

Società Chimica Italiana  
Divisione di Chimica dei Sistemi Biologici  
June 20<sup>th</sup> - 22<sup>nd</sup>, 2022

## Scientific Program

Monday, June 20 <sup>th</sup>	
12.30 – 14.20	Registration of Participants
14.20 – 14.30	Opening Remarks
<b>Session 1</b>	
<i>Chairpersons:</i> Michael Assfalg – Francesco Peri	
14.30 – 15.15	<b>PL01:</b> Alba Silipo <i>Unveiling the puzzle of microbial glycans: how to correlate the structure to the function</i>
15.15 – 15.35	<b>OR01:</b> Cristina Airoidi <i>Multivalent ligands for bacteria targeting</i>
15.35 – 15.55	<b>OR02:</b> Francesco Musiani <i>Computational studies on internal tunnels of the Helicobacter pylori UreDFG multimeric protein complex</i>
15.55 – 16.15	<b>OR03:</b> Francesco Bellia <i>Natural and synthetic effectors of alpha-synuclein: features and interplays</i>
16.15 – 16.55	Coffee Break & Poster Session 1 ( <b>PO01 – PO11</b> )
<i>Chairpersons:</i> Gianluca Caprini – Carla Isernia	
16.55 – 17.00	Italfarmaco “Gastone De Santis” Award Ceremony
17.00 – 17.30	<b>AL01:</b> Alessandro D’Urso <i>Porphyrins as chiroptical probe for biomolecule's conformations</i>
17.30 – 18.00	<b>AL02:</b> Francesca Munari <i>Ubiquitination of the Alzheimer’s disease related protein Tau by enzymatic and chemical methods: effects on the mechanism of amyloids formation</i>
18.00 – 18.15	<b>OR04:</b> Aurane Froux <i>G-quadruplex binding by transition metal complexes: the whole pathway from design to synthesis, to in cellulo anticancer investigations</i>
18.15 – 18.30	<b>OR05:</b> Claudia Riccardi <i>Design, synthesis and characterization of lipophilic Ru(III) complexes as potential antitumor agents</i>
18.30 – 19.30	<i>Assemblea dei Soci della Divisione di Chimica dei Sistemi Biologici</i>

Tuesday, June 21 <sup>st</sup>	
Session 2	
Chairpersons: Massimiliano Coletta – Roberto Fattorusso	
9.00 – 9.45	<b>PL02:</b> Maurizio Pellecchia <i>NMR- and structure-guided design of potent ligands and molecular degraders to protein-protein interactions</i>
9.45 – 10.05	<b>OR06:</b> Daniela Arosio <i>Triazine-based small molecules as novel PD-L1 inhibitors</i>
10.05 – 10.25	<b>OR07:</b> Cecilia Pozzi <i>Structural characterization of YAP-TEAD4 protein-protein interaction: an emerging target for cancer treatment</i>
10.25 – 10.45	<b>OR08:</b> Luigi Russo <i>High-resolution NMR-based approach for studying receptor-ligand interactions on living cells surface</i>
10.45 – 11.30	Coffee Break & Poster Session 2 ( <b>PO12 – PO22</b> )
Chairpersons: Roberta Pierattelli – Michele Saviano	
11.30 – 11.45	<b>OR09:</b> Angelo Gallo <i>Protein-protein interaction in polyketides producing antibiotic</i>
11.45 – 12.00	<b>OR10:</b> Gianluca D'Abrosca <i>Screening a molecular fragment library to modulate PED/PEA15-Phospholipase D1 interaction in cellular lysate environments</i>
12.00 – 12.15	<b>OR11:</b> Giusy Tassone <i>Identification of phosphate-containing compounds as new inhibitors of 14-3-3/c-Abl protein-protein interaction</i>
12.15 – 12.30	<b>OR12:</b> Giovanna Viola <i>Elucidating the interaction between ultrasmall gold nanoparticles and the amyloidogenic protein tau</i>
12.30 – 12.45	<b>OR13:</b> Valeria Lanza <i>Interactions between trehalose-silybins conjugates and A<math>\beta</math> oligomers: a biophysical and in vitro study</i>
12.45 – 13.00	<b>OR14:</b> Rita Pagano <i>Silybin-tyrosol conjugates as promising Multitarget Ligands (MTLs) to contrast neurodegenerative diseases</i>
13.00 – 14.30	Lunch

Tuesday, June 21 <sup>st</sup>	
Session 3	
<i>Chairpersons:</i> Jussara Amato – Daniela Montesarchio	
14.30 – 15.15	<b>PL03:</b> Roberto Improta <i>Photophysics and photochemistry of DNA: insights from Quantum Mechanical calculations</i>
15.15 – 15.30	<b>OR15:</b> Angelo Spinello <i>Unraveling the molecular basis of aberrant splice sites recognition by the SF3b splicing factor via all-atom simulations</i>
15.30 – 15.45	<b>OR16:</b> Riccardo Rozza <i>Unraveling the molecular recognition and inhibition mechanism of the U2AF2 splicing factor</i>
15.45 – 16.00	<b>OR17:</b> Silvia Rinaldi <i>A dynamic recognition of t1-adenosine sheds new lights on human Argonaute-2 protein target affinity</i>
16.00 – 16.30	Coffee Break
16.30 – 16.45	<b>OR18:</b> Gabriele Travagliante <i>Interactions between achiral porphyrins and a mature miRNA</i>
16.45 – 17.00	<b>OR19:</b> Rita Tosto <i>Porphyrin-KLVFF conjugates as theranostic tools in Alzheimer's disease</i>
17.00	Guided Tour
20.00	Social Dinner

Wednesday, June 22 <sup>nd</sup>	
Session 4	
Chairpersons: Danilo Milardi – Gaetano Malgieri	
09.00 – 09.45	<b>PL04:</b> Antonio Rosato <i>A bird's eye view of metalloproteins</i>
09.45-10.05	<b>OR20:</b> Laura Cipolla <i>Gelatin-based hydrogels: preparation and applications</i>
10.05 – 10.25	<b>OR21:</b> Marilisa Leone <i>Design and evaluation of potential anticancer agents targeting the Sam domain of EphA2 receptor and its interactome</i>
10.25 – 10.45	<b>OR22:</b> Anna Maria Santoro <i>Bio-inspired proteasome enhancers</i>
10.45 – 11.30	Coffee Break & Poster Session 3 ( <b>PO23 – PO34</b> )
Chairpersons: Alessandra Magistrato – Antonio Rosato	
11.30 – 11.45	<b>OR23:</b> Federica Moraca <i>Structural insights of the ubiquitylation effects on the human Bardet-Biedl Syndrome (BBS) complex through Coarse-Grained Molecular Dynamics simulations</i>
11.45 – 12.00	<b>OR24:</b> Laura Rigobello <i>Computational study of pathogenetic mutations in the transmembrane domain of Complex I of the respiratory chain</i>
12.00 – 12.15	<b>OR25:</b> Matteo Castelli <i>Conformational selection at atomic level: the effects of glycosylation and modulators on Grp94</i>
12.15 – 12.30	<b>OR26:</b> Massimiliano Gaeta <i>DOPA-melanin polymers as versatile bio-inspired material for multipurpose applications</i>
12.30 – 12.45	<b>OR27:</b> Veronica Ghini <i>Profiling metabolites and lipoproteins in COMETA, an Italian cohort of COVID-19 patients</i>
12.45 – 13.00	<b>OR28:</b> Alessia Vignoli <i>Risk stratification in patients with atrial fibrillation on oral anticoagulants: an NMR-based metabolomics and lipoproteomics study</i>
13.00 – 13.15	Closing Remarks