

XXVII  
National Meeting on  
Medicinal Chemistry

<sup>7</sup>N <sup>15</sup>P <sup>6</sup>C <sup>9</sup>F 14

14<sup>th</sup> Young Medicinal Chemists' Symposium  
Nuove Prospettive in Chimica Farmaceutica

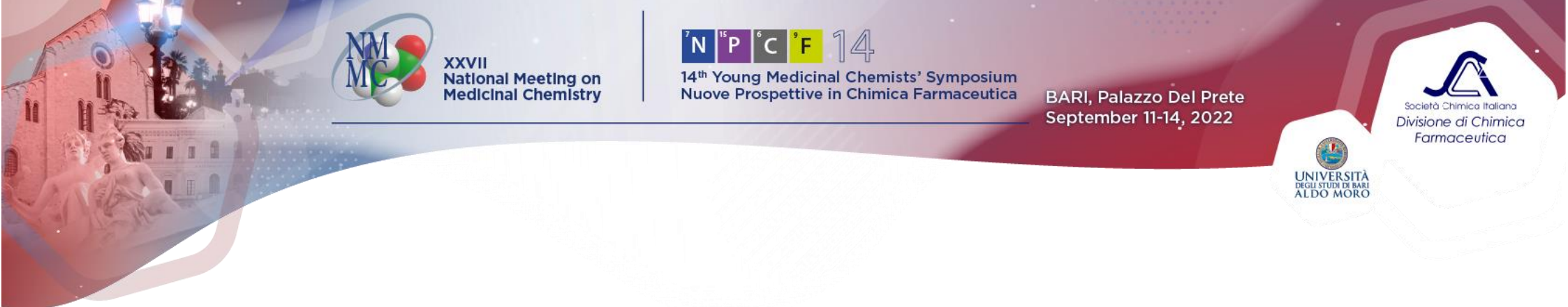
BARI, Palazzo Del Prete  
September 11-14, 2022



Società Chimica Italiana  
Divisione di Chimica  
Farmaceutica

## Sunday, September 11<sup>th</sup>, 2022

14.30-16.45	<b>REGISTRATION</b>
	<b>Aldo Moro Hall</b>
17.00-17.45	<b>OPENING CEREMONY</b> <b>Stefano Bronzini</b> – Rector of the University of Bari Aldo Moro <b>Antonio F. Uricchio</b> – President of ANVUR <b>Francesco Leonetti</b> – Head of the Department of Pharmacy-Pharmaceutical Sciences <b>Luigi D'Ambrosio Lettieri</b> – Vice-president of F.O.F.I. <b>Regional Political Authorities</b> <b>Gianluca Sbardella</b> – Chair of the Meeting <b>Maria Laura Bolognesi</b> – President of the Medicinal Chemistry Division <b>Cosimo D. Altomare</b> – Chair of the Local Organizing Committee
17.45-18.15	<b>Medicinal Chemistry Division of the Italian Chemical Society's Awards</b> <b>Francesco Merlino</b> , <i>University of Naples Federico II, Italy</i> <b>Laura Scavini</b> , <i>University of Parma, Italy</i> <b>Best Doctoral Thesis Awards</b> Design and Synthesis of new PET radiotracers in drug discovery <b>Marco Maspero</b> , <i>University of Milan, Italy</i> Design and synthesis of (pro)electrophilic compounds for investigating the multifactorial nature of neurodegenerative diseases: focus on inflammation-driven events <b>Filippo Basagni</b> , <i>University of Bologna, Italy</i>
18.15-18.45	<b>Musajo Medal of the Medicinal Chemistry Division of the Italian Chemical Society</b> Recipient: <b>Gabriele Costantino</b> , <i>University of Parma, Italy</i> <b>Chair: Maria Laura Bolognesi</b> – President of the Medicinal Chemistry Division
18.45-19.45	<b>PL1: Exploring molecular promiscuity through activity data analysis and explainable artificial intelligence</b> <b>Jürgen Bajorath</b> , <i>University of Bonn, Germany</i>
20.00	<b>WELCOME BUFFET</b>



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## Monday, September 12<sup>th</sup>, 2022

	<b>Aldo Moro Hall</b>	
	Chair: <b>Cosimo D. Altomare</b>	
<b>9.00-9.50</b>	<b>PL2:</b> Going with the flow - The use of continuous processing for synthesizing Active Pharmaceutical Ingredients <b>C. Oliver Kappe</b> , <i>University of Graz, Austria</i>	
	<b>Aldo Moro Hall</b>	<b>Vincenzo Starace Hall</b>
	Chairs: <b>Vincenza Andrisano, Orazio Nicolotti</b>	Chairs: <b>Violetta Cecchetti, Stefano Alcaro</b>
<b>10.00-10.30</b>	<b>KN1:</b> Computational approaches to the design of covalent drugs <b>Marco Mor</b> , <i>University of Parma, Italy</i> <i>ChemMedChem Lecture</i>	<b>KN2:</b> Unleashing the potential of Translocator Protein as a therapeutic and diagnostic target: a successful MedChem tale <b>Sabrina Taliani</b> , <i>University of Pisa, Italy</i>
<b>10.30-10.50</b>	<b>OC1:</b> SQM-Score: Universal Quantum-Mechanical Scoring Function for Structure-based Drug Design <b>Adam Pecina</b> , <i>Czech Academy of Sciences Prague, Czech Republic</i>	<b>OC2:</b> Functionalized 6H-dibenzo[c,e]thiazine 5,5-dioxides are potent suppressors of the toxicity mediated by the cellular prion protein <b>Giuseppe Manfroni</b> , <i>University of Perugia, Italy</i>
<b>10.50-11.00</b>	<b>FC1:</b> Machine learning applied to early prediction of drug metabolism <b>Marta Lettieri</b> , <i>S-IN Soluzioni Informatiche srl, Vicenza, Italy</i>	<b>FC2:</b> Extra virgin olive oil extracts enriched in secoiridoids induce an anti-inflammatory profile in PBMCs from obese children <b>Stefania De Santis</b> , <i>University of Bari, Italy</i>
<b>11.00-11.20</b>	<b>COFFEE BREAK</b>	
<b>11.20-11.40</b>	<b>OC3:</b> The 3D-QSAR.COM portal as tool to develop predictive ligand-based and structure-based models for SARS-CoV-2 main protease inhibitors <b>Rino Ragno</b> , <i>Sapienza University of Rome, Italy</i>	<b>OC6:</b> Discovery of orexant and anorexant agents with indazole scaffold endowed with peripheral antiedema activity <b>Adriano Mollica</b> , <i>University of Chieti-Pescara G. D'Annunzio, Italy</i>
<b>11.40-12.00</b>	<b>OC4:</b> Development of a LC-MS platform for monoclonal antibody characterization to assist the production of a rituximab biosimilar from plants <b>Francesca Rinaldi</b> , <i>University of Pavia, Italy</i>	<b>OC7:</b> New class of potential antidiabetes agents targeting DPPIV and CAs enzymes <b>Laura Fumagalli</b> , <i>University of Milan, Italy</i>
<b>12.00-12.20</b>	<b>OC5:</b> A proof-of-concept of the analgesic effect of non-psychoactive <i>Cannabis sativa</i> L. and its main components on peripheral neuropathy <b>Federica Pellati</b> , <i>University of Modena and Reggio-Emilia, Italy</i>	<b>OC8:</b> Towards the characterization of corrector ARN23765 mechanism of action via photo-affinity labeling (PAL) approach <b>Francesco Saccoliti</b> , <i>Italian Institute of Technology, Genoa, Italy</i>
<b>12.30-14.00</b>	<b>LUNCH</b>	
<b>14.00-15.30</b>	<b>POSTER SESSION &amp; COMMERCIAL EXHIBITION</b>	



## Monday, September 12<sup>th</sup>, 2022

	Aldo Moro Hall	Vincenzo Starace Hall
	Chair: <b>Gabriele Costantino, Giovanni Lentini</b>	Chair: <b>Maria Laura Bolognesi, Roberto Di Santo</b>
15.30-16.00	<b>KN3:</b> Synthetic lethality for next generation precision oncology <b>Andrea Cavalli, University of Bologna, Italy</b>	<b>KN4:</b> A nature inspired approach to develop covalent enzyme inhibitors with anti-infective and anticancer activity <b>Paola Conti, University of Milan, Italy</b>
16.00-16.20	<b>OC9:</b> New nicotinamide mimic scaffold allowed nanomolar inhibition of human PARP enzymes <b>Oriana Tabarrini, University of Perugia, Italy</b>	<b>OC11:</b> Broad spectrum metallo $\beta$ -lactamases inhibitors: new tools against clinically relevant carbapenemases <b>Loretta Lazzarato, University of Turin, Italy</b>
16.20-16.40	<b>OC10:</b> Spindlin-1 degraders: stairway to heaven (?) <b>Monica Viviano, University of Salerno, Italy</b>	<b>OC12:</b> Novel dipeptide nitriles as antitrypanosomal agents targeting rhodesain of <i>Trypanosoma brucei rhodesiense</i> : development and combination studies <b>Roberta Ettari, University of Messina, Italy</b>
16.40-17.00	<b>COFFEE BREAK</b>	
17.00-17.20	<b>OC13:</b> TRPM8 ion channel: new target in the treatment of castration-resistant prostate cancer (CRPC) <b>Veronica Di Sarno, University of Salerno, Italy</b>	<b>OC15:</b> The PADAM oxidation route for the synthesis of SARS-CoV-2 main protease inhibitors <b>Sveva Pelliccia, University of Naples Federico II, Italy</b>
17.20-17.40	<b>OC14:</b> Challenge transability of "in vitro" to "in vivo": gene-expression biomarkers and fluorescent image-guided surgery probes identification for ovarian cancer <b>Antonio Scilimati, University of Bari, Italy</b>	<b>OC16:</b> Discovery of diketo acid derivatives targeting the SARS-CoV-2 NSP13 helicase <b>Valentina Madia, Sapienza University of Rome, Italy</b>
17.40-17.50	<b>FC3:</b> Combining mass spectrometry and nuclear magnetic resonance for the study of ligand: G-quadruplex interaction <b>Erika Oselladore, University of Brescia, Italy</b>	<b>OC17:</b> An integrated medicinal chemistry workflow for the development of new peptides as SARS-CoV-2 MPro covalent inhibitors <b>Simona Musella, University of Salerno, Italy</b>
17.50-18.00	<b>FC4:</b> Carbazole derivatives as multi-target agents in breast cancer treatment <b>Jessica Ceramella, University of Calabria, Italy</b>	
18.00-19.00	<b>NETWORKING</b>	
	<b>Tavola rotonda</b> <b>Malattia di Lafora: dalla ricerca di farmaci ai diritti dei pazienti</b> <b>Per una stretta cooperazione tra ricerca e assistenza</b> <b>G. d'Orsi, T. Bressanello, G. Annichiarico, A. Liantonio, G. Costantino, C. Altomare</b>	<b>Workshop</b> <b>Why was my paper rejected? Optimizing manuscripts for successful submission and publication</b> <b>David Peralta, Editor-in-Chief ChemMedChem, Wiley-VCH</b>
19:30	<b>CONCERT OF CORUS HARMONIA – BASILICA DI S. NICOLA</b>	



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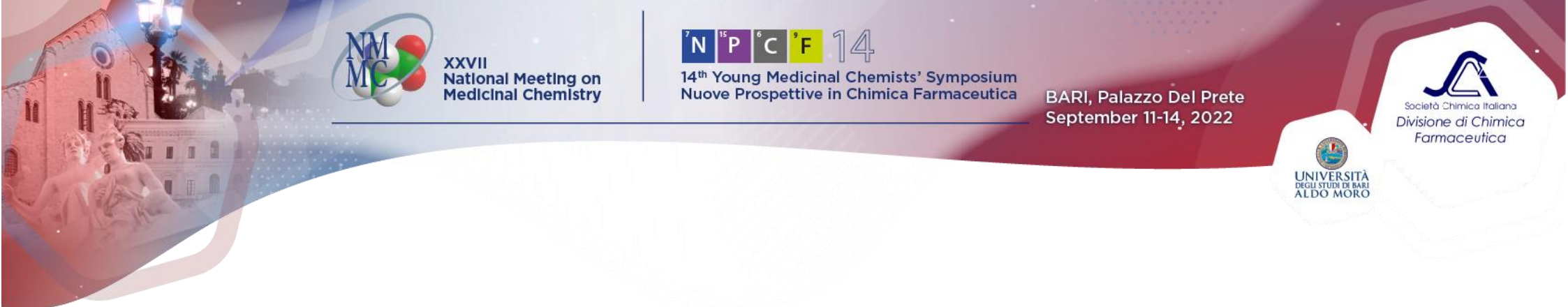
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## Tuesday, September 13<sup>th</sup>, 2022

	<b>Aldo Moro Hall</b>	
	Chair: <b>Nicola A. Colabufo</b>	
<b>9.00-9.50</b>	<b>PL3:</b> Innovative strategies to target non-coding RNAs with synthetic ligands <b>Maria Duca</b> , <i>Université Côte d'Azur Nice, France</i>	
	<b>Aldo Moro Hall</b>	<b>Vincenzo Starace Hall</b>
	Chairs: <b>Patrizia Diana, Francesco Leonetti</b>	Chairs: <b>Enza Lacivita, Tiziano Bandiera</b>
<b>10.00-10.30</b>	<b>KN5:</b> Targeting dopamine D <sub>4</sub> receptor as a thrilling challenge to explore new therapeutic opportunities <b>Fabio Del Bello</b> , <i>University of Camerino, Italy</i>	<b>KN6:</b> Identification of ARN21641, an orally available and CNS penetrant Acid Ceramidase inhibitor with target engagement in mouse models of Gaucher and Krabbe diseases <b>Rita Scarpelli</b> , <i>Italian Institute of Technology, Genoa, Italy</i>
<b>10.30-10.50</b>	<b>OC18:</b> Development of novel enzyme inhibitors of the endocannabinoids' catabolism for the treatment of epilepsy and neuroinflammatory conditions <b>Stefania Butini</b> , <i>University of Siena, Italy</i>	<b>OC19:</b> Hijacking the folding process for targeted protein degradation <b>Andrea Astolfi</b> , <i>University of Perugia, Italy</i>
<b>10.50-11.00</b>	<b>FC5:</b> Targeting the mycobactin biosynthesis pathway in <i>M. tuberculosis</i> : a step towards the improvement of the anti-virulence activity of MbtI inhibitors <b>Matteo Mori</b> , <i>University of Milan, Italy</i>	<b>FC6:</b> Development of hydrogen sulfide-releasing hybrids as novel multitarget drugs <b>Angela Corvino</b> , <i>University of Naples Federico II, Italy</i>
<b>11.00-11.20</b>	<b>COFFEE BREAK</b>	
<b>11.20-11.40</b>	<b>OC20:</b> The pivotal role of pyrrolidine ring as multitarget scaffold in neurodegenerative diseases <b>Antonio Carrieri</b> , <i>University of Bari, Italy</i>	<b>OC23:</b> Nucleic acid aptamers: potential therapeutic agents for cancer and neurodegenerative disorders <b>Jussara Amato</b> , <i>University of Naples Federico II, Italy</i>
<b>11.40-12.00</b>	<b>OC21:</b> Pursuing the complexity of bipolar disorder: rational design and optimization of first-in-class D <sub>3</sub> R/GSK-3 $\beta$ modulators towards an in vivo proof of concept <b>Rita M.C. Di Martino</b> , <i>Italian Institute of Technology, Genoa, Italy</i>	<b>OC24:</b> Combining quantum mechanics and machine learning in the search of the bioactive conformation of drug-like compounds <b>Antonio Viayna</b> , <i>University of Barcelona, Spain</i>
<b>12.00-12.20</b>	<b>OC22:</b> S.M.A.R.T. steroids: synthesis and structure-activity relationship study towards allosteric modulators of N-methyl-D-aspartate receptors <b>Eva Kudova</b> , <i>Czech Academy of Sciences Prague, Czech Republic</i>	<b>OC25:</b> Challenging bioisosteric switch in AChE-MAO B dual-targeting hit optimization <b>Leonardo Pisani</b> , <i>University of Bari, Italy</i>
<b>12.30-14.00</b>	<b>LUNCH</b>	
<b>14.00-15.30</b>	<b>POSTER SESSION &amp; COMMERCIAL EXHIBITION</b>	



Tuesday, September 13 <sup>th</sup> , 2022		
	<b>Aldo Moro Hall</b>	<b>Vincenzo Starace Hall</b>
	Chair: <b>Giannamaria Annunziato, Laura Scalvini</b>	Chair: <b>Isabella Romeo, Francesco Merlino</b>
<b>15.30-16.00</b>	<b>KN7:</b> From the catalytic mechanism to the enzyme substrate selectivity: a study on <i>N</i> -acylethanolamine acid amidase <b>Laura Scalvini, University of Parma, Italy</b>	<b>KN8:</b> From natural resource to preclinical candidate: our experience with the temporin-derived peptide antimicrobial agents <b>Francesco Merlino, University of Naples Federico II, Italy</b>
<b>16.00-16.10</b>	<b>FC7:</b> Discovery of 2-(4-hydroxy-3,5-dimethylphenyl)- <i>N</i> -(pyridin-2-yl)-1 <i>H</i> -benzo[d]imidazole-6-sulfonamide as BET inhibitor with selectivity for the first bromodomain <b>Alessandra Cipriano, University of Salerno, Italy</b>	<b>FC11:</b> Tetrahydropyran and cyclohexane linked novel bacterial topoisomerase inhibitors with improved balanced antibacterial activity and safety profile <b>Maja Kokot, National Institute of Chemistry, Ljubljana, Slovenia</b>
<b>16.10-16.20</b>	<b>FC8:</b> First-in-class selective inhibitors of the histone acetyltransferase KAT8 <b>Francesco Fiorentino, Sapienza University of Rome, Italy</b>	<b>FC12:</b> Miconazole-like scaffold is a promising lead for developing <i>Naegleria fowleri</i> - specific brain permeable CYP51 inhibitors <b>Valeria Tudino, University of Rome Tor Vergata, Italy</b>
<b>16.20-16.30</b>	<b>FC9:</b> Design, synthesis, and biological evaluation of new hybrid MOR agonist/HDACi compounds: an innovative approach for persistent pain management <b>Giuliana Costanzo, University of Catania, Italy</b>	<b>FC13:</b> Structural modifications of triazine-based compounds for high-efficiency PDK inhibition <b>Camilla Pecoraro, University of Palermo, Italy</b>
<b>16.30-16.40</b>	<b>FC10:</b> Visible-light photocatalytic activity of isocyanides: from the proof-of-concept to the synthetic application in Ugi-like chemistry <b>Camilla Russo, University of Naples Federico II, Italy</b>	<b>FC14:</b> In silico assisted discovery of dual 5-LOX/sHE inhibitors: in vitro characterization and in vivo anti-inflammatory properties <b>Tania Ciaglia, University of Salerno, Italy</b>
<b>16.40-17.00</b>	<b>COFFEE BREAK</b>	
<b>17.00-17.30</b>	<b>In memoriam of Prof. Vincenzo Tortorella (1932-2022) Celebration of retired colleagues</b>	
<b>17.30-19.30</b>	<b>DCF-SCI GENERAL MEETING (ASSEMBLEA DELLA DIVISIONE DI CHIMICA FARMACEUTICA)</b>	
<b>20.30</b>	<b>SOCIAL DINNER AT RISTORANTE ZONNO (Lungomare di Bari)</b>	



## Wednesday September 14<sup>th</sup>, 2022

	<b>Aldo Moro Hall</b>	
	Chair: <b>Marcello Leopoldo</b>	
<b>9.00-9.50</b>	<b>PL4:</b> Targeting chemokine receptor CCR2 - From insurmountable antagonists to affinity-based probes <b>Laura Heitman, Leiden University, The Netherlands</b>	
	<b>Aldo Moro Hall</b>	<b>Vincenzo Starace Hall</b>
	Chairs: <b>Marco Catto, Marcello Leopoldo</b>	Chairs: <b>Gianluca Sbardella, Cosimo D. Altomare</b>
<b>10.00-10.30</b>	<b>KN9:</b> Development and hands-on application of PyRMD: a new AI-powered virtual screening tool <b>Sandro Cosconati, Luigi Vanvitelli University, Naples, Italy</b>	<b>KN10:</b> The discovery of potent and selective agonists of human transient receptor potential Cation Channel Subfamily M member 5: from HTS to early hit validation <b>Alessio Barilli, Aptuit, an Evotec Company, Verona, Italy</b>
<b>10.30-10.50</b>	<b>OC26:</b> Exploring CCRL2 Chemerin binding using accelerated molecular dynamics <b>Antonio Coluccia, Sapienza University of Rome, Italy</b>	<b>OC28:</b> The first in vivo proof-of-concept for the efficacy of selective HDAC6 inhibition in cystic fibrosis: anti-inflammatory profile, effects on bacterial load, formulation and biodistribution studies <b>Margherita Brindisi, University of Naples Federico II, Italy</b>
<b>10.50-11.10</b>	<b>OC27:</b> Functionalized ligands targeting G protein-coupled adenosine receptors <b>Stephanie Federico, University of Trieste, Italy</b>	<b>OC29:</b> New insights in the development of cannabinoid receptor subtype 2 (CB2R) ligands <b>Marialessandra Contino, University of Bari, Italy</b>
<b>11.10-11.30</b>	<b>COFFEE BREAK</b>	
<b>11.30-11.50</b>	<b>OC30:</b> Optimizing the choice of 3D query structures in ligand-based virtual screenings with PHARMSCREEN <b>Giorgia Zaetta, Parc Científic de Barcelona, Spain</b>	<b>OC32:</b> Novel cyclic uPA-derived decapeptides reduce in vivo lung dissemination and re-educate CAF phenotype by acting through integrin $\alpha v \beta 5$ <b>Alfonso Carotenuto, University of Naples Federico II, Italy</b>
<b>11.50-12.10</b>	<b>OC31:</b> A computational grid-based analysis to map drug-like peptide binding pockets of peptide-protein interactions systems <b>Daniela Trisciuzzi, University of Bari, Italy</b>	<b>OC33:</b> Screening of amino-acid-anthraquinone click chemistry conjugates targeting human telomeric G-quadruplexes <b>Giovanni Ribaudo, University of Brescia, Italy</b>
	<b>Aldo Moro Hall</b>	
	Chair: <b>Gianluca Sbardella</b>	
<b>12.10-13.10</b>	<b>PL5:</b> COVID-19 pandemic: what we learnt in antiviral drug discovery, successes, and failures <b>Vincenzo Summa, University of Naples Federico II, Italy</b>	
<b>13.10-13.30</b>	<b>CLOSING REMARKS and POSTER PRIZES</b>	
<b>13.30</b>	<b>LUNCH</b>	