

Programma dei LAVORI di DIVISIONE - 17 settembre pomeriggio

Divisione CHIMICA ANALITICA (ANA)

ANA 07

15.00 - 15.20	ANA PZ003	Mariosimone Zoccali	<i>Is There a Real Need for Multidimensional Chromatography Strategies with the Current Availability of Powerful Mass Spectrometry Platforms?</i>
15.20 - 15.40	ANA KN008	Giovanni Ventura	<i>AllerT: a Matlab-based workflow for putative allergens identification in novel foods via LC-ESI-MS/MS analysis</i>
15.40 - 16.00	ANA OR051	Domenica Mangraviti	<i>Differentiation and profiling of Morocco species belonging to Lamiaceae Family by Ambient Mass Spectrometry methods</i>
16.00 - 16.15	ANA OR052	Nicole Marittimo	<i>Advancements in Direct-MS using SPME coupled to Liquid-El and CI</i>
16.15 - 16.30	ANA OR053	Katia Arena	<i>Characterization of bioactive compounds from natural products using focusing-modulated comprehensive two-dimensional liquid chromatography coupled to mass spectrometry</i>
16.30 - 16.45	ANA OR054	Eleonora Oliva	<i>Analysis of phenolic compounds in plant matrices by means of HPLC-MS/MS with targeted and semi-untargeted approach</i>
16.45 - 17.00	ANA OR055	Tania Salerno	<i>The Coupling of Gas Chromatography - Mass Spectrometry with Infrared Spectroscopy for Reliable Identification of Unknowns in Complex Samples</i>
17.00 - 17.15	ANA OR056	Danilo Sciarrone	<i>Reliability of monodimensional vs multidimensional GC-C-IRMS data: a critical evaluation</i>
17.15 - 17.30	ANA OR057	Peter Q. Tranchida	<i>Options of 1D GC, flow-modulation signal-enhanced 1D GC and flow-modulation comprehensive 2D GC in a single instrument: a proof-of-concept study</i>
17.30 - 17.45	ANA OR058	Cecile Valsecchi	<i>Enhanced LC-MS/MS spectra matching through multi-task neural networks and molecular fingerprints</i>

ANA 08

15.20 - 15.40	ANA IL005	Alessandra Bianco Prevot	<i>Organic Pollutant Removal using Photo-Fenton Processes in the presence of Fe(III) complexing agents</i>
15.40 - 16.00	ANA IL006	Paola Fermo	<i>In-situ and micro-destructive investigation for the analysis of degradation products present on marble surfaces</i>
16.00 - 16.15	ANA OR059	Francisco Ardini	<i>Evaluation of potential source areas for atmospheric lead reaching Ny-Ålesund (Svalbard) from 2010 to 2019</i>
16.15 - 16.30	ANA OR060	Stefano Bertinetti	<i>Strontium isotopic analysis of microsamples by inductively coupled plasma - tandem mass spectrometry</i>

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16.30 - 16.45	ANA OR061	Luca Carena	<i>Photochemistry of furfuryl alcohol in/on snow at -30°C: photoreactivity with singlet oxygen and by direct photolysis</i>
16.45 - 17.00	ANA OR062	Silvia Illuminati	<i>Year-round records of bulk aerosol composition over the Victoria Land (Antarctica)</i>
17.00 - 17.15	ANA OR063	Elisa Calà	<i>Identification of aloe and other dyes by means of SERS and HPLC-DAD-MS in the embroidery of a 15th century English folded almanac</i>
17.15 - 17.30	ANA OR064	Emilio Catelli	<i>Rediscovering the lost color. Advanced vector quantization algorithm and hyperspectral imaging for digital restoration of color films</i>
17.30 - 17.45	ANA OR065	Giovanna Marussi	<i>The Third-Century monetary crisis: chemical analysis of Denarii and Antoniniani</i>
17.45 - 18.00	ANA OR066	Rosaria Anna Picca	<i>Synthesis and spectroscopic characterization of synergistic nanomaterials for stone artwork protection</i>

ANA 09

15.20 - 15.40	ANA KN009	Paolo Bollella	<i>Enzyme based Amperometric Biosensors: From Direct Electron Transfer to Chimeric Enzymes</i>
15.40 - 16.00	ANA OR067	Giuseppe Arrabito	<i>Printing Biology: engineering analytical platforms by molecular inks</i>
16.00 - 16.15	ANA OR068	Noemi Bellasai	<i>Design of dual-functional polymer on plasmonic biosensor for detection of circulating tumor DNA point mutations</i>
16.15 - 16.30	ANA OR069	Alessandro Bertucci	<i>Artificial Biomolecular Communication Regulated by Synthetic DNA Translators</i>
16.30 - 16.45	ANA OR070	Alessandra Maria Bossi	<i>Soft molecularly imprinted nanoparticles for protein recognition in sensing and assays</i>
16.45 - 17.00	ANA OR071	Stefano Cinti	<i>A microfluidic paper-based chip patterned with Prussian Blue to determine sweat urea</i>
17.00 - 17.15	ANA OR072	Erica Del Grosso	<i>Transient control of DNA-based systems</i>
17.15 - 17.30	ANA OR073	Marco Giannetto	<i>Smart immunosensors for point-of-care serologic test to determine the level of immunity by Covid-19 infection or by SARS-CoV-2 vaccination</i>
17.30 - 17.45	ANA OR074	Antonia Lopreside	<i>Reagent-free paper biosensor based on genetically modified bioluminescent protein for cancer biomarker detection</i>
17.45 - 18.00	ANA OR075	Lucia Sarcina	<i>Selective detection of Xylella fastidiosa with a Surface Plasmon Resonance based immunoassay</i>

Divisione CHIMICA DELL'AMBIENTE E DEI BENI CULTURALI (ABC)

ABC 04

15.00-15.15	ABC OR051	Dominique Scalarone	<i>CAPuS project: research and higher education allied for the Conservation of Art in Public Spaces</i>
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15.15-15.30	ABC OR013	Ilaria Serafini	<i>Advances in analytical methodologies applied to cultural heritage: first application of DLLME to characterize dyes in ancient textiles</i>
15.30-15.45	ABC OR014	Slimani Sawssen	<i>Caput Mortuum purple hematite pigment: Investigation of magnetic properties</i>
15.45-16.00	break		
16.00-16.15	ABC OR015	Andrea Brunelli	<i>Colloidal behavior of titanium dioxide nanoparticles in artificial and in Venice lagoon waters in the presence of standard or natural colloidal particles</i>
16.15-16.30	ABC OR016	Felice Simeone	<i>Assessment of the Cytotoxicity of Metal oxide Nanoparticles on the Basis of Immediately Available Physical-Chemical Parameters.</i>
16.30-16.45	ABC OR017	Cristina De Ceglie	<i>The effect of a karst-fractured aquifer on wastewater quality: an UHPLC-HRMS study</i>
16.45-17.00	ABC OR018	Francesco Saliu	<i>Plastic and its associated contaminants: determination of PAEs in coral reef invertebrates by in vivo SPME-LC-MS/MS</i>
17.00-17.15			
17.15-17.30	ABC OR019	Armando Zarrelli	<i>Characterization of degradation byproducts of Sartans: elucidation of their degradation pathway and ecotoxicity assessment</i>
17.30-17.45	ABC OR020	Marco Mantovani	<i>Microalgal treatment of the liquid fraction from hydrothermal carbonization process (HTC) in a circularity perspective</i>
17.45-18.00	ABC OR021	Giulia Guidotti	<i>Poly(diethylene 2,5-furanoate): a biobased promising candidate for compostable high-performant packaging</i>
18.00-18.15	ABC OR022	Valeria D'Ambrosio	<i>Lipids extraction from sewage sludge using green biosolvent for a sustainable production of biodiesel</i>

Divisione CHIMICA INDUSTRIALE (IND)

IND 04

Sessione congiunta con Gruppo Interdivisionale Energie Rinnovabili - Enerchem

15.00 - 15.30	IND KN005 Chini Lecture	Carlo Perego	<i>CO2 utilization: from waste to resource</i>
15.30 - 15.40	IND OR033	Martina Serafini	<i>Nanostructured Cu-based Electrocatalysts on a Carbonaceous Gas Diffusion Layer for the Electrochemical Reduction of CO2</i>
15.40 - 15.50	IND OR034	Simelys Hernandez	<i>How to exploit thermochemical catalysts to make efficient & sustainable CO2 electroreduction to added value products</i>
15.50 - 16.00	IND OR035	Ivan Grigioni	<i>High rate CO2 electroreduction to formate with a InP colloidal quantum dots derived catalyst</i>
16.00 - 16.10	IND OR036	Federico Bella	<i>Preliminary investigation of anodic materials for potassium batteries</i>
16.10 - 16.20	IND OR037	Maria Grazia Musolino	<i>Solvothermal synthesis of doped hematite/reduced graphene oxide nanocomposites for sodium-ion batteries</i>

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16.20 - 16.30	IND OR038	Emilia Paone	<i>Reductive Upgrading of Biomass Derived Furan promoted by Spent Lithium-Cobalt Batteries as an Efficient Heterogeneous Catalyst</i>
16.30 - 16.40	IND OR039	Matteo Bonomo	<i>Thermosetting polyurethanes resins: application as cheap, sustainable and scalable encapsulants for (flexible) Perovskite Solar Cells</i>
16.40 - 16.55	Discussion		
16.55 - 17.10	break		
17.10 - 17.20	IND OR040	Andrea Fasolini	<i>Low Temperature Methane Steam Reforming in a H₂-selective Pd Membrane Reactor</i>
17.20 - 17.30	IND OR041	Tiziano Montini	<i>Visible-light-driven coproduction of diesel precursors and hydrogen from lignocellulose-derived methylfurans</i>
17.30 - 17.40	IND OR042	Nicola Sangiorgi	<i>Improved water stability of CsPbBr₃ thin film photoelectrodes</i>
17.40 - 17.50	IND OR043	Cosimo Micheletti	<i>Luminescent Solar concentrators based on Aggregation-Induced Emission</i>
17.50 - 18.00	IND OR022	Giuseppe Pipitone	<i>Aqueous phase reforming of biorefinery by-products towards sustainable hydrogen production</i>
18.00 - 18.10	IND OR045	Francesco Conte	<i>H₂ production by photoreforming of glucose</i>
18.10 - 18.30	Discussion		

Divisione CHIMICA ORGANICA (ORG)

ORG 08

15.00 - 15.30	ORG PZ006	Daniela Montesarchio	Premio alla ricerca Chimica Organica per le Scienze della Vita <i>G-Quadruplexes to the fore: towards DNA-targeting magic bullets</i>
15.30 - 16.00	Break		
16.00 - 16.15	ORG PZ014	Anna Esposito	Premio Tesi di Dottorato Chimica Organica per le Scienze della Vita <i>Exploring the therapeutic potential of L-deoxyiminosugars in rare diseases</i>
16.15 - 16.30	ORG OR045	Cristina Minnelli	<i>Epigallocatechin-3-gallate-based Inhibitors Targeting EGFR to Overcome Drug Resistance in Advanced NSCLC</i>
16.30 - 16.45	ORG OR046	Lucía Morillas Becerril	<i>Specific and nondisruptive interaction of guanidium-functionalized gold nanoparticles with neutral phospholipid bilayers</i>
16.45 - 17.00	ORG OR047	Maria Luisa Navacchia	<i>Dihydroartemisinin-bile acid hybridization as an effective approach to enhance dihydroartemisinin anticancer activity</i>
17.00 - 17.30	Break		
17.30 - 17.45	ORG OR048	Ferran Nieto Fabregat	<i>Gram-negative bacteria LPS recognition by DC-SIGN</i>

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17.45 - 18.00	ORG OR049	Anna Notaro	<i>Mimiviruses possess the biosynthetic pathways to produce bacteria-like sugars in a clade-specific manner</i>
18.00 - 18.15	ORG OR050	Alessandro Palmioli	<i>On-cell saturation transfer difference NMR for the identification of FimH ligands and inhibitors</i>
18.15 - 18.30	ORG OR051	Daniela Perrone	<i>Synthesis and preclinical evaluation of antisense oligonucleotides conjugated with ursodeoxycholic acid for the treatment of Duchenne muscular dystrophy</i>

ORG 09

16.00 - 16.15	ORG PZ013	Mirko Maturi	Premio Tesi di Dottorato Chimica Organica per l'Ambiente, l'Energia e le Nanoscienze <i>Advanced Functional Organic-Inorganic Hybrid (Nano)Materials: from Theranostics to Organic Electronics and Additive Manufacturing</i>
16.15 - 16.30	ORG OR052	Mariacecilia Pasini	<i>Sustainable by Design Carbon Dots as promising material for luminescent and biomedical applications</i>
16.30 - 16.45	ORG OR053	Vincenzo Patamia	<i>A new hybrid porous multifunctional material based on Loofah-Halloysite</i>
16.45 - 17.00	ORG OR054	Marina Massaro	<i>Synthesis and characterization of different mussel inspired materials for several applications</i>
17.00 - 17.30	Break		
17.30 - 17.45	ORG OR055	Giulia Neri	<i>Fluorinated Polymers and Fluorescent Graphene as Innovative Nanotheranostic Materials</i>
17.45 - 18.00	ORG OR056	Alessandra Operamolla	<i>Cellulose nanocrystals for paper consolidation</i>
18.00 - 18.15	ORG OR057	Luca Pettazoni	<i>Transamidation-based vitrimers from renewable sources</i>
18.15 - 18.30	ORG OR058	Serena Riela	<i>Improvement of properties of halloysite and some other «friends» by chemical modifications</i>

ORG 10

16.00 - 16.15	ORG OR059	Claudio Curti	<i>Merging Vinylogy with Organocatalysis: Direct, Asymmetric Entry to Chiral Fused Uracil Derivatives</i>
16.15 - 16.30	ORG OR060	Daniele Fiorito	<i>Synthetic studies towards Bastimolide B</i>
16.30 - 16.45	ORG OR061	Paola Costanzo	<i>Highly oleophilic and reusable polyurethane composites for the removal of oils from fresh water and seawater</i>
16.45 - 17.00	ORG OR062	Andrea Mezzetta	<i>Reactive Deep Eutectic Solvents (ReDESS): an underexploited option for organic chemistry</i>
17.00 - 17.30	Break		
17.30 - 17.45	ORG OR063	Lorenzo Di Terlizzi	<i>Visible light-driven α-arylation of enol silyl ethers via arylazo sulfones.</i>

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17.45 - 18.00	ORG OR064	Lucia Ferrazzano	<i>Greening peptide synthesis: new options for a sustainable chemistry</i>
18.00 - 18.15	ORG OR065	Valeria Nori	<i>Organocatalysed Michael addition of masked acetaldehyde to nitroalkenes in water</i>
18.15 - 18.30	ORG OR066	Rita Mocci	<i>Mechanochemical Fischer Indolisation: Exploration of a Timeless Reaction in a New Guise</i>

ORG 11

16.00 - 16.15	ORG OR067	Allegra Franchino	<i>Merging organo- and Au(I) catalysis for asymmetric or silver-free reactions of alkynes</i>
16.15 - 16.30	ORG OR068	Gianluigi Albano	<i>Infrared irradiation-assisted solvent-free Palladium-catalyzed (hetero)aryl-aryl coupling via C-H bond activation</i>
16.30 - 16.45	ORG OR069	Fabio Bellina	<i>Pd/Ag-mediated dehydrogenative alkynylation of imidazoles</i>
16.45 - 17.00	ORG OR070	Silvia Gaspa	<i>Photocatalyzed amides synthesis from alcohols by visible light</i>
17.00 - 17.30	Break		
17.30 - 17.45	ORG OR071	Fabrizio Medici	<i>Stereoselective [2+2] photocycloaddition: a viable strategy for the synthesis of enantiopure cyclobutane derivatives</i>
17.45 - 18.00	ORG OR072	Francesco Messa	<i>Ligand-Free Cobalt-Catalyzed Cross-Coupling Reaction Between Organoaluminum Reagents and (Hetero)Aryl and Alkyl Bromides</i>
18.00 - 18.15	ORG OR073	Giorgia Zanchin	<i>Imino-pyridine Cr complexes as precatalyst for the polymerization of olefins: synthesis and catalytic tests with NEt₃ as additive</i>

Divisione CHIMICA DEI SISTEMI BIOLOGICI (CSB)

CSB 03

15.00 - 15.30	CSB KN003	Luc Brunsveld	<i>Stabilization of Protein-Protein Interactions; from the fundamentals of cooperativity to applications in drug discovery</i>
15.30 - 15.45	CSB OR014	Alessio Romerio	<i>Design, synthesis and Biological evaluation of New, glycolipid-based Toll-Like Receptor 4 (TLR4) Modulators</i>
15.45 - 16.00	CSB OR015	Giusy Tassone	<i>Evidence of amino-thiadiazoles as innovative inhibitors of human glutaminy cyclase, validated target for neurodegenerative disorders</i>
16.00 - 16.15	CSB OR016	Francesco Tadini-Buonisegni	<i>Modulation of Ca²⁺-ATPase transport activity by pharmacologically relevant compounds</i>
16.15 - 16.30	CSB OR017	Michela Pisani	<i>Insulin loaded in liquid crystalline mesophases: effects on carrier structure and insulin stability</i>
16.30 - 17.00	Break		

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17.00 - 17.30	CSB KN004	Elena Sgaravatti	<i>Research and development of active ingredients from vegetable cells or crops to be used in the Health care, Food and Personal care sectors</i>
17.30 - 17.45	CSB OR018	Valeria Romanucci	<i>New curcumin mimics based on tyrosol scaffold: investigation of neuroprotective and anticancer activity</i>
17.45 - 18.00	CSB OR019	Roberto Tira	<i>Modulation of Tau aggregation with natural coffee compounds</i>
18.00 - 18.10	CSB OR020	Rita Pagano	<i>Phosphate-linked Silybin dimers: synthesis and investigation of biological activity</i>
18.10 - 18.20	CSB OR021	Massimiliano Gaeta	<i>Hybrid Porphyrin/DOPA-melanin Film as Versatile Biomaterial for Water Remediation</i>
18.20 - 18.50	Discussione		

Divisione DIDATTICA CHIMICA (DID)

DID 02

15:00-15:30	DID IL002	Carlo Fiorentini	<i>The teaching of chemistry from the perspective of citizenship</i>
15:30-15:45	DID OR010	Teresa Cecchi	<i>Chemistry: a Precious Discovery in the Dantesque World</i>
15:45-16:00	DID OR011	Maria Irene Donnoli	<i>A Carbon atom journey</i>
16:00-16:15	DID OR012	Elena Lenci	<i>Peer review of scientific articles: a teaching experience</i>
16:15-16:30	DID OR013	Silvia Prati	<i>Increasing the engagement of non-chemistry major students: examples of didactic strategic</i>
16:30-18:30	Panel Discussion	Silvia Bencivelli (coordinator) Pellegrino Conte Paola Govoni Piersandro Pallavicini Valentina Domenici	<i>Chemistry: how, where, when and why</i>

Divisione SPETTROMETRIA DI MASSA (MAS)

MAS 02

15.00 - 15.40	MAS PL003	Nikolai Kuhnert	<i>Mass spectrometry in coffee science: From bean to drink to human</i>
15.40 - 16.10	MAS KN001	Tata Alessandra	<i>Non-targeted authentication of food products: the synergic combination of ambient mass spectrometry, data fusion and machine learning"</i>
16.10 - 16.25	MAS OR006	M.A. Acquavia	<i>Influence of mixed starter cultures of Hanseniaspora osmophila and Saccharomyces cerevisiae on wine flavor profile explored through HS-SPME/GC-MS</i>
16.25 - 16.35	Break		

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16.35 - 17.05	MAS KN002	Linda Monaci	<i>Future challenges in MS based technologies applied to the safety of foods.</i>
17.05 - 17.20	MAS OR007	Rosalia Zianni	<i>Lipidomic approach to evaluate the effect of X-ray irradiation treatment on the lipid profile of Camembert cheese</i>
17.20 - 17.35	MAS OR008	Fabiola De Marchi	<i>High-resolution mass spectrometry approaches finalized to identification of new glycoside compounds in grape</i>
17.35 - 17.50	MAS OR009	Ciro Cannavacciuolo	<i>Analysis by high-resolution mass spectrometry of polyphenolic alkaloids fraction from <i>Portulaca oleracea</i></i>
17.50 - 18.05	MAS OR010	Lucia Bartella	<i>Paper Spray tandem mass spectrometry: an innovative approach to assess flavonoid content in citrus drinks</i>

Divisione TEORICA E COMPUTAZIONALE (TEO)

TEO 02

15.00 - 15.30	TEO KN002	Alfonso Pedone	<i>Exploiting Machine Learning Methods in Atomistic Simulations of Oxide Glasses</i>
15.30 - 15.45	FIS OR059	Adriana Pecoraro	<i>First-principles study of Mn and Fe co-doped BaZrO₃ as PC-SOFC cathode for the Oxygen Reduction Reaction</i>
15.45 - 16.00	TEO OR013	Leonardo Guidoni	<i>Quantum Chemistry using Quantum Computers</i>
16.00 - 16.15	FIS OR061	Marco Medves	<i>TDDFT methods for large systems: new computational schemes and automatic generation of density fitting basis</i>
16.15 - 16.30	TEO OR014	Elena Tocci	<i>Molecular view on crystals nucleation and growth on different PVDF polymorphs</i>
16:30 - 17:00	Discussion		

TEO 03

15:00 - 15:10	TEO OR015	Matteo Capone	<i>Multi-Scale Charge-Transfer Modeling in Enzyme Catalysis</i>
15:10 - 15:20	TEO OR016	Guelber Cardoso Gomes	<i>Computational study of dicationic ionic liquids based on imidazole</i>
15:20 - 15:30	TEO OR017	Elisa Bernes	<i>An experimental and theoretical investigation on the electronic structure of indole, 2,3-dihydro-7-azaindole, and 3-formylindole in the gas phase by synchrotron-based spectroscopic techniques</i>
15:30 - 15:40	TEO OR018	Yasi Dai	<i>Addressing the Frenkel and charge transfer character of exciton states with a model Hamiltonian based on dimer calculations: application to large aggregates of perylene bisimide</i>

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15:40 - 15:50	TEO OR019	Stefano Motta	<i>Study of ligand binding to HIF-2α through Path-Metadynamics</i>
15:50 - 16:00	TEO OR020	Alessandra Gilda Ritacca	<i>The multifaceted roles of copper ion in human body explored by computational tools</i>
16:00 - 16:10	TEO OR021	Anna Rovaletti	<i>Unravelling the reaction mechanism of Mo/Cu CO dehydrogenase using QM/MM calculations</i>
16:10 - 16:20	TEO OR022	Sara Del Galdo	<i>How water density responds to the presence of a crowding agent</i>
16:20 - 16:30	TEO OR023	Francesco Ferdinando Summa	<i>SYSMOIC: A Program Package for the Calculation of Origin-Independent Electron Current Density and Derived Magnetic Properties in Molecular Systems</i>
16:30 - 17:00	break		
17:00 - 17:20	TEO KN003	Fabrizia Negri	<i>Modelling extended-core π systems and their aggregates: charge transport and optoelectronic properties</i>
17:20 - 17:40	TEO PZ003	Giovanni Di Liberto	<i>Rational Design of Semiconductor Interfaces for Photocatalysis</i>
17:40 - 18:00	TEO PZ004	Eduardo Schiavo	<i>First Principles Approaches for Heterogeneous Functional Materials</i>
18:00 - 18:30	Discussion		