

Programma dei LAVORI di DIVISIONE - 15 settembre pomeriggio**Divisione CHIMICA ANALITICA (ANA)****ANA 01**

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|---------------|------------------|------------------------------|---|
| 15.00 - 15.10 | ANA PL001 | Claudio Minero | INTRODUZIONE |
| 15.10 - 15.30 | ANA PZ001 | Luigia Sabbatini | <i>Contaminarsi fa bene alla ricerca</i> |
| 15.30 - 15.50 | ANA PZ002 | Luigi Mondello | <i>Recent Developments in Mass spectrometry and Cutting Edge Scientific Innovation to Characterize Complex Samples</i> |
| 15.50 - 16.10 | ANA IL001 | Susy Piovesana | <i>New trends for the enrichment and liquid chromatography-mass spectrometry analysis of peptides with protein post-translational modifications</i> |
| 16.10 - 16.30 | ANA KN001 | Flavio A. Franchina | <i>The value of multidimensional chromatography coupled to mass spectrometry for the non-targeted metabolite profiling of natural products</i> |
| 16.30 - 16.45 | ANA OR001 | Alessia Arena | <i>Mineral oil investigation in omega-3 rich lipid supplements by using multidimensional liquid-gas chromatography</i> |
| 16.45 - 17.00 | ANA OR002 | Carmela Maria Montone | <i>Untargeted characterization and quantitative analysis of underivatized fatty acids in <i>Chlorella vulgaris</i> microalgae</i> |
| 17.00 - 17.15 | ANA OR003 | Lorenzo Cucinotta | <i>Simultaneous Enantiomeric and Isotopic Ratio evaluation of target terpenes in <i>Cannabis sativa</i> essential oils through Enantio-MDGC-C-IRMS</i> |
| 17.15 - 17.30 | ANA OR004 | Gemma De Grazia | <i>Evaluation of cryogenic effect for target VOCs isolation by a preparative multidimensional gas chromatographic system</i> |
| 17.30 - 17.45 | ANA OR005 | Rosangela Elliani | DEVELOPMENT OF A RAPID AND SIMPLE PROTOCOL FOR THE ASSAY OF PARABENS AND BISPHENOLS IN HUMAN SALIVA BY SOLID-PHASE MICROEXTRACTION-GAS CHROMATOGRAPHY-TRIPLE QUADRUPOLE MASS SPECTROMETRY |
| 17.45 - 18.00 | ANA OR006 | Antonio Ferracane | <i>Simultaneous determination of 88 multi-class pesticide residues in four vegetable matrices using reduced QuEChERS extraction and flow-modulated comprehensive two-dimensional gas chromatography-triple quadrupole mass spectrometry</i> |
| 18.00 - 18.15 | ANA OR007 | Micaela Galletta | <i>Evaluation of use of hydrogen as carrier gas in flow-modulation comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry</i> |

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| 18.15 - 18.30 | ANA OR008 | Anna Illiano | <i>LC-MRM/MS assay for the quantification of some hormonal proteins in serum and follicular fluid of women undergoing in vitro fertilization</i> |
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ANA 02

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| 15.50 - 16.10 | ANA KN002 | Clemente Bretti | <i>Removal of environmentally relevant cations: polymer inclusion membranes (PIMs)</i> |
| 16.10 - 16.30 | ANA KN003 | Francesco Pellegrino | <i>A New Strategy for Overcoming the Volcano in Water Photosplitting: Controlled Periodic Illumination</i> |
| 16.30 - 16.45 | ANA OR009 | Raghav Dogra | <i>Preliminary evaluation of Magnetic Nanoparticles for glyphosate contaminated water remediation</i> |
| 16.45 - 17.00 | ANA OR010 | Federico Girolametti | <i>Evaluation of mercury content in red mullet (<i>Mullus barbatus</i>) muscle from the Adriatic Sea in relation to biological factors and sampling area: risk assessment for human consumption</i> |
| 17.00 - 17.15 | ANA OR011 | Marco Minella | <i>Experimental evaluation of Fenton oxidation coupled with membrane distillation for produced water treatment: benefits, challenges and effluent toxicity</i> |
| 17.15 - 17.30 | ANA OR012 | Donatella Nardiello | <i>Nanoconfined liquid phase nanoextraction: an innovative extraction technique for ex-situ and in-situ rapid and quantitative determination of benzene derivatives in seawater</i> |
| 17.30 - 17.45 | ANA OR013 | Gabriella Pinto | <i>Characterization of polyphenolic compounds in food and industrial wastes</i> |
| 17.45 - 18.00 | ANA OR014 | Luca Rivoira | <i>Iterative protocols for the extraction and quantitation of microplastics from marine sediments and oysters</i> |
| 18.00 - 18.15 | ANA OR015 | Saul Santini | <i>Validation of a new method for the simultaneous determination of different classes of PBT chemicals in biota samples</i> |
| 18.15 - 18.30 | ANA OR016 | Davide Vivado | <i>Study of iron speciation in coastal seawater samples of the Ross Sea (Antarctica) by CLE-AdSV</i> |

ANA 03

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| 15.50 - 16.10 | ANA IL002 | Erika Scavetta | <i>Organic Electrochemical Transistors as low cost chemical sensors</i> |
| 16.10 - 16.30 | ANA IL003 | Chiara Zanardi | <i>Graphene-based electrodes for the detection of biomarkers in sweat</i> |
| 16.30 - 16.45 | ANA OR017 | Andrea Bonini | <i>A Label-free impedance biosensing assay based on CRISPR/Cas12a collateral activity for bacterial DNA detection</i> |

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| 16.45 - 17.00 | ANA OR018 | Tiziano Di Giulio | <i>Molecularly imprinted polymers-based impedimetric sensor for metal-ion mediated recognition of a dipeptide</i> |
| 17.00 - 17.15 | ANA OR019 | Laura Fabiani | <i>Magnetic beads combined with carbon black-based screen-printed electrodes for COVID-19: A reliable and miniaturized electrochemical immunosensor for SARS-CoV-2 detection in saliva</i> |
| 17.15 - 17.30 | ANA OR020 | Eleonora Macchia | <i>Selective Single-Molecule Detection of clinically relevant biomarkers with an Organic Transistor</i> |
| 17.30 - 17.45 | ANA OR021 | Federica Mariani | <i>Healthcare monitoring using wearable pH sensors</i> |
| 17.45 - 18.00 | ANA OR022 | Vincenzo Mazzaracchio | <i>A TiO₂ /KuQuinone modified screen-printed photoelectrochemical sensor for NADH detection</i> |
| 18.00 - 18.15 | ANA OR023 | Gheorghe Melinte | <i>Enhancement of lysozyme detection process by using a gold clusters-based electrochemical aptasensor</i> |
| 18.15 - 18.30 | ANA OR024 | Filippo Silveri | <i>Redox-active graphene film integrated into a smart device for pesticide biosensing</i> |

Divisione CHIMICA FARMACEUTICA (FAR)
FAR 03

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| 15.00 - 15.45 | FAR MD001 | Kenneth A. Jacobson | <i>Pratesi Medal Lecture - Design and Therapeutic Potential of Adenosine and P2Y Receptor Ligands</i> |
| 15.45 - 16.00 | FAR PZ001 | Ciro Milite | <i>Modulators of Coactivator-Associated Arginine Methyltransferase 1 (CARM-1): There and Back Again</i> |
| 16.00 - 16.15 | FAR PZ002 | Mariateresa Giustiniano | <i>Isocyanide Chemistry from the Ground (state) to the Star(s): what's the point for a medicinal chemist?</i> |
| 16.15 - 17.00 | FAR MD002 | Antonello Mai | <i>Giacomello Medal Lecture - Lecture for the receipt of the "Giordano Giacomello" medal by the Medicinal Chemistry Division of the Italian Chemical Society</i> |
| 17.00 - 17.15 | break | | |
| 17.15 - 17.30 | FAR OR011 | Marilia Barreca | <i>Inhibition of non-Hodgkin lymphoma cell growth by pyrrolo[1,2]oxazole derivatives</i> |
| 17.30 - 17.45 | FAR OR012 | Laura Braconi | <i>A new strategy to overcome multidrug resistance (MDR) in cancer cells: P-gp and hCAXII multitarget inhibitors</i> |
| 17.45 - 18.00 | FAR OR013 | Daniela Carbone | <i>Synthesis and preclinical evaluation of a new generation of 1,2,4-triazine-based PDK modulators: a novel therapeutic approach to halt cancer growth.</i> |

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| 18.00 - 18.15 | FAR OR014 | Arianna Gelain | <i>Unraveling the interaction mechanism of a benzothiadiazole-2,2-dioxide derivative with STAT3: towards novel direct inhibitors</i> |
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FAR 04

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| 17.15 - 17.30 | FAR OR015 | Lucia Tamborini | <i>Flow-based redox biotransformations for food and pharma applications</i> |
| 17.30 - 17.45 | FAR OR016 | Federica Ianni | <i>Stability of chlorogenic acid as model system after household microwave treatment</i> |
| 17.45 - 18.00 | FAR OR017 | Ilaria Frosi | <i>Comparison of different extraction methods to recover bioactive compounds from corn waste (Zea mays L.)</i> |
| 18.00 - 18.15 | FAR OR018 | Martina Contente | <i>Valorization of food wastes and residues through glycosidases</i> |

Divisione CHIMICA INDUSTRIALE (IND)

IND 01

Sessione congiunta con Gruppo Interdivisionale Catalisi

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|---------------|--|----------------------------|---|
| 15.00 - 15.30 | IND KN001 Medaglia Piero Pino | Nicoletta Ravasio | <i>Catalysis and Green Deal</i> |
| 15,30 - 15,40 | IND OR001 | Eleonora Aneggi | <i>Solvent free selective oxidation of benzyl alcohol over supported Ru catalysts</i> |
| 15.40 - 15.50 | IND OR002 | Denise Cavuoto | <i>The role of support wettability and acidity in the hydrogenation of γ-valerolactone over Cu/SiO₂ catalyst</i> |
| 15.50 - 16,00 | IND OR003 | Tommaso Tabanelli | <i>Improved Catalytic Transfer Hydrogenation of alkyl levulinates with alcohols over ZrO₂ based catalysts</i> |
| 16.00 - 16.10 | IND OR004 | Eleonora Vottero | <i>Reconstruction phenomena in a Pt/γ-Al₂O₃ catalyst under hydrogenation conditions</i> |
| 16.10 - 16.20 | IND OR005 | Maila Danielis | <i>Structural Evolution and Enhanced Steam Deactivation Resistance of PtPd/CeO₂ Methane Oxidation Catalysts Prepared by Dry Milling</i> |
| 16.20 - 16.30 | IND OR006 | Gabriella Garbarino | <i>Effect of promoters on the performances of Ni-Al₂O₃ catalysts for CO₂ hydrogenation</i> |
| 16.30 - 16.45 | Discussion | | |
| 16.45 - 17.00 | break | | |
| 17.00 - 17.20 | IND KN002 | Walter Cabri | <i>The Twelve Principles of Green Chemistry Translation Guide for Palladium Catalyzed Cross Coupling Reactions for Active Pharmaceutical Ingredients Sustainable Productions"</i> |
| 17.20 - 17.30 | IND OR007 | Roberto Sole | <i>The alkoxy carbonylation of protected propargyl alcohols</i> |

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| 17.30 - 17.40 | IND OR008 | Aleksandr Voronov | <i>Unexpected O-5-exo-dig Cyclization of Propargyl Ureas to Oxazoline-2-amines Catalyzed by Silver Salts</i> |
| 17.40 - 17.50 | IND OR009 | Francesco Taddeo | <i>Kinetics of solketal synthesis promoted by Iron(III) complex</i> |
| 17.50 - 18.00 | IND OR010 | Vinayak. Botla | <i>Palladium/Norbornene-Catalyzed Synthesis of 2-Iodobiphenyls</i> |
| 18.00 - 18.10 | IND OR011 | Stefano Econdi | <i>Heterogeneous catalysts for the liquid-phase degradation of simulants of organophosphorus chemical warfare agents</i> |
| 18.10 - 18.30 | Discussion | | |

Divisione CHIMICA ORGANICA (ORG)

ORG 01

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|---------------|--|-------------------|--|
| 15.00 - 15.30 | Benvenuto e premiazione (sessioni unificate) | | |
| 15.30 - 16:00 | ORG PZ001 | Anna Bernardi | Medaglia Adolfo Quilico <i>At the crossroad between Chemistry and Biology: interfering with the sugar code using glycomimetics</i> |
| 16.00 - 16.15 | ORG OR001 | Alessandro Ajo | <i>Nanocages and capsules for drug and peptides delivery</i> |
| 16.15 - 16.30 | ORG OR002 | Silvana Alfei | <i>Cationic Copolymers: A Promising Option in the Treatment of Drug Resistance in Neuroblastoma Cells</i> |
| 16.30 - 16.45 | ORG OR003 | Davide Audisio | <i>Direct Carbon Isotope Exchange of Pharmaceuticals via Reversible Decyanation</i> |
| 16.45 - 17.00 | ORG OR004 | Sara Battista | <i>Antibacterial and physicochemical properties of quatsomes formulated with L-prolinol-derived surfactants</i> |
| 17.00 - 17.30 | Break | | |
| 17.30 - 17.45 | ORG OR005 | Roberta Bernini | <i>Hydroxytyrosol, much more than an antioxidant</i> |
| 17.45 - 18.00 | ORG OR006 | Andrea Calcaterra | <i>Diels-Alder type adducts from Morus nigra as potent inhibitors of Micobacterium tuberculosis PtpB</i> |
| 18.00 - 18.15 | ORG OR007 | Fabrizio Chiodo | <i>Carbohydrate-Mediated "Innate" Considerations in Designing Vaccine-Candidates</i> |
| 18.15 - 18.30 | ORG OR008 | Martina Cirillo | <i>Selective Integrin Ligands Promote Cell Internalization of the antineoplastic agent Fluorouracil</i> |

ORG 02

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| 16.00 - 16.15 | ORG OR009 | Mariapina D'Onofrio | <i>Chemoselective disulfide-coupling for the semisynthesis of ubiquitinated forms of the Alzheimer's associated protein tau</i> |
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| 16.15 - 16.30 | ORG OR010 | Maria Giulia Davighi | <i>New potential carbonic anhydrase inhibitors based on mono and multivalent sugars and iminosugars</i> |
| 16.30 - 16.45 | ORG OR011 | Cristina De Castro | <i>N-glycan from Paramecium bursaria Chlorella virus MA-1D: reevaluation</i> |
| 16.45 - 17.00 | ORG OR012 | Jenny Desantis | <i>Design, synthesis, and evaluation of small molecules Proteolysis Targeting Chimeras (PROTACs) to induce androgen receptor degradation</i> |
| 17.00 - 17.30 | Break | | |
| 17.30 - 17.45 | ORG OR013 | Cristina Di Carluccio | <i>Investigation of the molecular recognition of sialoglycans bound to Siglec-like adhesins of Streptococcus gordonii</i> |
| 17.45 - 18.00 | ORG OR014 | Rossella Di Guida | <i>Structural characterization of the lipooligosaccharide and capsular polysaccharide from the psychrotrophic bacterium Pseudoalteromonas nigrifaciens Sq02</i> |
| 18.00 - 18.15 | ORG OR015 | Maria Funicello | <i>Switching the anticancer effect to HIV protease inhibition: new heteroaryl-amidic compounds with a pseudo-symmetric core</i> |
| 18.15 - 18.30 | ORG OR016 | Dario Gentili | <i>Synthesis of small molecules with potential antiviral activity against Sars-CoV-2</i> |

ORG 03

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| 16.00 - 16.15 | ORG OR017 | Vincenzo Algieri | <i>Regioselective Synthesis of 1,3,4,5-Tetrasubstituted Pyrazoles by Eliminative Enaminone-Nitrilimine 1,3-Dipolar Cycloaddition</i> |
| 16.15 - 16.30 | ORG OR018 | Michael Andresini | <i>Nitrogen transfer to sulfenamides: synthesis of sulfinamidines and unexplored sulfinimidate esters as valuable precursors of protected sulfilimines</i> |
| 16.30 - 16.45 | ORG OR019 | Marco Ballarotto | <i>Substituted 6H-benzo[c]chromenes: synthetic approach via a Diels-Alder/aromatization sequence and computational investigation</i> |
| 16.45 - 17.00 | ORG OR020 | Bruno Mattia Bizzarri | <i>Aminomaleonitrile inspired prebiotic chemistry as a novel microwave assisted multicomponent tool for the synthesis of imidazole and purine derivatives with anti-influenza activity</i> |
| 17.00 - 17.30 | Break | | |
| 17.30 - 17.45 | ORG OR021 | Diego Caprioglio | <i>The oxidation of phytocannabinoids: a systematic investigation</i> |
| 17.45 - 18.00 | ORG OR022 | Marco Colella | <i>Use of flow technology for the development of a sustainable synthesis of azetines and azetidines</i> |
| 18.00 - 18.15 | ORG OR023 | Dario Corbisiero | <i>Enantioselective Synthesis of Polyfunctionalized Isoxazoline Rings: Development of a Methodology for the preparation of Tumor-Oriented Small Molecules</i> |

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| 18.15 - 18.30 | ORG OR024 | Massimiliano Cordaro | <i>Synthetic Approaches to Molecular Diversity of BODIPY</i> |
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ORG 04

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| 16.00 - 16.15 | ORG OR025 | Vincenzo Mirco Abbinante | <i>Highly-fluorinated aromatic diimides for organic electronics: from synthesis to thin-film preparation</i> |
| 16.15 - 16.30 | ORG OR026 | Rita Argenziano | <i>Functional films from 5,6-dihydroxyindole oligomers and long chain diamines partnership</i> |
| 16.30 - 16.45 | ORG OR027 | Giacomo Biagiotti | <i>Tailoring the structure of the BODIPY probe in the design of functional fluorescent materials</i> |
| 16.45 - 17.00 | ORG OR028 | Davide Blasi | <i>Trityl-brominated radicals as building blocks for doublet CPL emitters</i> |
| 17.00 - 17.30 | Break | | |
| 17.30 - 17.45 | ORG OR029 | Alberto Bossi | <i>Porphycenes, a lesser known tetrapyrrolic macrocycle with intriguing properties suitable for in situ sensing</i> |
| 17.45 - 18.00 | ORG OR030 | Adriano Parodi | <i>Polyhydroxybutyrate as a sustainable platform for the production of chemicals and bio-polymers</i> |
| 18.00 - 18.15 | ORG OR031 | Simone Di Noja | <i>Transfer of Axial Chirality to the Nanoscale Endows Carbon Dots with Circularly Polarized Luminescence</i> |
| 18.15 - 18.30 | ORG OR032 | Claudio Ferdeghini | <i>Synthesis and thermal behavior of dicationic ionic liquids</i> |

Divisione CHIMICA DEI SISTEMI BIOLOGICI (CSB)

CSB 01

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| 15.00 - 15.05 | Opening Remarks Presidente Michael Assfalg | | |
| 15.05 - 15.35 | CSB KN001 | Rommie Amaro | <i>Computational Microscopy of SARS-CoV-2</i> |
| 15.35 - 16.00 | CSB PZ001 | Luca Mazzei | <i>Talking about urease: How the grasp on the molecular aspects of this enzyme can help in counteracting its role in microbiological pathogenesis and environmental issues</i> |
| 16.00 - 16.15 | CSB OR001 | Marta De Zotti | <i>A pH-Induced Reversible Conformational Switch able to control the Photocurrent Efficiency in a Peptide Supramolecular System</i> |
| 16.15 - 16.30 | CSB OR002 | Ottavia Bellotto | <i>Supramolecular hydrogels from unprotected dipeptides: a comparative study on stereoisomers and structural isomers the Photocurrent Efficiency in a Peptide Supramolecular System</i> |
| 16.30 - 17.00 | Break | | |
| 17.00 - 17.30 | CSB PZ002 | Claudia Bonfio | <i>Uncovering the emergence of modern cells</i> |
| 17.30 - 17.45 | CSB OR003 | Gianantonio Battistuzzi | <i>Molecular basis of myoglobinopathy, a newly discovered molecular disease</i> |
| 17.45 - 18.00 | CSB OR004 | Lidietta Giorno | <i>Selectivity and stability of biological macromolecules heterogenized to nanostructured artificial membranes</i> |

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| 18.00 - 18.15 | CSB OR005 | Claudia Riccardi | <i>Design, synthesis and characterization of cyclic TBA analogues</i> |
| 18.15 - 18.50 | Discussione | | |

Divisione DIDATTICA CHIMICA (DID)

DID 01

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| 15:00-16:00 | DID PL001 | Jan Apotheker | <i>Developments in chemistry education</i> |
| 16:00-16:30 | DID IL001 | Mariano Venanzi | <i>Sustainable chemistry for a sustainable teaching. A proposal for a first level curriculum in Chemistry at University</i> |
| 16:30-16:45 | DID OR001 | Federica Branchini | <i>Teaching the notion of chemical bonding: a didactic challenge</i> |
| 16:45-17:00 | DID OR002 | Maria Antonietta Carpentieri | <i>A new didactic pathway to introduce Spectroscopy by historical-epistemological/STEM laboratorial/distance learning blended approach</i> |
| 17:00-17:15 | DID OR003 | Maria Costa | <i>Virtual Reality visualizations of complex molecular structures in chemistry education. The β-CD-ASA example</i> |
| 17:15-17:30 | DID OR004 | Sandro Jurinovich | <i>A didactic sequence for teaching chromatography: observation, model and practical applications</i> |
| 17:30-17:45 | DID OR005 | Dora Stella Lombardi | <i>'Light and Molecules': an experimental approach to the understanding of basic concepts of Quantum Mechanics</i> |
| 17:45-18:00 | DID OR006 | Alma Moretta | <i>Additional Learning Requirements (OFA) in Math for Environmental Science degree course: a review for a better understanding of the difficulties of students entering university</i> |
| 18:00-18:15 | DID OR007 | Davide Peddis | <i>From the astro to the nano scale: a learning by doing teaching pathway</i> |
| 18:15-18:30 | DID OR008 | Antonio Testoni | <i>Chemistry, history and complexity</i> |
| 18:30-18:45 | DID OR009 | Sergio Palazzi | <i>A colorful new morning - teaching applied chemistry in pandemic times</i> |

Divisione SPETTROMETRIA DI MASSA (MAS)

MAS 01

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| 15.00 - 15.15 | Welcome | | |
| 15.15 - 15.55 | MAS PL001 | Giuseppina Maccarone | <i>The Role of Mass Spectrometry in the – omics Era</i> |
| 15.55 - 16.10 | MAS OR001 | Daniela Cecconi | <i>Integrated lipidomics and proteomics reveal cardiolipin remodelling, upregulation of HADHA and long chain fatty acids in pancreatic cancer stem cells</i> |
| 16.10 - 16.25 | MAS OR002 | Silvia Pedretti | <i>Metabolomic approaches to investigate the role of the mitochondrial</i> |
| 16.25 - 16.35 | Break | | |

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| 16.35 - 17.15 | MAS PL002 | John A. McLean | <i>High dimensional molecular phenomics in systems, synthetic, and chemical biology</i> |
| 17.15 - 17.30 | MAS OR003 | Isabella Piga | <i>Spatial proteomics to map tissue alterations during the progression of fibrosis in an IPF and Nintedanib-treated mouse model</i> |
| 17.30 - 17.45 | MAS OR004 | Federico Fanti | <i>Quantitative analysis of resolvins in biological matrices by means LLE-μSPE-HPLC-MS/MS</i> |
| 17.45 - 18.00 | MAS OR005 | Elettra Barberis | <i>A Combined GCxGC-MS and GC-MS Approach to Discovery and Validate New Potential Biomarkers for Prostate Cancer Diagnosis</i> |

Divisione TEORICA E COMPUTAZIONALE (TEO)

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| 15:00 - 15:20 | TEO KN001 | Emilia Sicilia | <i>Computations for investigating anticancer activity of metal-based compounds beyond cisplatin</i> |
| 15:20 - 15:40 | TEO PZ001 | Greta Donati | <i>Exploring Chemistry through Multiple Time and Size Scales</i> |
| 15:40 - 15:50 | TEO OR001 | Marco Bertani | <i>Improving empirical force fields for molecular dynamics simulations of oxide glasses. The importance of three-body interactions in rigid-ion models</i> |
| 15:50 - 16:00 | TEO OR002 | Arianna Massaro | <i>First-principles study of Oxygen redox activity in P2-type $\text{Na}_x\text{Ni}_{0.25}\text{Mn}_{0.68}\text{O}_2$ high energy cathode for Na-ion batteries</i> |
| 16:00 - 16:10 | TEO OR003 | Mirko Vanzan | <i>An atomistic insight on the hot-electron injection mechanism</i> |
| 16:10 - 16:20 | TEO OR004 | Sergio Tosoni | <i>Computational characterization of single-atom species on metal-supported oxide thin films</i> |
| 16:20 - 16:30 | TEO OR005 | Ida Ritacco | <i>Spontaneous Production of Ultrastable Reactive Oxygen Species on Titanium Oxide Surfaces Modified with Organic Ligands</i> |
| 16:30 - 17:00 | break | | |
| 17:00 - 17:20 | TEO PZ002 | Alessandro Erba | <i>The Role of Fock Exchange in Relativistic Density Functional Theory</i> |
| 17:20 - 17:30 | TEO OR006 | Luca Brugnoli | <i>Development and application of a ReaxFF Reactive Force Field for Cerium Oxide/Water Interfaces</i> |
| 17:30 - 17:40 | TEO PO005 | Anna Ranaudo | <i>Computational study on the structural stability of mutated Affitins</i> |
| 17:40 - 17:50 | TEO OR008 | Noelia Faginas-Lago | <i>Molecular Simulations of $\text{CO}_2/\text{N}_2/\text{H}_2\text{O}$ Gaseous Mixture Separation in Graphtriyne Membrane</i> |
| 17:50 - 18:00 | TEO OR009 | Francesca Fasulo | <i>Electrode-electrolyte interface in solid-state lithium batteries: new insights from density functional embedding theory</i> |

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| 18:00 - 18:10 | TEO OR010 | Mariagrazia Fortino | <i>Multi-replica biased sampling for photoswitchable p-conjugated polymers</i> |
| 18:10 - 18:30 | discussion | | |