein maturation.</i>
11.50 – 12.05	CSB OR14: <u>D. Sala</u> , S. Ciambellotti, A. Giachetti, P. Turano and A. Rosato. <i>Investigation of the iron(II) release mechanism from human ferritin as a function of pH.</i>
12.05 – 12.20	CSB OR15: <u>D. Capasso</u> , S. Di Gaetano, V. Celentano, D. Diana, L. Festa, R. Di Stasi, L. De Rosa, R. Fattorusso and L. D. D’Andrea. <i>Unveiling a VEGF-mimetic peptide sequence in IQGAP1 protein.</i>

12.20 – 12.35	CSB OR16: <u>M. Scognamiglio</u> and B. Schneider. <i>Metabolomics studies of allelopathy: unravelling chemical interactions between Mediterranean plants through an omics approach.</i>
12.35 – 12.50	CSB OR17: <u>A. P. Falanga</u> , N. Borbone, S. D’Errico, B. Pinto, M. Marzano, G. Piccialli and G. Oliviero. <i>Targeting of the G-quadruplex-forming bcl2G4-1 region in the human Bcl-2 gene with Peptide Nucleic Acid: an anti-gene approach for cancer treatment.</i>
12.50 – 13.05	CSB OR18: <u>M. De Zotti</u> , A. Bortolotto, I. Elmaghraby, L. Sella, F. Favaron. <i>Peptaibols: naturally occurring peptides as biopesticides.</i>
13.05 - 14.00	Intervallo Pranzo
	<i>Sala Paestum B</i>
14:00-15:00	<i>Sessione Poster 2 (CSB PO01 – CSB PO20)</i>

Divisione Didattica

Lunedì 11 Settembre 2017

<i>Sala Medusa</i>	
Sessione di apertura	
Chairperson: Giovanni Villani	
8:30 – 9:00	<i>Registrazione Partecipanti</i>
9:00 – 9:15	<i>Saluti</i>
9:15 – 10:00	DID-PL01: Margherita Venturi. <i>Chimica e creatività</i>
10:00 - 10:30	DID-KN01: Eleonora Aquilini. <i>Formazione Iniziale degli insegnanti: Legge aprile 2017</i>
10:30 – 11:00	Coffee Break
Sessione: Insegnare Chimica, che cosa e a chi	
Chairperson: Maria Funicello	
11:00 – 11:20	DID-OR01: Anna Madaio, Giuseppina Andreotti, Massimo Poletto, Renzo Stio <i>Insieme nel Reale e nel Virtuale per la chimica sostenibile – Progetto per le Scuole Secondarie di I grado</i>
11:20 – 11:40	DID-OR02: Patrick Marcantelli, Giovanni Villani, Silvana Saiello, Cecilia Giordano, Fabiana Tescione <i>Un approccio didattico alle Trasformazioni fisiche e chimiche della materia</i>
11:40 – 12:00	DID-OR03: Elena Lenci <i>La Chimica per la Luce: un percorso didattico attraverso la storia delle reazioni chimiche sfruttate dall'uomo per ottenere luce</i>
12:00 – 12:20	DID-OR04: Marilena Muraglia, Teresa Turi, Graziano De Scisciolo, Ivana Defrenza, Filomena Corbo, Maria Lisa Clodoveo, Franchini Carlo <i>Teknologia: A novel Project Based Learning (PBL) laboratory education program between Highschool and R&D</i>
12:20 – 12:40	DID-OR05: Francesca Vergine, Liberato Cardellini <i>La Chimica al Liceo – Il sogno di Giovanni</i>
12:40 – 13:00	DID-OR06: Enrico Mansueti, Liberato Cardellini <i>L'inclusione degli alunni con BES attraverso la realtà compensativa</i>
13:00 - 14:00	Intervallo Pranzo

<i>Sala Medusa</i>	
Sessione: Metodi e approcci all'insegnamento scientifico	
Chairperson: Anna Caronia	
15:00 – 15:20	DID-OR07: Laura Orian, Camilla Ferrante <i>Interdisciplinarietà, Co-progettazione e altro ancora nel PLS</i>
15:20 – 15:40	DID-OR08: Simonetta Antonaroli, Gabriella Bandini, Alessandra D'Epifanio, Mariano Venanzi <i>Chimica ed Energia: dalle parole ai fatti</i>
15:40 – 16:00	DID-OR09: Luca Scalzullo, Francesco Piero Paolicelli, Domenico Aprile, Rosanna Dell'Università, Daniele Sofia, Massimo Poletto <i>Un progetto civico per una centralina a basso costo per il monitoraggio delle polveri sottili</i>
16:30 – 17:00	Coffee Break
Sessione Tavola Rotonda	
Chairperson: Giovanni Villani	

17:00 – 18:30	Angela Agostiano, Ugo Cosentino, Antonio Floriano, Maria Rosaria Tinè <i>Corsi e Dottorati in Didattica della Chimica/Scienze</i>
18:30 – 20:00	<i>Riunione Consiglio Direttivo e Assemblea dei Soci della Divisione di Didattica.</i>

Martedì 12 Settembre 2017

<i>Sala Medusa</i>	
Sessione Tavola Rotonda	
9:00 – 10:30	Le associazioni AIF-ANISN-DDSCI-SIRD <i>Le competenze per insegnare</i>
10:30 – 11:00	Coffee Break
Sessione: Il Chimico verso il lavoro: esperienze formative	
Chairperson: Silvana Saiello	
11:00 – 11:30	DID-KN02: <u>Damiano Manigrassi</u> <i>Titolo della conferenza da definire</i>
11:30 – 11:50	DID-OR10: <u>Martino Di Serio</u> <i>Il Chimico nell'Industria: le competenze richieste</i>
11:50 – 12:10	DID-OR11: <u>Maria Funicello</u> <i>L'Università come luogo di lavoro per i giovani</i>
12:10 – 12:30	DID-OR12: <u>Anna Caronia</u> <i>Valutare l'alternanza per competenze</i>
13:00 - 14:00	Intervallo Pranzo
<i>Sala Paestum B</i>	
14:00 – 15:00	Sessione poster I (DID P001 – DID P012)

Mercoledì 13 Settembre 2017

<i>Sala Medusa</i>	
Sessione: Comunicare la Chimica: a chi e per che cosa	
Chairperson: Federica Bella	
15:00 – 15:30	DID-KN03: <u>Sara Tortorella</u> <i>Research at 360°: the novel mission of dissemination</i>
15:30 – 16:00	DID-KN04: <u>Valentina Domenici</u> <i>Perception of Chemistry and its relationship with Teaching and Communicating Chemistry</i>
16:00 – 16:20	DID-OR13: <u>Cristina Lazzerini, Valentina Domenici</u> <i>"Chemistry of Soap": an example of vertical curriculum developed in collaboration with a Science Museum</i>
16:20 – 16:40	DID-OR14: <u>Alice Soldà</u> <i>A European Video Contest to promote Chemistry among High Schools</i>
16:40 – 17:00	Coffee Break
Sessione Tavola rotonda	
Chairperson: Pietro Greco	
17:00 – 18:30	Luciano D'Alessio, Luigi Campanella, Luigi Amodio, Valentina Dominici <i>Comunicare le Scienze (e la Chimica) al grande pubblico</i>

Divisione di Spettrometria di Massa

Lunedì 11 Settembre 2017

<i>Sala Cassandra</i>	
Sessione Metabolomica e Lipidomica	
Chairperson: Donatella Caruso	
9:00 – 9:30	<i>Apertura lavori divisione</i>
9:30-10:10	MAS PL01: <u>Nico Mitro</u> , Matteo Audano, Silvia Pedretti, Maurizio Crestani, Enrique Saez, Emma De Fabiani and Donatella Caruso <i>Metabolomic approaches to unravel the role of a novel mitochondrial regulator</i>
10:10-10:30	MAS OR01: <u>Laura Goracci</u> , Sara Tortorella, Paolo Tiberi, Roberto Maria Pellegrino, Alessandra Di Veroli, Aurora Valeri, Lucia Cesarini, Gabriele Cruciani <i>Lipostar, a novel platform-neutral cheminformatics tool for untargeted and targeted lipidomics</i>
10:30 – 11:00	Coffee Break
Sessione Metabolomica e Lipidomica	
Chairperson: Donatella Caruso	
11:00 – 11:20	MAS OR02: <u>Gianluca Giorgi</u> <i>Metabolic fingerprinting of plants and wines</i>
11:20 – 11:40	MAS OR03: <u>Simona Scarpella</u> , Arthur Moseley, Chris Hughes, Erik J. Soderblom, Keith Richardson, Will Thompson, Johannes PC Vissers, Jason Wildgoose, James Langridge <i>Qualitative and quantitative characterization of a novel DIA method for omics analysis</i>
11:40 – 12:00	MAS OR04: <u>Calogera Monastero</u> , Angela Cuttitta, Antonella Maggio, Antonio Mazzola, Santino Orecchio, Bernardo Patti <i>Qualitative and quantitative analysis of fatty acids extracted from pelagic species of the Sicilian Channel, comparison with endogenous variables</i>
12:00 – 12:20	MAS OR05: <u>Gilda D'Urso</u> , Cosimo Pizza, Sonia Piacente, Paola Montoro <i>LC-MS based metabolomics and evaluation of the antioxidant activity of <i>Fragaria vesca</i> leaves</i>
12:20 – 12:40	MAS OR06: <u>Luisa Mattoli</u> , Cangi Francesca, Burico Michela, Anna Gaetano, Lorenzo Tafini, Fodaroni Giada, Stella Bedont, Sara Tamimi, Denise De Carli, Simona Propersi, Veronica Ercolani, Valentina Fiordelli, Enrico Flamini, Luca Grigi <i>Mass Spectrometry and natural complex products metabolomic analysis</i>
12:40 – 13:00	MAS OR07: Mariateresa Maldini <i>-OMICS world: take it easy! Solutions to Advance your Metabolomics Research</i>
13:00 – 14:00	Intervallo Pranzo

<i>Sala Cassandra</i>	
Sessione Congiunta Chimica Analitica Spettrometria di Massa	
Chairperson: Tommaso Cataldi	
15:00 – 15:30	ANA/MAS KN01: <u>Cosima Damiana Calvano</u> , Marco Glaciale, Sara Granafei, Anna Maria Sardanelli, Luana Bellanova, Antonella Mastrorocco, Francesco Palmisano, Tommaso R.I Cataldi <i>Advanced mass spectrometric techniques for the untargeted lipidome characterization of fibroblasts in early on-set Parkinson's disease patients</i>
15:30 – 15:50	ANA/MAS OR01: <u>Simone Nicolardi</u> , Yuri E.M. van der Burgt, Jeroen D.C. Codée, Manfred Wuhler, Cornelis, H. Hokke, Fabrizio Chiodo <i>Structural characterization of bio-functionalized gold nanoparticles by ultrahigh resolution mass spectrometry.</i>

15:50 – 16:10	ANA/MAS OR02: Lucia Cenci, Graziano Guella, <u>Alessandra Maria Bossi</u> <i>Molecularly imprinted materials coupled to MALDI-TOF Mass Spectrometry for the targeted analysis of peptides and proteins.</i>
16:10 – 16:30	ANA/MAS OR03: <u>Rossana Scarpone</u> , Roberta Rosato, Federico Bacá, Manuel Sergi, Dario Compagnone <i>Unknown and non-target analysis to determine pesticides in fruit and vegetables by means of UHPLC-HRMS (Orbitrap)</i>
16:30 – 17:00	Coffee Break
Sessione Congiunta Chimica Analitica Spettrometria di Massa	
Chairperson: Paola Montoro	
17:00 – 17:30	ANA/MAS KN02: <u>Daniilo Sciarrone</u> , Antonino Schepis, Luigi Mondello <i>Advanced analytical capabilities exploiting isotope ratio mass spectrometry and quadrupole mass spectrometry coupled to multidimensional gas chromatography</i>
17:30 – 17:50	ANA/MAS OR04: <u>Andreina Ricci</u> , Paola Cimino, Anna Troiani, Federico Pepi, Stefania Garzoli, Chiara Salvitti and Vincenzo Barone <i>From ascorbic acid to furan molecules: a theoretical and experimental study on the gas phase acid catalyzed degradation of vitamin C</i>
17:50 – 18:10	ANA/MAS OR05: <u>Veronica Termopoli</u> , Pierangela Palma, Giorgio Famiglini, Maurizio Piergiovanni, Achille Cappiello <i>Liquid-EI (LEI) Atmospheric Pressure Mechanism for the introduction of liquid streams into an unmodified electron ionization source of a mass spectrometer.</i>
18:10 – 18:30	ANA/MAS OR06: Chiara Salvitti, Andreina Ricci, Federico Pepi, Stefania Garzoli, Anna Troiani, Giulia De Petris, Marzio Rosi <i>Selective gas-phase conversion of D-fructose to 5-hydroxymethylfuraldehyde through a base-assisted dehydration process</i>

Martedì 12 Settembre 2017

Sala Cassandra	
Sessione Isotopi stabili	
Chairperson: Gianluca Giorgi	
9:00 – 9:40	MAS PL02: <u>Federica Camin</u> , Matteo Perini, Luana Bontempo <i>Stable isotope ratios for food authentication and traceability</i>
9:40 – 10:00	MAS OR08: <u>Antonella Macrì</u> , Paola Iacumin <i>Stable isotopes in fossil remains and environmental reconstruction</i>
10:00 – 10:20	MAS OR09: <u>Alessandro Pratesi</u> , Tiziano Marzo, Damiano Cirri, Luigi Messori <i>Mass spectrometry and metallomics: a powerful technique to delineate the mode-of-action of anticancer metallodrugs. The case of Oxaliplatin and its analogues</i>
10:20 – 10:40	MAS OR10: Lionel Mounier, <u>Luca Simonotti</u> , Andreas Hilkert <i>Chromatography-based EA-IRMS: redesigning the elemental analyzer around modern chromatographic principles to match the challenges of today's and tomorrow's applications</i>
10:40 – 11:00	Coffee Break
Sessione Life Sciences	
Chairperson: Nico Mitro	
11:00 – 11:40	MAS PL03: Violette Gautier, Linsey Raaijmakers, Christian K. Frese, Renske Penning, Charlotte A.G.H. van Gelder, Thierry Schmidlin, Gianluca Maddalo, Kristel Kemper, Oscar Krijgsman, Marina Mikhaylova, Riccardo Stucchi, Qingyang Liu, Harm Post, Markus Brockmann, Vincent A. Blomen, Joppe Nieuwenhuis, Elmer Stickel, Matthijs Raaben, Onno B. Bleijerveld, Lucas T. Jae, Thijn R. Brummelkamp, Shabaz Mohammed, Albert J. R. Heck, Casper C. Hoogenraad, Daniel S. Peeper and <u>A.F. Maarten Altaelaar</u> <i>High-resolution proteomics, integrative phosphoproteomics and targeted mass spectrometry to unravel complex biology</i>

11:40 – 12:00	MAS OR11: <u>Maurizio Piergiovanni</u> , Achille Cappiello, Giorgio Famigliani, Veronica Termopoli, Pierangela Palma <i>Determination of benzodiazepines in beverages using green extraction methods and HPLC-UV detection</i>
12:00 – 12:20	MAS OR12: <u>Marcello Manfredi</u> , Eleonora Conte, Elisa Robotti, Elettra Barberis, Fabio Gosetti, Eleonora Mazzucco, Valeria Caneparo, Ester Vanni, Santo Landolfo, Marisa Gariglio, Marco De Andrea, Emilio Marengo <i>Quantification of Plasma Proteins with micro-LC SWATH®-MS for Biomarker Discovery in Inflammatory Bowel Disease</i>
12:20 – 12:40	MAS OR13: <u>Ilaria Santoro</u> , Giovanni Sindona, Monica Nardi, Cinzia Benincasa <i>Improvements of extraction and identification methodologies of PUFA from algae</i>
12:40 – 13:00	MAS OR14: <u>Roberto Spezzano</u> , Gaia Cermenati, Mariateresa Maldini, Silvia Pedretti, Matteo Audano, Silvia Giatti, Marzia Pesaresi, Roberto Cosimo Melcangi, Nico Mitro, Donatella Caruso <i>Lack of sterol regulatory element binding protein-1c induces alteration of neuroactive steroid levels in sciatic nerve</i>
13:00 – 14:00	Intervallo Pranzo
Sala Paestum B	
14:00 – 15:00	Sessione Poster 2 (MAS PO01 – MAS PO05)

Divisione di Chimica Teorica e Computazionale

Lunedì 11 Settembre 2017

<i>Hotel Savoy Sala Puccini</i>	
<i>Sessione DCTC</i>	
<i>Chairperson: Mauro Stener</i>	
9.00 – 9.40	TEO KN01: <u>Massimiliano Aschi</u> <i>Toward a Computational Modelling of Charge-Transfer Reactions in Condensed Phase: from Ultrafast Photo-Induced to Slow Thermal Processes</i>
9.40 – 10.00	TEO OR01: <u>Cristina Puzzarini</u> , Alessio Melli, Nicola Tasinato, Julien Bloino, Vincenzo Barone <i>Astrochemistry: A Computational Spectroscopy's View</i>
10.00 – 10.20	TEO OR02: <u>Alessandro Landi</u> , Raffaele Borrelli, Andrea Peluso <i>Modeling Charge Transport in Organic Materials</i>
10.20 – 10.40	TEO OR03: <u>Umberto Raucci</u> , Nadia Rega <i>Ab Initio Molecular Dynamics to Simulate Excited State Proton Transfer to Solvent: the Strange Case of a Super Photoacid in Water and Methanol Solutions</i>
10.40 – 11.10	Coffee Break
<i>Sessione DCTC</i>	
<i>Chairperson: Maria Cristina Menziani</i>	
11.10 – 11.30	TEO OR04: <u>Silvio Pipolo</u> , Roberto Cammi, Stefano Corni <i>Real-Time Coupling between Molecules and a Continuum Environment</i>
11.30 – 11.50	TEO OR05: <u>Oscar Baseggio</u> , Mauro Stener, Giovanna Fronzoni, Daniele Toffoli, Alessandro Fortunelli, Stan van Gisbergen, Erik van Lenthe <i>A New Efficient Time Dependent Density Functional Algorithm for Large Systems: Theoretical Study and Applications to Plasmonic Systems</i>
11.50 – 12.10	TEO OR06: <u>M. Gabriella Chiariello</u> , Nadia Rega <i>Exploring Nuclear Photorelaxation and Photoreactivity by Excited State Ab-Initio Dynamics and Time Resolved Vibrational Analysis</i>
12.10 – 12.30	TEO OR07: <u>Alessandra Serva</u> , Valentina Migliorati, Francesco Sessa, Paola D'Angelo <i>Lanthanoid(III) Ions: Transferable Lennard-Jones and Buckingham Pair Potentials from Aqueous to Complex Media</i>
12.30 – 12.50	TEO OR08: <u>Marco Fusè</u> , Julien Bloino, Franco Egidi, Alberto Baiardi, Vincenzo Barone <i>Unraveling Chiral Properties of Metal Complexes Through Computational Vibrational Spectroscopy</i>
12.50 – 13.10	TEO OR09: <u>Francesco Tavanti</u> , Erika Ferrari, Alfonso Pedone Maria Cristina Menziani <i>Computational Study of Curcumin-derivatives for Alzheimer's Disease Treatment</i>

13.10 - 14.00	Intervallo Pranzo
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<i>Sala Paestum B</i>	
14:00 – 15:00	<i>Sessione Poster I (TEO PO01 – TEO PO11)</i>

<i>Hotel Savoy Sala Puccini</i>	
<i>Sessione DCTC</i>	
<i>Chairperson: Carlo Adamo</i>	
15.00 – 15.40	TEO KN02: <u>Giuseppe B. Suffritti</u> , Pierfranco Demontis <i>Reverse Mössbauer Effect as a Source of "Hot" Protons in Hydrogen Absorbing Metals</i>
15.40 – 16.00	TEO OR10: <u>Eduardo Schiavo</u> , Ana B. Muñoz-García, Michele Pavone <i>First-Principles Design of P-Type Semiconductor Oxides as Alternative to NiO in P-Type Dye-Sensitized Solar Cells</i>

16.00 – 16.20	TEO OR11: Marco Dalla Tiezza, <u>Laura Orian</u> <i>Toward a Rational Design of Half-Sandwich Group 9 Catalysts for [2+2+2] Alkynes Cycloadditions</i>
16.20 – 16.40	TEO OR12: <u>Stefano Piotta</u> , Anna Montano, Simona Concilio, Lucia Sessa, Pio Iannelli, Barbara Panunzi, Rosita Diana <i>Ramachandran Energy Approach for Protein Folding</i>
16.40 – 17.10	Coffee Break
Sessione DCTC	
Chairperson: Cristina Puzzarini	
17.10 – 17.30	TEO PZ01: <u>Julien Bloino</u> <i>Accurate Spectra of Medium-Large Molecules: Recent Developments and New Challenges</i>
17.30 – 17.50	TEO PZ02: <u>Alfonso Pedone</u> <i>From First-Principle Chemical Shift and EFG Tensors Calculations to Solid-State 1D and 2D NMR Spectra Simulations of Complex Systems</i>
17.50 – 18.10	TEO PZ03: <u>Franco Egidi</u> <i>Development of Theoretical and Computational Models for the Calculation of Spectroscopic Properties of Molecules in the Gas Phase and in Solution</i>
18.10 – 18.20	TEO PZ04: <u>Greta Donati</u> , Alessio Petrone, Nadia Rega <i>Wavelet Analysis for Non-Equilibrium Processes in Chemistry</i>
18.20 – 18.25	TEO PZ05: <u>Marco Mendolicchio</u> , Nicola Tasinato, Vincenzo Barone <i>New Models and Computational Strategies for Molecular Structure Prediction</i>
Sala Puccini	
18.30 – 20.00	<i>Assemblea dei Soci della Divisione di Chimica Teorica e Computazionale</i>

Martedì 12 Settembre 2017

Hotel Savoy Sala Puccini	
Sessione congiunta DCTC-INO	
Chairperson: Gianluca Ciancaleoni	
9.00 – 9.40	TEO/INO KN01: <u>Bartolomeo Civalleri</u> <i>Ab Initio Modeling of Metal-Organic Frameworks: from Gas Adsorption to Stimuli Responsive Properties</i>
9.40 – 10.00	TEO/INO OR01: <u>Ana B. Muñoz-García</u> , Michele Pavone <i>Computational Design of Sr₂Fe_{1.5}Mo_{0.5}O_{6-Δ} (SFMO)-based Bifunctional Electrodes for Proton-Conducting Solid Oxide Electrochemical Cells</i>
10.00 – 10.20	TEO/INO OR02: <u>Cutini Michele</u> , Marta Corno, Piero Ugliengo <i>Insight from DFT Simulations on the Collagen/Hydroxyapatite Interface: a Simple Model Based on the Poly-Proline Polymer</i>
10.20 – 10.40	TEO/INO OR03: <u>Laura Falivene</u> , Sergey Kozlov, Luigi Cavallo <i>A DFT Rationalization of a Two Metals Strategy to Tune Selectivity in Catalysis</i>
10.40 – 11.10	Coffee Break
Sessione congiunta DCTC-INO	
Chairperson: Emilia Sicilia	
11.20 – 12.00	TEO/INO KN02: Iogann Tolbatov, Cecilia Coletti, Alessandro Marrone, <u>Nazzareno Re</u> <i>Insight into the Electrochemical Reduction Mechanism of Pt(IV) Anticancer Complexes</i>
12.00 – 12.20	TEO/INO OR04: <u>Tiziana Marino</u> , Mario Prejano, Paolo Piazzetta, Nino Russo <i>The Role of Metal Substitution in the Metallo-Enzymes: a Theoretical Point of View</i>
12.20 – 12.40	TEO/INO OR05: <u>Gianluca Ciancaleoni</u> , Niccolò Bartalucci, Leonardo Belpassi, Fabio Marchetti <i>Back-Donation in d⁰ Metal Complexes: Does it Exist? The case of Nb(V)</i>

12.40 – 13.00	TEO/INO OR06: <u>Gloria Mazzone</u> , Claudia Regina, Nino Russo <i>Combination of Porphyrin and Ruthenium-arene Moieties for a Dual Anticancer Function. A Theoretical Investigation</i>
13.00 - 14.00	Intervallo Pranzo

Mercoledì 13 Settembre

<i>Hotel Savoy Sala Puccini</i>	
Sessione congiunta DCTC-FIS	
Chairperson: Michele Pavone	
15.00 – 15.40	TEO/FIS KN01: <u>Chiara Cappelli</u> <i>A Fully Polarizable Embedding Model for Molecular Spectroscopy of Aqueous Solutions</i>
15.40 – 16.00	TEO/FIS OR01: <u>Roberto Dovesi</u> , Simone Salustro, Francesco Gentile, Yves Noel <i>Hydrogen defects in Diamond. A quantum mechanical approach</i>
16.00 – 16.15	TEO/FIS OR02: <u>Lorenzo Zamirri</u> , Marta Corno, Albert Rimola, Piero Ugliengo <i>Forsterite Surfaces as Models of Interstellar Core Dust Grains: Computational Study of Carbon Monoxide Adsorption</i>
16.15 – 16.30	TEO/FIS OR03: <u>Mattia Melosso</u> , Claudio Degli Esposti, Luca Dore, Cristina Puzzarini, Lorenzo Spada <i>Prebiotic Molecules in Interstellar Space: Aminoacetonitrile and C-Cyanomethanimine</i>
16.30 – 17.00	Coffee Break
Sessione congiunta DCTC-FIS	
Chairperson: Ludovico Valli	
17.00 – 17.15	TEO/FIS OR04: <u>M. Vincenzo La Rocca</u> , Lorella Izzo, Simona Losio, Massimo Mella <i>Should we Introduce Pre-Equilibria into Markov Models for Homogeneously Catalyzed Copolymerization?</i>
17.15 – 17.30	TEO/FIS OR05: <u>Francesco Di Maiolo</u> , Carlotta Pieroni, Anna Painelli <i>Intermolecular Energy Transfer in Real Time</i>
17.30 – 17.50	TEO/FIS OR06: <u>Enrico Bodo</u> , Andrea Le Donne <i>Proton Mobility in Protic Ionic Liquids: New Results from Theoretical Calculations</i>
17.50 – 18.10	TEO/FIS OR07: <u>Nicola Tasinato</u> , Lorenzo Spada, Cristina Puzzarini, Vincenzo Barone <i>Computational Tools for the Interpretation of Rotational Spectra within the Virtual Multifrequency Spectrometer</i>
18.10 – 18.25	TEO/FIS OR08: <u>Alessandro Mariani</u> , Ruggero Caminiti, Lorenzo Gontrani <i>A Spotlight on The Complex Hierarchical Structure of Some Ionic Liquid-Molecular Liquid Binary Mixtures</i>
18.25 – 18.40	TEO/FIS OR09: <u>Olga Russina</u> , Ruggero Caminiti <i>Fluorous Mesoscopic Domains in Room Temperature Ionic Liquids</i>
18.40 – 18.55	TEO/FIS OR10: <u>Ettore Fois</u> , Rossella Arletti, Lara Gigli, Giovanna Vezzalini, Simona Quartieri, Gloria Tabacchi <i>Supramolecular Organization of Water-Ethanol Solution in Ferrierite under Pressure</i>

Sessione del Gruppo Senior

Mercoledì 13 Settembre 2017

Chimica e Sport - Chemistry and Sport	
<i>Sala Diana</i>	
Chairperson Domenico Misiti	
15:00-15:40	GRS IL01 Santo Davide Ferrara <i>Doping-Antidoping e ruolo delle Scienze Biomedicolegali</i>
15:45-16:25	GRS IL02 Luigi Nicolais <i>I grandi cambiamenti nella 4° rivoluzione industriale</i>
16:30-17:00	Coffee Break
Chairperson Rosario Nicoletti	
17.00-17.30	Aracne Editrice – Comitato Editoriale SCI <i>Presentazione della Collana “Molecole in primo piano”</i>
	Assemblea Gruppo Senior SCI

Eventi Satellite di Interesse Industriale

Grafene e sue possibili applicazioni industriali

Giovedì 14 Settembre 2014

<i>Auditorium Giove</i>	
Chairperson: Vincenzo Palermo	
14:30-14:45	ESG IL01 Gaetano Granozzi <i>Second and third generation graphenes for energy conversion</i>
14:45-15:00	ESG IL02 Giovanni Bruno <i>CVD graphene: transparency, conductivity and flexibility, three inseparable properties to develop innovative applications</i>
15:00-15:15	ESG IL06 Maurizio Peruzzini <i>Black Phosphorus: from Ugly Duckling to Black Swan</i>
15:15-15:30	ESG IL04 Michele Maggini <i>Continuous flow synthesis of functionalized graphene</i>
15:30-15:45	ESG IL05 Zhenyuan Xia <i>Functionalization and applications of graphene-based materials</i>
15:45-16:00	ESG IL03 Maurizio Galimberti <i>Facile and sustainable functionalization method for preparing graphene layers with different solubility parameters</i>
16:00-16:30	Coffee Break
Chairperson: Gaetano Guerra	
16:30-16:45	ESG IL07 Manuela Melucci <i>Tailored polysulfone-graphene oxide adsorbers for water remediation</i>
16:45-17:00	ESG IL08 Maria Rosaria Acocella <i>New Application of Oxidized Nanocarbons: from Catalysis to Nanocomposites</i>
17:00-17:15	ESG IL09 Pellegrino Musto <i>Vibrational spectroscopy investigations on graphene/Poly(lactic acid) composites</i>
17:15-17:30	ESG IL10 Marino Lavorgna <i>Porous graphene-based polyurethane foams-aerogel composites prepared via unidirectional freeze-drying process</i>

17:30-17:45	ESG IL11 Michele Giordano <i>Multifunctional properties of Graphene Nanoplatelets based nanolaminates</i>
17:45-17:55	Paolo Ciambelli <i>Presentazione del progetto europeo Marie Curie – RISE Graphene 3D (Multifunctional Graphene-based Nanocomposites with Robust Electromagnetic and Thermal Properties for 3D-printing Application)</i>

Formulazioni nell'industria chimica e farmaceutica

Giovedì 14 Settembre 2014

<i>Sala Mercurio</i>	
Chairperson: Gerardino D'Errico, Martino Di Serio	
14:30-14:35	<i>Introduction by Chairperson</i>
14:35-14:50	ESF IL01 Vittorio Maglia <i>Chimica delle formulazioni e chimica delle specialità: le esigenze dell'industria</i>
14:50-15:05	ESF IL02 Marco Adami <i>Formulation challenges and emerging technologies in the pharmaceutical industry: an overview</i>
15:05-15:20	ESF IL03 Sesto Viticoli <i>I formulati, nuova frontiera della chimica italiana</i>
15:20-15:35	ESF IL04 <u>Andrea Casazza</u> <i>Trimbow: un nuovo successo formulativo nel mondo delle combinazioni</i>
15:35-15:50	ESF IL05 Giorgio Ferrari <i>Studio della struttura alla scala nanometrica di formulati cementizi</i>
15:50-16:05	ESF IL06 Salvatore Mercuri <i>Innovative approaches to tailor a particle size distribution</i>
16:05-16:30	Coffee Break
Chairperson: Rita Patrizia Aquino, Gianluca Sbardella	
16:30-16:45	ESF IL07 Franco Gasparri <i>I cosmetici per pelli sensibili: strategie formulative per la modulazione dell'attività lenitiva ed anti-infiammatoria</i>
16:45-17:00	ESF IL08 Stefano Resta <i>Challenges in formulating Ace Bleach products</i>
17:00-17:15	ESF IL09 Antonino Bagnulo <i>Formulazioni nel settore della nutraceutica: stato dell'arte e prospettive future</i>
17:15-17:30	ESF IL10 Massimo Bonini <i>Colloidi e Nanoscienze: Formulazioni e nuove sfide</i>
17:30-17:45	ESF IL11 Pasquale Del Gaudio <i>Polysaccharides based in situ gelling powders as promising wound healing medical devices</i>
17:45-18:00	ESF IL12 Martino Di Serio <i>Formulazioni industriali, un nuovo indirizzo di laurea</i>