

Programma dei LAVORI di DIVISIONE - 21 settembre pomeriggio

Divisione CHIMICA ANALITICA (ANA)

ANA10

15.00 - 15.20	ANA PZ004	Martina Catani	<i>Boosting the downstream processing of biopharmaceuticals by means of multicolumn continuous chromatography</i>
15.20 - 15.40	ANA IL007	Maurizio Quinto	<i>Rotating Magnetic Chromatography, a new technique for micro-particle and cell separation</i>
15.40 - 16.00	ANA IL008	Roccardo Sardella	<i>Role of mobile phase composition in enantioselective liquid chromatography</i>
16.00 - 16.15	ANA OR076	Federica Bianchi	<i>Nanomaterials for improved sensitivity in sample treatment</i>
16.15 - 16.30	ANA OR077	Irene Coralli	<i>Secondary reactions in the analysis of microplastics by Py-GC-MS</i>
16.30 - 16.45	ANA OR078	Simona Felletti	<i>Investigation of the chemoselectivity of normal phase stationary phases towards the separation of cannabinoids</i>
16.45 - 17.00	ANA OR079	Giuseppina Gullifa	<i>Potential Health Impact Assessment of New Pocket Pen- Vaporizers: Vapor Characterization Using SPME-GC/MS</i>
17.00 - 17.15	ANA OR080	Jacopo La Nasa	<i>Analytical pyrolysis coupled with gas chromatography/mass spectrometry and solvent extraction for the characterization of microplastics and polymer additives</i>
17.15 - 17.30	ANA OR081	Roberta La Tella	<i>Evaluation of carbon - clad zirconia columns as stationary phases for superheated water liquid chromatography</i>
17.30 - 17.45	ANA OR082	Marcello Locatelli	<i>Fabric Phase Sorptive Extraction: an innovative tool for TDM and pharmacotoxicological studies using unconventional biological matrices</i>
17.45 - 18.00	ANA OR083	Sara Palmieri	<i>Molecular imprinted polymer coupled to LC-MS/MS for maleic hydrazide determination in food samples</i>
18.00 - 18.15	ANA OR084	Marco Roverso	<i>Determination of lactose in low-lactose milk by direct liquid injection and high-resolution mass spectrometry</i>

ANA11

15.20 - 15.40	ANA KN010	Silvia Berto	<i>Study and application of chemical models to measure the urine saturation with calcium salts</i>
15.40 - 16.00	ANA OR085	Chiara Abate	<i>Sequestering ability of carnosine towards some potentially toxic divalent metal cations in aqueous solution</i>

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16.15 - 16.30	ANA OR087	Denise Bellotti	<i>Understanding the thermodynamics and coordination chemistry of metal-binding proteins: the common thread to elucidate metal acquisition processes at host/pathogen interface</i>
16.30 - 16.45	ANA OR088	Rosita Cappai	<i>Complex formation equilibria of a kojic acid derivative with different metal ions</i>
16.45 - 17.00	ANA OR089	Salvatore Cataldo	CYCLODEXTRIN-BASED NANOSPONGES FOR LEAD(II) ION ADSORPTION FROM AQUEOUS SOLUTIONS
17.00 - 17.15	ANA OR090	Ottavia Giuffrè	<i>O-phosphorylethanolamine and O-phosphorylcholine in aqueous solution: acid-base behavior and speciation with Mg²⁺</i>
17.15 - 17.30	ANA OR091	Anna Irto	<i>Thermodynamic parameters on the interaction of divalent and trivalent metal cations with 3-hydroxy-4-pyridinones</i>
17.30 - 17.45	ANA OR092	Luana Malacaria	<i>Studies on the complexation between quercetin and some first-row transition metal cations in aqueous solution</i>
17.45 - 18.00	ANA OR093	Rossella Migliore	<i>Recognition of antibiotics by calixarene-based micellar aggregates in aqueous solution: binding features and driving forces</i>
18.00 - 18.15	ANA OR094	Davide Spanu	<i>On-line ion trapping by frontal chromatography ICP-MS: a low-cost strategy for the fast speciation of inorganic pollutants</i>

ANA12

15.20 - 15.40	ANA KN011	Flavio Della Pelle	<i>2D Nanomaterials: among functional natural compounds and affordable sensor designs</i>
15.40 - 16.00	ANA KN012	Barbara Roda	<i>Selector(R): the cell chromatography for quality control of living cells</i>
16.00 - 16.15	ANA OR095	Jessica Brandi	<i>Identification of protein biomarkers responsible for meat tenderness in bovine Longissimus dorsi muscle by Kohonen self-organizing maps and multivariate analysis</i>
16.15 - 16.30	ANA OR096	Simone Cavalera	<i>Anti-Retroviral Drugs Monitoring in Urine and Saliva: A Rapid and Sensitive Lateral Flow Immunoassay for Tenofovir</i>
16.30 - 16.45	ANA OR097	Andrea Cerrato	<i>An innovative analytical platform for cannabis chemovar differentiation based on untargeted metabolomics and chemometrics</i>

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16.45 - 17.00	ANA OR098	Angela Di Capua	<i>Use of online buffer exchange coupled to native-mass spectrometry to elucidate the stoichiometry of the Salmonella FraR (transcriptional repressor)-DNA complex</i>
17.00 - 17.15	ANA OR099	Fabio Di Nardo	<i>Exploiting silver nanoplates as colorimetric label in Lateral Flow Immunoassay</i>
17.15 - 17.30	ANA OR100	Nicolò Interino	<i>UPLC-Q-TOF-MS/MS analysis of bile acids and their main metabolite profile in farm animal faeces and species-specific correlation with gut microbiota</i>
17.30 - 17.45	ANA OR101	Valentina Marassi	<i>Nanosphere, polymer, self-assembled material? Clearing up the confusion on polydopamine through multidetection-FFF</i>
17.45 - 18.00	ANA OR102	Monica Mattarozzi	<i>Insights into aptamer-protein interactions for analytical applications: egg white lysozyme as case study</i>
18.00 - 18.15	ANA OR103	Lapo Renai	<i>Untargeted metabolomics reveals different postprandial serum metabolome profiles after single intake of Vaccinium myrtillus and Vaccinium corymbosum</i>

Divisione CHIMICA INDUSTRIALE (IND)

IND 04

Sessione congiunta con Gruppo Interdivisionale Green Chemistry - Chimica Sostenibile

15.00 - 15.20	IND KN006	Rafael Luque	<i>Benign by design strategies for a more sustainable future: the valorisation concept</i>
15.20 - 15.30	IND OR049	Anna Gagliardi	<i>Upgrading of Ethanol: Boosting the Guerbet Reaction with a Redox Co-Catalyst</i>
15.30 - 15.40	IND OR050	Ilenia Rossetti	<i>Sustainable process design for the valorization of bioethanol as platform chemical</i>
15.40 - 15.50	IND OR051	Maela Manzoli	<i>Enabling technologies to boost cellulose selective valorisation over bifunctional catalyst</i>
15.50 - 16.00	IND OR052	Silvia Tabasso	<i>Green deep eutectic solvents and microwave technology towards a closed loop biorefinery</i>
16.00 - 16.10	IND OR053	Nicola Di Fidio	<i>Microwave-assisted FeCl₃-catalysed production of glucose from giant reed and cardoon cellulose fraction and its fermentation to new generation oil by oleaginous yeasts</i>
16.10 - 16.20	IND OR054	Alessia Ventimiglia	<i>Theoretical study of glucose oxidation to glucaric acid using gold based catalyst</i>
16.20 - 16.35	Discussion		
16.35 - 16.50	break		
16.50 - 17.10	IND KN007	Volker Hessel	<i>Sustainability as Process Design Guidance for Flow and Plasma Chemistry</i>
17.10 - 17.20	IND OR055	Valeria Pappalardo	<i>Heterogeneous catalysis in the esterification of natural antioxidants</i>

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17.20 - 17.30	IND OR056	Carmelina Rossano	<i>Amberlite IR120 as catalyst for the levulinic acid esterification reaction in batch and continuous operation</i>
17.30 - 17.40	IND OR057	Silvia Giorgi	<i>Synthesis of new biopolymers by biomasses valorization</i>
17.40 - 17.50	IND OR058	Riccardo Bacchiocchi	<i>Innovative heterogeneous catalysts for the reduction of levulinic acid derivatives to γ-valerolactone and consecutive reduction products</i>
17.50 - 18.00	IND OR059	Francesco Mauriello	<i>Hydrogenolysis of aromatic ethers under lignin-first conditions</i>
18.00 - 18.30	Discussion		

Divisione CHIMICA ORGANICA (ORG)**ORG 15**

15.00 - 15.30	ORG PZ002	Paolo Tecilla	Medaglia Angelo Mangini <i>Self-organized Supramolecular Systems for Catalysis, Sensing and Transport</i>
15.30 - 16.00	ORG PZ009	Elena Lenci	Premio alla ricerca Chimica Organica per le Scienze della Vita Junior <i>Combining Diversity-Oriented Synthesis and chemoinformatics to generate small molecules libraries</i>
15.50 - 16.00	Break		
16.00 - 16.15	ORG OR092	Molly Pither	<i>Elucidation of the Chemical Structure of Lipopolysaccharides Isolated from the Commensal Bacteria Veillonella parvula</i>
16.15 - 16.30	ORG OR093	Debora Pratesi	<i>The glycomimetic approach for selective inhibition of Carbonic Anhydrases</i>
16.30 - 16.45	ORG OR094	Deborah Quaglio	<i>Resorc[4]arene-based site directed immobilization of antibodies for immunosensors development</i>
16.45 - 17.00	ORG OR095	Roberto Rossi	<i>Problem solving in Pharmaceutical processes: isolation, characterization and synthetic preparation of unknown impurities in 4-piperidinepropanol manufacture</i>
17.00 - 17.30	Break		
17.30 - 17.45	ORG OR096	Laura Russo	<i>Chemoselective synthesis of triple-functionalized nanoparticles for multimodal in vivo imaging of pancreatic β-cells</i>
17.45 - 18.00	ORG OR097	Giovanni Sacco	<i>Affinity enhancement of peptide ligands for tumor overexpressed receptors</i>
18.00 - 18.15	ORG OR098	Cristina Manuela Santi	<i>Synthesis of an analogue of Neisseria meningitidis A capsular polysaccharide for the development of a glycoconjugate vaccine</i>
18.15 - 18.30	ORG OR099	Federica Santino	<i>Rational Design of Pseudoproline-Containing K-Opioid Receptor-Selective Peptidomimetics</i>

ORG 16

			Premio alla ricerca Chimica Organica nei suoi Aspetti Metodologici Junior Catalyst Design via Computational Means: <i>Correlations Bridge Experiments and Calculations</i>
15.30 - 16.00	ORG PZ010	Manuel Orlandi	
16.00 - 16.15	ORG OR100	Valentina Pirota	<i>Selective hydrolysis of water-soluble naphthalene diimides driven by core-substitution</i>
16.15 - 16.30	ORG OR101	Simone Potenti	<i>4-Fluorothreonine as a test case: the effects of fluorination on molecular properties</i>
16.30 - 16.45	ORG OR102	Michele Ricci	<i>Application of ASCA modelling tools on a PDO hard cheese: Analysis of the effects on physical parameters of Trentingrana</i>
16.45 - 17.00	ORG OR103	Federica Sabuzi	<i>Computational study of substituted phenols pKa</i>
17.00 - 17.30	Break		
17.30 - 17.45	ORG OR104	Carla Rizzo	<i>New supramolecular fluorescent NDI-gels as bioimaging materials</i>
17.45 - 18.00	ORG OR105	Maria Sologan	<i>Functionalized gold nanoparticles for MRI applications</i>
18.00 - 18.15	ORG OR106	Benedetta Maria Squeo	<i>Thiophene substituted aza-BODIPY as promising metal-free, pure NIR emitter for OLEDs</i>
18.15 - 18.30	ORG OR107	Kristian Vasa	<i>Design and synthesis of macromolecular and nanostructured carbonic anhydrases-based materials</i>

ORG 17

			Premio alla ricerca Chimica Organica per l'Ambiente, l'Energia e le Nanoscienze Junior Powerful Strategies to Functionalized Molecules in One- Pot, Mild Conditions and Benign Solvents
15.30 - 16.00	ORG PZ011	Sara Meninno	
16.00 - 16.15	ORG OR108	Giulio Bertuzzi	<i>Novel Visible-Light Mediated Protocols for the Synthesis of N Heterocycles and Site-Selective Functionalizations</i>
16.15 - 16.30	ORG OR109	Tommaso Bortolato	<i>Radical α-Trifluoromethoxylation of Ketones by Means of Organic Photoredox Catalysis</i>
16.30 - 16.45	ORG OR110	Mattia Di Maro	<i>A ball-milling green synthetic procedure for the preparation of novel macromolecular stabilizers for polyolefinic-based materials</i>
16.45 - 17.00	ORG OR111	Salvatore Marullo	<i>Cholinium-based ionic liquids as catalysts for the glycolysis of post-consumer PET waste</i>
17.00 - 17.30	Break		
17.30 - 17.45	ORG OR112	Angelica Mero	<i>Treatment of biomass food waste by exploiting Natural Deep Eutectic Solvents and bio based-Ionic Liquids</i>

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17.45 - 18.00	ORG OR113	Elisabetta Monciatti	<i>Hydroaminomethylation of terminal alkenes in water: microwave and micellar catalysis roles</i>
18.00 - 18.15	ORG OR114	Matteo Tiecco	<i>Organocatalytic activity of chiral L-Proline-based Deep Eutectic Solvents</i>
18.15 - 18.30	ORG OR115	Federica Valentini	<i>Catalytic biomass valorization towards hydrogen transfer reactions using formic acid and derivatives as safe H-source</i>

ORG 18

15.30 - 16.00	ORG PZ012	Nicolas D'Imperio	Premio alla ricerca Chimica Organica per lo Sviluppo di Processi e Prodotti nell' Industria Junior Olefins from carbonyls. Development of new phosphorus-based cross-coupling reactions
16.00 - 16.15	ORG OR116	Valerio Fasano	<i>How Big is the Pinacol Boronic Ester as a Substituent?</i>
16.15 - 16.30	ORG OR117	Susanna Bertuletti	<i>From carbonyls to chiral alcohols via asymmetric biocatalysis: exploiting the substrate promiscuity of hydroxysteroid dehydrogenases (HSDHs)</i>
16.30 - 16.45	ORG OR118	Denisa Bisag	<i>Catalyst- and substrate- dependent chemodivergent reactivity of stabilised sulfur ylides with salicylaldehydes</i>
16.45 - 17.00	ORG OR119	Giulia Brufani	<i>Imidazolium based heterogenous catalyst for the synthesis of cyanohydrintrimethylsilyl ether and β-azido ketones</i>
17.00 - 17.30	Break		
17.30 - 17.45	ORG OR120	Emanuela Calcio Gaudino	<i>Highly Efficient Microwave-assisted synthetic protocols under Pd based β-cyclodextrin heterogeneous catalyst</i>
17.45 - 18.00	ORG OR121	Francesco Calogero	<i>Photoredox allylation and propargylation of aldehydes catalytic in titanium</i>
18.00 - 18.15	ORG OR122	Vincenzo Campisciano	<i>Al(III) Porphyrin-Imidazolium Salt Copolymer onto Carbon Nanotubes as Catalyst for the Synthesis of Cyclic Carbonates</i>
18.15 - 18.30	ORG OR123	Francesca Foschi	<i>Copper-Catalyzed/Hypervalent Iodine(III)-Mediated Dimerization/Cyclization of 2-Benzylamino-phenols: Synthesis of Fluorescent Oxazolo-phenoxazines</i>

Divisione CHIMICA DEI SISTEMI BIOLOGICI (CSB)**CSB 04**

15.00 - 15.30	CSB KN005	Angela Casini	<i>Gold-templated reactions in biological systems: from medicine to catalysis</i>
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15.30 - 15.45	CSB OR022	Francesco Bellia	<i>Hyaluronate–Carnosine conjugates: copper(II) complexes and antioxidant properties</i>
15.45 - 16.00	CSB OR023	Daniele Vitone	<i>The speciation of zinc complexes with chloroquine ligand</i>
16.00 - 16.15	CSB OR024	Valentina Oliveri	<i>8-Hydroxyquinoline Hybrids Differentially Interact with α-Synuclein</i>
16.15 - 16.30	CSB OR025	Giancarlo Terraneo	<i>Halogenation Dictates Architectures and Properties of Amyloid Peptides</i>
16.30 - 17.00	Break		
17.00 - 17.30	CSB KN006	Amedeo Cafilisch	<i>Fragment-based drug design</i>
17.30 - 17.45	FIS OR066	Federica Rizzi	<i>Role of the FZD10 delivering exosomes in cellular proliferation of gastrointestinal cancer</i>
17.45 - 18.00	FIS OR062	Ivana Miletto	<i>Functionalized Upconversion Nanoparticles for Theranostic</i>
18.00 - 18.15	CSB OR028	Gabriele Travagliante	<i>Spectroscopic study on interactions of porphyrins and micro-RNA</i>
18.15 - 18.50	Discussione		

Divisione DIDATTICA CHIMICA (DID)**DID 03**

15:00-15:30	DID IL003	Eleonora Aquilini	<i>Caring for yourself, the environment and others in primary school</i>
15:30-15:45	DID OR014	Sergio Palazzi	<i>Towards a material archive of dyestuffs from the XX century</i>
15:45-16:00	DID OR015	Ugo Cosentino	<i>The School-University joint interventions provided in the National Recovery and Resilience Plan</i>
16:00-18:00	Panel Discussion	Riccardo Iacona (Coordinator) Vincenzo Balzani Andrea Segrè Vittorio Maglia Giovanni De Feo	<i>360-degree sustainability</i>

Divisione SPETTROMETRIA DI MASSA (MAS)**MAS 03**

15.00 - 15.40	MAS PL004	Encarnación Moyano	<i>Mass spectrometry for the environmental analysis of halogenated organic pollutants</i>
15.40 - 16.10	MAS KN003	Sara Bogialli	<i>Mass spectrometry for the monitoring and protection of the environment</i>
16.10 - 16.25	MAS OR011	Carolina Barola	<i>Temporal trend of per- and polyfluoroalkyl substances in air samples collected at the rural site of Monte Martano (Central Italy)</i>
16.25 - 16.35	Break		

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16.35 - 17.15	MAS PL005	Antony Memboeuf	<i>How can energetics in CID MS/MS help the analytical chemists?</i>
17.15 - 17.30	MAS OR012	Angela Tartaglia	<i>Fabric Phase Sorptive Membrane Array: A Novel Approach for Non-Invasive In Vivo Sampling</i>
17.30 - 17.45	MAS OR013	Raffaella Pascale	<i>An interplay between FT-ICR MS and LC-LTQ MS/MS for Metabolic Profiling of Peperoni di Senise PGI Bell Peppers</i>
17.45 - 18.00	MAS OR014	Eugenio Aprea	<i>Volatile organic compounds in Gorgonzola cheese and their relationship with sensory descriptors and consumers' liking</i>
18.00 - 18.15	MAS OR015	Flaminia Vincenti	<i>New Synthetic Opioids: Development of Analytical Methods for Their Characterization and Determination by Means of HPLC-HRMS/MS</i>

Divisione TEORICA E COMPUTAZIONALE (TEO)

TEO 04

15:00 - 15:20	TEO KN004	Mauro Stener	<i>Predictive optical photoabsorption of metal clusters via efficient TDDFT simulations</i>
15:20 - 15:40	TEO PZ005	Lorenzo Cupellini	<i>Multiscale investigation of chlorophyll fluorescence quenching in plant light-harvesting complexes</i>
15:40 - 15:50	TEO OR024	Chiara Aieta	<i>Quantum nuclear densities from semiclassical on-the-fly molecular dynamics</i>
15:50 - 16:00	TEO OR025	Filippo Lipparini	<i>An easy and efficient strategy to compute an accurate SCF guess for ab-initio molecular dynamics simulations</i>
16:00 - 16:10	TEO OR026	Marco Mendolicchio	<i>Accuracy and Reliability in the Simulation of Vibrational Spectra: A Comprehensive Benchmark of Generalized Vibrational Perturbation Theory to the Second Order (GVPT2)</i>
16:10 - 16:20	TEO OR027	Fulvio Perrella	<i>Improving accuracy and efficiency of ADMP Extended Lagrangian Molecular Dynamics</i>
16:20 - 16:30	TEO OR028	Diego Sorbelli	<i>Probing the electronic structure of gold dihydride with state-of-the-art relativistic approaches</i>
16:30 - 17:00	break		
17:00 - 17:20	TEO PZ006	Nicola Tasinato	<i>Computational Strategies for Environmental Chemistry</i>
17:20 - 17:30	TEO OR029	Francesco Di Maiolo	<i>Theoretical Approaches to Quantum Molecular Dynamics in Out of Equilibrium Environments</i>
17:30 - 17:40	TEO OR030	Lorenzo Donà	<i>Extending and assessing composite electronic structure methods to the solid state</i>
17:40 - 17:50	TEO OR031	Federica Lodesani	<i>An in-depth look into the mechanism of crystallization of lithium disilicate: a metadynamics study</i>

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17:50 - 18:00	TEO OR032	D. K. Andrea Phan Huu	<i>Molecular spectroscopy in condensed phases: an antiadiabatic approach to the medium polarizability</i>
18:00 - 18:10	TEO OR033	Pierpaolo Pravatto	<i>Tunneling splitting and the stochastic description of activated processes</i>
18:10 - 18:30	discussione finale		