



MERCK & ELSEVIER Young Chemists Symposium



An event by



Società Chimica Italiana
Gruppo Giovani



Hotel Ambasciatori & Hotel Sporting
Rimini (Italy)
November 19th – 21st, 2018



ELSEVIER

MERCK

MONDAY, 19TH NOVEMBER

11:30 **Registration and Check-in** – Conference desk (Hotel Ambasciatori)

14:30 **Opening ceremony** – Sala Quarzo (Hotel Ambasciatori)

15:00 **Session #1** – Sala Quarzo (Hotel Ambasciatori) **Chair: Alessandro D'Urso**

Plenary lecture – **Pierangelo Metrangolo** (PoliMI)

Self-organization and emerging properties of halogenated peptide assemblies

15:40 **Claudio Carrara** (Industrie De Nora S.p.A.) – *Water electrolysis: case study of innovation at De Nora*

Giulia Piana (PoliTO) – *Novel sustainable processes and materials for polymer electrolytes in sodium-ion batteries*

Michele Cutini (UniTO) – *What is the driving force for collagen protein folding? Insights from hybrid DFT simulations*

Carlos Rodriguez Del Rio (Elsevier) – *Reaxys: don't reinvent the wheel. Drive it!*

16:30 **Coffee break** – American bar (Hotel Ambasciatori)

17:00

Session #2

Materials and processes for advanced technologies

Sala Quarzo (Hotel Ambasciatori)

Chair: Raffaele Cucciniello

Emilia Paone (UniRC) – *Transfer hydrogenolysis of benzyl phenyl ether promoted by the bimetallic Pd/Co catalyst*

Luca Lavagna (PoliTO) – *Cellulose functionalization: comparison between wet-chemistry hydrophobization vs. photopolymerization*

Federico Begni (UniUPO) – *On the toluene adsorption on hyper cross-linked polymers*

Federica Lazzari (UniMI) – *PGSE NMR studies on complex formulation of aminoacid deriving polymers and sodium deoxycholate micelle*

Session #3

Frontiers in organic chemistry

Sala Ametista (Hotel Ambasciatori)

Chair: Samuele Staderini

Nicola Zappimbulso (UniBA) – *Solvent-free Pd-catalyzed heteroaryl-aryl coupling reactions via C–H bond activation*

Costanza Vanni (UniFI) – *Multivalent glycomimetics: anchoring iminosugars on dendrimeric and globular scaffolds*

Stefano Valente (UNITS) – *Design, synthesis and characterization of fluorinated gold nanoparticles as theranostic agents*

Federica Rogati (UniUPO) – *Triterpenoids hydroxamates as HIF prolyl hydrolase inhibitors*

Session #4

Flash talks on the bio, pharma and organic scenario

Sala Smeraldo (Hotel Sporting)

Chair: Lorenzo Botta

Emanuele Azzi (UniTO) – *Photocatalytic synthesis of tetrahydropyridazines*

Mariateresa Badolato (UniCAL) – *1,4-naphthoquinones: discovery and mechanistic elucidation of a new class of yriple-negative breast cancer antiproliferative agents targeting GPR55*

Fabio Bologna (UniBO) – *High-throughput virtual screening to design protein-gadofullerene hybrids*

Margherita Bazzoni (UniPR) – *Efficient active-template synthesis of calix[6]arene-based oriented rotaxanes and pseudorotaxanes*

Session #5

Current trends in analytical methods

Sala Rubino (Hotel Sporting)

Chair: Placido Franco

Denise Bellotti (UniFE) – *Investigation on Zn(II) and Cu(II) binding sites in C4YJH2, a putative metal transporter of Candida albicans*

Tatiana Chenet (UniFE) – *Adsorption of L-lysine on L and ZSM-5 zeolites*

Eleonora Conca (UniTO) – *Methods for elemental analysis of PM samples collected on aluminum foils: results of an inter-comparison exercise*

Simona Felletti (UniFE) – *Thermodynamic comparison of zwitterionic teicoplanin-based 2µm superficially and sub-2µm fully porous particles for ultrafast chiral liquid chromatography*

Aurelio Bifulco (UniNA) – *Silica coated hemp fabrics and microfibers through a green ecofriendly chemical approach*

Enrico Casamassa (CNR) – *Chemistry and friction: a new method to investigate tribological problems*

Jacopo De Maron (UniBO) – *Alkyl carbonates as non-toxic reagents for selective gas-phase alkylation of phenolics*

Valeria Loise (UniCAL) – *Multiwalled carbon nanotubes: chemical physical characterization and rheological effect on bitumen*

Nicola Di Fidio (UniPI) – *An integrated and versatile biorefinery model to produce lipids from second generation biomass*

Carmelina Rossano (UniNA) – *Kinetic study of the levulinic acid esterification with ethanol promoted by Amberlyst-15*

Giulio Latini (PoliTO) – *Advances in CO₂ capture by task specific bio-based ionic liquids*

Freddy Liendo (PoliTO) – *Intensification of calcium carbonate precipitation in a packed bed reactor*

Maria J. Moran Plata (UniTO) – *Copper (0) nanoparticles in glycerol: an efficient and versatile catalyst for hydride-free reduction of nitro derivatives*

Angelo Nicosia (UniCT) – *Structure-effects correlation on symmetry breaking phenomenon in supramolecular aggregates of porphyrin based polymers*

Domenica Raciti (UniCT) – *Interface dynamics at oscillating air bubbles*

Giorgio Rizzo (UniBA) – *Structural characterization of regenerated silk fibroin through CeCl₃ solubilization protocol*

Antonia Rinaldi (UniFI) – *Tandem gold(I)-catalyzed cyclization for the synthesis of pentannulated N-hetero and carbacycles*

Stefano Nejrotti (UniTO) – *Natural deep eutectic solvents as an efficient catalytic system for the Nazarov cyclization*

Roberta Puglisi (UniCT) – *Supramolecular detection of nerve agents simulant: from mono-topic to multi-topic approach*

Andrea Mezzetta (UniPI) – *A new class of solvents for sustainable cellulose functionalisation*

Giulia Marafon (UniPD) – *Intrinsically photoswitchable α/β peptides toward two-state foldamers*

Vincenzo Marsicano (UnivAQ) – *Synthesis of polycyclic quinolines by means of Brønsted acid catalyzed reaction of β -(2-aminophenyl)- α,β -ynones with ketones*

Alessandro Manfrin (ETH) – *Substituent effect on the direct photodegradation of benzotrifluorides*

Maria Cristina Ligi (UniFI) – *Application of carbon nanotubes to tissue regeneration*

Giorgio Grillo (UniTO) – *Microwave-assisted synthesis of 1,4-pentanediol over Au catalysts: a metal/support coordinative effect*

Chiara Gangemi (UniCT) – *Structure beyond sequence: which role for miRNA conformations?*

Cosmin Butnaru (UniTO) – *A biosimilar mucus model to evaluate the diffusion of drugs for more efficient cystic fibrosis therapies*

Alessandra Benassi (UniPV) – *Photoactivable 2,5-diaryl tetrazoles as novel scaffolds for assembling selective G-quadruplex ligands*

Gabriele Carullo (UniCAL) – *Quercetin-3-oleate: bio-catalytic synthesis and efficacy validation in diabetic foot ulcers*

Linda Bertato (UnINSUBRIA) – *Integrating bioaccumulation assessment tools for mammals: from data collection to in silico modelling*

Gianluca Casotti (UniPI) – *Uncatalyzed organozinc halides conjugate addition to enones*

Federica Guarra (UniPI) – *Development of radiolabeled gold(III) N-heterocyclic carbenes*

Kelly Bugatti (UniPR) – *Synthesis of new small-molecule peptidomimetics as selective $\alpha\beta_6$ integrin ligands*

Giulio Lucarelli (UniROMA-1) – *Enantioselective preparation of the first key intermediate in the synthesis of (+)-oryzaalexin S*

Maria Sole Burali (UniPG) – *Heterocyclic compounds inhibitors of NS5 RNA-dependent RNA polymerase of Dengue virus*

Margherita Pirola (UniMI) – *Trichlorosilane: a versatile reagent for nitroalkanes transformations*

Sarah Mazzotta (Univ Sevilla) – *Piperazine thiourea derivatives against clinical strains of colistin-resistant *Acinetobacter baumannii*. Synthesis and in vitro biological evaluation*

Chiara Giorio (UniPD) – *Formation of metal-ligand complexes in atmospheric aerosol from an urban environment in Padua (Italy)*

Elisa Musella (UniBO) – *New electrochemical strategy for the preparation of layered double hydroxides (LDHs)*

Session #6

Flash talks on materials chemistry for nanotech

Sala Rubino (Hotel Sporting)

Chair: **Leonardo Triggiani**

Enrico Catizzone (UniCAL) – *Catalytic assessment of zeolite-based systems for dimethyl ether synthesis*

Lucia Fagiolari (PoliTO) – *Ambient condition fabrication of perovskite solar cells*

Fortuna Ponte (UniCAL) – *Metadynamics as a tool for studying the reduction mechanism of Asplatin, a Pt(IV) prodrug*

Stefano Marchesi (UniUPO) – *Sequestration of lanthanide ions from aqueous solutions with synthetic saponite slays*

Chiara Ivaldi (UniUPO) – *Creating hierarchical sapo-34 architectures with tunable acid properties using bottom-up synthetic strategies*

Emanuela Manfredi (UniGE) – *Identification of artistic pigments: a comparison of different approaches to image acquisition and analytical data processing*

Daniela Dolciemi (UniPG) – Structure-based screening campaign to identify new SAHRMs with immunomodulatory profile

Ilaria Casartelli (UnINSUBRIA) – In silico approaches for the refinement of bioaccumulation in mammals

Dario Telese (UniBO) – Synthesis of benzisoxazoles and their application in the Kemp elimination

Valeria Cavalloro (UniPV) – From nature a new compound against *Leishmania infantum*

Marco Giordano (UniTO) – Synthesis and characterization of copper complexes as redox mediators in DSSCs

Maria Marzano (UniNA) – Doubler-end-linked-oligonucleotides: the rules and effects of the linker size on the topology and stability of G-quadruplexes

Maria Giulia Nizi (UniPG) – Methoxylated 2-phenylquinoline blocking the *S. aureus* NorA efflux pump

Junwei Zhao (UniBO) – Introducing imidazolidin-2-one scaffolds in peptides promotes the formation of ϵ -turn

Maria Chiara Gullo (UniPR) – Pyridine-2,6-bis(1H-1,2,3-triazol-4-yl): a selective chelating unit for Minor Actinide extraction from radioactive wastes

Cristina Santi (UniMI) – Synthesis of phosphonodisaccharide analogue from *Neisseria meningitidis* A capsular polysaccharide

Arcangelo Celeste (IIT) – Ionic liquids based electrolytes for advanced cathode materials

Martina Marinelli (UniBO) – Double-cable copolymers for polymeric solar cells

Stefano Mariotti (UniTO) – Investigation on paint thinners quality: development of analytical methods for determination of composition and metal content

Marcello Condorelli (UniCT) – Sensing features of silver nanoparticles green generated and reshaped

Giulia Costamagna (UniTO) – By-products analysis of a pyrolysis plant powered by plastic waste materials for energy's production

Erica Rebba (UniTO) – Hydrophobization of nanomaterials for application in leather finishing

Emanuele Porru (UniBO) – Serum bile acid quantification in anti-TNF alpha treatment for intestinal bowel disease combined to multivariate chemometric data analysis


Serena Della Volpe (UniPV) – Elucidation of HuR-small ligand binding modes: a combined STD-NMR and in silico approach

Gioele Giordanengo (UniTO) – Synthesis and characterization of a novel azo dye-based cerium(III) metal organic framework

Francesca Valentini (UniROMA-2) – Spectroelectrochemical characterization of kuquinones anions

19:45	Free time
20:30	Elsevier social dinner – <i>Ristorante Topazio (Hotel Sporting)</i> Dress code: <u>Top Elegance</u>
22:00	Poster session – <i>Sala Ametista (Hotel Ambasciatori)</i> Authors of <i>Flash Talks</i> will present their poster
23:30	Welcome drink – <i>American bar (Hotel Ambasciatori)</i> <i>First cocktail offered by SCI Giovani</i>

TUESDAY, 20TH NOVEMBER

7:30	Breakfast – <i>In your hotel</i>
9:30	Session #7 – <i>Sala Quarzo (Hotel Ambasciatori)</i> Chair: Federico Bella
	Plenary lecture – Luisa Torsi (UniBA) <i>Single molecule detection of markers with a label-free bio-electronic sensor</i>
10:10	Plenary lecture – Michele Pavone (UniNA) <i>Addressing renewable energy challenges with quantum chemistry</i>
10:50	Massimiliano Bearzot (Elsevier) – <i>How to write great papers: from title to references, from submission to publication</i>
11:20	Assegnazione “Premio Primo Levi 2017” – <i>Premio per la migliore pubblicazione dell'anno 2017 ad opera di un socio giovane</i> 
11:30	Authors of <i>Flash Talks</i> must remove the poster from <i>Sala Ametista (Hotel Ambasciatori)</i> Authors of <i>Posters</i> must hang the poster in <i>Sala Ametista (Hotel Ambasciatori)</i>
11:35	Coffee break – <i>American bar (Hotel Ambasciatori)</i>
12:00	Session #8 – <i>Sala Quarzo (Hotel Ambasciatori)</i> Chair: Michele Schlich
	Claudia Bonfio (MRC-LMB) – <i>Prebiotic synthesis of redox-active iron-sulfur catalysts</i> Daniele Martella (LENS@UniFI) – <i>From liquid crystals to microrobotic legs and hands</i> Riccardo Rigo (UniPD) – <i>Dissection of the folding pathway of a G-rich region within c-KIT promoter</i> Sergio Rossi (UniMI) – <i>Metal-free α-trifluoromethylthiolation and α-trifluoromethylselenolation of carbonyl derivatives</i> Francesco Tavanti (UniMORE) – <i>Silver nanocubes for reproducible and controlled raman detection of proteins</i> Matteo Atzori (UniFI) – <i>Scaling-up electronic spin qubits into extended molecular frameworks</i> Cristina Pizzolitto (UniVE) – <i>Optimization of grafting SBA-15 synthesis for Levulinic acid production</i> Chiara Nardon (UniPD) – <i>From the tumor microenvironment to the development of an innovative technology</i>

13:20 **Group picture**


13:30 **Business lunch** – *Ristorante Topazio (Hotel Sporting)*

14:45 **Session #9** – *Sala Quarzo (Hotel Ambasciatori)* Chair: **Roberto Spezzano**

Dario Smacchia (Vinavil S.p.A.) – *A possible solution for substitution of substances of very high concern: formaldehyde and perfluoroalkyl substances*

Invited lecture – **Nicola Cavallini** (UniMORE)

Come to chemometrics: we have cookies (and whisky, and beer)

15:25 **Roberta Costantini** and **Federica La Dogana** (Merck) – *Come preparare un buon CV e come affrontare un'intervista di successo* 

Simone D'Agostino (UniBO) – *Luminescence modification via co-crystals formation: a crystal engineering approach*

Giulia Tuci (CNR) – *Unraveling surface basicity and bulk morphology relationship on covalent triazine frameworks with unique gas adsorption and catalytic properties*

Giovanni Valenti (UniBO) – *Single cell electrochemiluminescence imaging: from the proof-of-concept to disposable device-based analysis*

17:00 **Session #10** – *Sala Ametista (Hotel Ambasciatori)*

Poster session / Coffee provided

Rebecca Appiani (UniMI) – *Modified analogues of 4-(2-triethylaminoethoxy) stilbene as potential selective antagonists of neuronal nicotinic receptors $\alpha 7$*

Matteo Bartolini (UniSI) – *Synthesis of D- π -A dyes for dye-sensitized photocatalysis*

Maria Rita Battaglia (UniBO) – *FT-IR and LC-DAD-MS/MS for Cannabis analysis in (il)legal related products*

Federico Bella (PoliTO) – *Multivariate, theoretical and electrochemical approaches to investigate titanium dioxide electrodes in sodium batteries*

Lorenzo Botta (UniROMA-2) – *Regioselective IBX-mediated synthesis of coumarin derivatives with antioxidant and anti-influenza activities*

Veronica Caratelli (UniROMA-2) – *Origami multiple paper-based electrochemical biosensors for pesticide detection*

Francesca Clemente (UniFI) – *Design, synthesis and evaluation as potential pharmacological chaperones for Gaucher disease of 2-substituted trihydroxy piperidines*

Beatrice Cogliati (UniPR) – *Synthesis and investigation of croconates as smart organic coating for noble metals nanoparticles*

Raffaele Cucciniello (IPSSEOA) – *Recovery and recycling for a sustainable future in the chemical industry*

Mohamed Desoky (UniTO) – *Synthesis of dopant-free polymers for perovskite solar cells*

Riccardo Destefano (UniTO) – *Determination of heavy metals in cosmetic products*

Denise Lovison (UniUD) – *New phosphine/diimine ruthenium(II) complexes as promising anticancer agents: cytotoxicity and pro-apoptotic activity*

Ernestino Lufrano (UniCAL) – *Organo-modified nanoclays for composite gel polymer electrolytes in lithium-ion battery: a study of ionic transport and mechanical properties*

Roberto Mandrioli (UniBO) – *Miniaturised sample pre-treatment and LC-MS/MS analysis of artemisinin in plant extracts and supplements*

Laura Mangiardi (UniROMA-1) – *Synthesis of a new artificial linker resorc[4]arene-based system for protein immobilization*

Alessia Marino (UniCAL) – *Renewed PVC: new recycling strategies*

Nicole Mariotti (UniTO) – *Preparation and synthetic applications of a new class of α -nitro functionalized enolates*

Gloria Mazzone (Chimie ParisTech) – *Color prediction of flexible dyes in aqueous solution: a combined MD/QM approach*

Francesco Papi (UniFI) – *Revealing the nature of the interaction between a novel TF-Thr mimetic with Gal-3*

Costanza Papucci (UniSI) – *Benzo-bisthiazole derivatives: a new class of green/yellow emitting fluorophores for luminescent solar concentrators*

Jessica Passaro (UniNA) – *Electrospun polyvinylpyrrolidone for soundproofing*

Alessandra Riccio (UniPG) – *Insights into molecular recognition of PD-1/PD-L1 inhibitors*

Bianca Dumontel (PoliTO) – *Enhanced biostability and biocompatibility of zinc oxide nanocrystals shielded by a phospholipid bilayer*

Federica Faroldi (UniPR) – *Reversible energy transfer to lanthanoid ions mediated by calixarenes*

Gianluca Fazio (Industrie De Nora S.p.A.) – *Open innovation at De Nora*

Placido Franco (UniBO) – *Development of a new HPLC-ESI-MS/MS method to profile bile acid metabolism oxidation products in human feces*

Matteo Gastaldi (UniTO) – *Synthesis and characterization of polymethacrylates functionalized with azo compounds for 3D printing*

Veronika Gunjević (UniTO) – *Cocoa shell waste valorization – extraction from lab to pilot-scale cavitation reactors*

Elena Lenci (UniFI) – *Chemoinformatics analysis of the molecular diversity of an in-house library of morpholine peptidomimetics*

Isabella Romeo (UniCAL) – *Mechanistic insights of hydrolytic activity into a de novo functional “Frankenstein” protein framework*

Federica Sabuzi (UniROMA-2) – *Thymol derivatives into lignin microcapsules: synthesis, encapsulation and delivery*

Davide Sala (CERM@UniFI) – *An atomistic view of the YjiP structural changes upon zinc(II) binding*

Samuele Staderini (CNR) – *DSSC: a synthetic approach for FRET increasing LHE dyes*

Francesca Susa (PoliTO) – *Biomimetic hybrid nanoconstructs for cancer therapy*

Janeth Tafur Marinos (UniTO) – *Analysis of volatile organic compounds in packaging of mozzarella cheese and yogurt*

Giulia Vergine (UniFE) – *Occurrence of heavy metals in sediments and biota in Northern Adriatic Sea*

18:00 **Session #11** – Sala Quarzo (Hotel Ambasciatori)

Diffusione della Cultura Chimica 

Chemistry meets society: the new interdivisional group of the Italian Chemical Society

18:30 **Assemblea annuale dei soci del Gruppo Giovani** 

con presentazione dei candidati al Consiglio Direttivo 2019-2021

Ordine del giorno

1. Nomina del Presidente dell'Assemblea
2. Relazione del Coordinatore del Gruppo Giovani
3. Relazione del Tesoriere del Gruppo Giovani
4. Programmazione delle attività future del Gruppo Giovani
5. Presentazione delle candidature pervenute per il Direttivo 2019-2021
6. Varie ed eventuali

19:45 Authors of *Posters* must remove the poster from *Sala Ametista* (Hotel Ambasciatori)

19:50 **Free time**

20:50 **Merck social dinner** – Ristorante Topazio (Hotel Sporting)

Dress code: Glamour disco-club outfit

23:00 **Dance & Cocktail supreme party @ Rimini top-club** – Coconuts

First 2 cocktails offered by SCI Giovani

WEDNESDAY, 21ST NOVEMBER

7:30 **Breakfast** – In your hotel

9:10 **Check-out** – Rooms must be left strictly before 9:15, you can leave your suitcase at the reception

9:30

Session #12

Trends in organic and biological systems

Sala Quarzo (Hotel Ambasciatori)

Chair: Elena Lenci

Ivan Bassanini (UniMI) – Structural optimization, in vitro characterization and in silico pharmacophore modeling of a new antiplasmodial chemotype

Marta Da Pian (UniPD) – Aggregation paths of poly-3-(hexyl thiophene) in the presence of either PCBM or poly(ϵ -caprolactone)

Alessio Dessì (CNR) – Dye-sensitized ethanol photoreforming for H₂ production

Daniela Sorrentino (UniROMA-2) – Rational control of the activity of Cu²⁺-dependent DNase by re-engineering purely entropic disordered domains

Giacomo Biagiotti (UniFI) – Drug delivery system based on carbon nanotubes: synthesis and biological essays

Gabriella Leone (UniBA) – In vivo functionalization of diatom mesoporous biosilica for bone tissue engineering

Luca Capaldo (UniPV) – Uranyl cation as visible-light photocatalyst for C-C bond formation via hydrogen atom transfer

Session #13

Chemistry for energy, sensors and environment

Sala Ametista (Hotel Ambasciatori)

Chair: Alice Soldà

Serena Arnaboldi (UniMI) – “Inherently chiral” ionic-liquid media: effective chiral electroanalysis on achiral electrodes

Matteo Bonomo (UniROMA-1) – X-ray structure and ionic conductivity study of choline-chloride/carboxylic acid DESs

Marisa Falco (PoliTO) – Crosslinked poly(ethylene oxide)-based polymer electrolytes for advanced Li-ion batteries

Meng Liu (UniBO) – Graphite intercalation compounds as effective platforms for the preparation of highly active electrocatalysts toward oxygen reduction and evolution reactions

Elisa Maruccia (PoliTO) – Preparation and characterization of zinc oxide based photoanodes for aqueous dye-sensitized solar cells

Stefano Palumbo (PoliTO) – Laminated silicon-graphene hetero-structure as high-rate anode for Li-ion batteries

Cataldo Simari (UniCAL) – Non-fluorinated ionomers and nanocomposite electrolytes for fuel cell applications: recent development and ions diffusion study

Session #14

Advances in medicinal and pharmaceutical chemistry

Sala Smeraldo (Hotel Sporting)

Chair: Lorenzo Botta

Federica Sodano (UniTO) – A novel NO-photoresponsive polymeric platform as an enhancer of doxorubicin delivery

Alessio Bartocci (UniGE) – Interactions between negatively charged nanoparticles and phospholipid bilayers: insights from molecular dynamics simulations

Angela Abruzzo (UniBO) – Effect of Lactobacillus biosurfactant on hydrocortisone solubilization and skin permeation

Andrea Astolfi (UniPG) – Hit identification of novel p38 α MAPK inhibitors by in silico approaches

Xinyu Ge (UniTO) – Activated carbon adsorptive recovery of X-ray contrast agent in aqueous solution and adsorbent regeneration

Marta Campora (UniGE) – Novel naphtho- and anthraquinone derivatives as multi-functional ligands for the therapy of Alzheimer's disease

Francesco Bavo (UniMI) – Potent anti-glioblastoma agents by hybridizing an $\alpha 7$ nAChR antagonist and a mitocan

Session #15

Technologies and processes based on inorganic systems

Sala Rubino (Hotel Sporting)

Chair: Gloria Mazzone

Danny Zanardo (UniVE) – ZnO photocatalysts for enhanced CO₂ conversion

Marco Carlotti (UnivGRONINGEN) – Exploring design rules in molecular electronics: the journey from design principles to functional materials

Alessia Giordana (UniTO) – Microwave assisted synthesis of zirconia: solid catalyst for biomass valorisation

Jacopo Segato (UniUD) – Hydration of alkynes: homogeneous gold(I) catalysis in solvent and acid-free condition

Alessandra Bombace (UniCT) – Molecular depth profiling by nitric oxide-assisted secondary ion mass spectrometry

Eduardo Schiavo (UniNA) – Investigating photoelectrochemical properties of dye-semiconductor interfaces via a DFT-based embedding scheme

Hilmar Guzman (PoliTO) – Catalytic vs. electrocatalytic reduction of CO₂ to added-value products

Elisa Brambilla (UniMI) – *A new synthesis of indolin-3-one derivatives*
Massimiliano Gaeta (UniCT) – *Chiral aggregation of ZnTPPS on polylysine: chain length effects*

Eleonora Colombo (UniMI) – *Total synthesis of a triazole analogue of Ixabepilone*

Graziano di Carmine (UniFE) – *NHC-catalyzed external oxidative desymmetrization of pharmaceutically relevant dihydropyridines*

Carlo Diaferia (UniNA) – *Fmoc-FF and hexapeptides-based multicomponent hydrogels as scaffold materials*

Anna Testolin (UniMI) – *Potentialities of hybrid nanocomposites based on RGO and Au NPs towards electroanalytical applications*
Diego Quintero Balbas (UniBO)

– *Advanced methodology for the characterization of early synthetic dyes used in cultural heritage using TLC and μ -enhanced spectroscopy*

Luca Rivoira (UniTO) – *Silica based matrices for the controlled release of glyphosate in soils*

Alessandro Sangion (UNINSUBRIA) – *QSAR models for the screening, prediction and refinement of PBT properties of contaminant of emerging concern*

Veronica Santoro (UniTO) – *Mechanisms controlling P retention during Fe(II) oxidative coprecipitation*

Stephanie Federico (UniTS) – *A dual target kinase ligand as neuroprotective agent presenting two different mechanisms of enzymatic inhibition*

Rolando Cannalire (UniPG) – *Potent and selective inhibition of Dengue e Zika viruses replication by pyridobenzothiazole compounds*

Doriana Levrè (UniUPO) – *ZINClick v.18: the 1,2,3-triazoles chemical space*

Stefano Sainas (UniTO) – *New human dihydroorotate dehydrogenase inhibitors able to restore myeloid differentiation in AML*

Tommaso Felicetti (UniPG) – *C-6/C-7 functionalization of the 3-phenylquinolone scaffold to obtain potent nontuberculous efflux inhibitors*

Andrea Valenti (UniCT) – *Characterization of conductive molecular wires assembled onto oxide by means of ToF-SIMS*

Anna Lenarda (UniTS) – *Selective H_2O_2 electrocatalytic generation by cobalt@N-doped graphitic carbon core-shell nanohybrids*

Marta Stucchi (UniMI) – *AuPd bimetallic catalysts for lignin-derivatives alcohols valorization*

Mattia Bartoli (PoliTO) – *Biochar from pyrolysis of olive waste: natural template for nanostructured polymer filler*

Tainah D. Marforio (UniBO) – *A promising enzyme for novel chemoenzymatic synthesis: Linalool dehydratase-isomerase. The catalytic mechanism unveiled by computational investigations*

11:30 **Coffee break** – American bar (Hotel Ambasciatori)

12:00 **Session #16** – Sala Quarzo (Hotel Ambasciatori) **Chair: Stefano Cinti**

Manuela Vacatallo (Merck) – *Bridging the gap from biology to chemical production*

Tommaso Tabanelli (UniBO) – *New synthetic strategies towards organic carbonates and related innovative applications*

Edoardo Jun Mattioli (UniBO) – *Computational investigation of the effect of external electric fields on organic reactivity*

Alice Soldà (EYCN) – *EYCN - the European Young Chemists' Network*

13:00 **Closing ceremony** – Sala Quarzo (Hotel Ambasciatori)

Poster awards

Flash communication awards

Oral communication awards

SCI Giovani 2016-2018 Board: Farewell

13:30 **Business lunch** – Ristorante Topazio (Hotel Sporting)

14:30 **MEYCS 2018** – The end

Organizing & Scientific Committee

Federico Bella, *Chair*
Lorenzo Botta
Raffaele Cucciniello
Alessandro D'Urso
Placido Franco
Elena Lenci
Gloria Mazzone
Michele Schlich
Alice Soldà
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The scientific contributions of this conference are collected in an international volume with ISBN code.

You can cite your work in this way:

N. Surname, N. Surname, ... and N. Surname,
"Abstract title", in *"Proceedings of the Merck & Elsevier Young Chemists Symposium (MEYCS 2018)"*, Ed. F. Bella, L. Botta, R. Cucciniello, A. D'Urso, P. Franco, E. Lenci, G. Mazzone, M. Schlich, A. Soldà, R. Spezzano, S. Staderini and L. Triggiani, ISBN: 978-88-94952-03-2, page number, 2018, Rome.

