PROGRAM

Sunday, September 11th, 2022

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

Monday, September 12th, 2022

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

Monday, September 12th, 2022

	Aldo Moro Hall		**Vincenzo Starace Hall**
	Chair: **Gabriele Costantino**, **Giovanni Lentini**		Chair: **Maria Laura Bolognesi**, **Roberto Di Santo**
15.30-16.00	**KN3:** Synthetic lethality for next generation precision oncology **Andrea Cavalli,** *University of Bologna, Italy*		**KN4:** A nature inspired approach to develop covalent enzyme inhibitors with anti-infective and anticancer activity **Paola Conti**, *University of Milan, Italy*
16.00-16.20	**OC9:** New nicotinamide mimic scaffold allowed nanomolar inhibition of human PARP enzymes **Oriana Tabarrini**, *University of Perugia, Italy*		**OC11:** Broad spectrum metallo β-lactamases inhibitors: new tools against clinically relevant carbapenemases **Loretta Lazzarato**, *University of Turin, Italy*
16.20-16.40	**OC10:** Spindlin-1 degraders: stairway to heaven (?) **Monica Viviano,** *University of Salerno, Italy*		**OC12:** Novel dipeptide nitriles as antitrypanosomal agents targeting rhodesain of *Trypanosoma brucei rhodesiense*: development and combination studies **Roberta Ettari**, *University of Messina, Italy*
16.40-17.00	**COFFEE BREAK**		
17.00-17.20	**OC13:** TRPM8 ion channel: new target in the treatment of castration-resistant prostate cancer (CRPC) **Veronica Di Sarno,** *University of Salerno, Italy*		**OC15:** The PADAM oxidation route for the synthesis of SARS-CoV-2 main protease inhibitors **Sveva Pelliccia**, *University of Naples Federico II, Italy*
17.20-17.40	**OC14:** Challenge transability of "in vitro" to "in vivo": gene-expression biomarkers and fluorescent image-guided surgery probes identification for ovarian cancer **Antonio Scilimati,** *University of Bari, Italy*		**OC16:** Discovery of diketo acid derivatives targeting the SARS-CoV-2 NSP13 helicase **Valentina Madia**, *Sapienza University of Rome, Italy*
17.40-17.50	**FC3:** Combining mass spectrometry and nuclear magnetic resonance for the study of ligand: G-quadruplex interaction **Erika Oselladore**, *University of Brescia, Italy*		**OC17:** An integrated medicinal chemistry workflow for the development of new peptides as SARS-CoV-2 MPro covalent inhibitors **Simona Musella,** *University of Salerno, Italy*
17.50-18.00	**FC4:** Carbazole derivatives as multi-target agents in breast cancer treatment **Jessica Ceramella**, *University of Calabria, Italy*		
18.00-19:00	**NETWORKING**		
	Tavola rotonda ***Malattia di Lafora: dalla ricerca di farmaci ai diritti dei pazienti*** ***Per una stretta cooperazione tra ricerca e assistenza*** **G. d'Orsi, T. Bressanello, G. Annichiarico, A. Liantonio, G. Costantino, C. Altomare**		Workshop **Why was my paper rejected? Optimizing manuscripts for successful submission and publication** **David Peralta**, Editor-in-Chief ChemMedChem, Wiley-VCH
19:30	**CONCERT OF CORUS HARMONIA – BASILICA DI S. NICOLA**		

Tuesday, September 13th, 2022

	Aldo Moro Hall		Vincenzo Starace Hall
	Chair: **Nicola A. Colabufo**		
9.00-9.50	**PL3**: Innovative strategies to target non-coding RNAs with synthetic ligands **Maria Duca**, *Université Côte d'Azur Nice, France*		
	Aldo Moro Hall		**Vincenzo Starace Hall**
	Chairs: **Patrizia Diana**, **Francesco Leonetti**		Chairs: **Enza Lacivita**, **Tiziano Bandiera**
10.00-10.30	**KN5:** Targeting dopamine D_4 receptor as a thrilling challenge to explore new therapeutic opportunities **Fabio Del Bello,** *University of Camerino, Italy*		**KN6:** Identification of ARN21641, an orally available and CNS penetrant Acid Ceramidase inhibitor with target engagement in mouse models of Gaucher and Krabbe diseases **Rita Scarpelli**, *Italian Institute of Technology, Genoa, Italy*
10.30-10.50	**OC18:** Development of novel enzyme inhibitors of the endocannabinoids' catabolism for the treatment of epilepsy and neuroinflammatory conditions **Stefania Butini,** *University of Siena, Italy*		**OC19:** Hijacking the folding process for targeted protein degradation **Andrea Astolfi**, *University of Perugia, Italy*
10.50-11.00	**FC5:** Targeting the mycobactin biosynthesis pathway in *M. tuberculosis*: a step towards the improvement of the anti-virulence activity of MbtI inhibitors **Matteo Mori,** *University of Milan, Italy*		**FC6:** Development of hydrogen sulfide-releasing hybrids as novel multitarget drugs **Angela Corvino**, *University of Naples Federico II, Italy*
11.00-11.20	**COFFEE BREAK**		
11.20-11.40	**OC20**: The pivotal role of pyrrolidine ring as multitarget scaffold in neurodegenerative diseases **Antonio Carrieri,** *University of Bari, Italy*		**OC23:** Nucleic acid aptamers: potential therapeutic agents for cancer and neurodegenerative disorders **Jussara Amato**, *University of Naples Federico II, Italy*
11.40-12.00	**OC21:** Pursuing the complexity of bipolar disorder: rational design and optimization of first-in-class D_3R/GSK-3β modulators towards an in vivo proof of concept **Rita M.C. Di Martino**, *Italian Institute of Technology, Genoa, Italy*		**OC24:** Combining quantum mechanics and machine learning in the search of the bioactive conformation of drug-like compounds **Antonio Viayna,** *University of Barcelona, Spain*
12.00-12.20	**OC22:** S.M.A.R.T. steroids: synthesis and structure-activity relationship study towards allosteric modulators of *N*-methyl-D-aspartate receptors **Eva Kudova**, *Czech Academy of Sciences Prague, Czech Republic*		**OC25:** Challenging bioisosteric switch in AChE-MAO B dual-targeting hit optimization **Leonardo Pisani,** *University of Bari, Italy*
12.30-14.00	**LUNCH**		
14.00-15.30	**POSTER SESSION & COMMERCIAL EXHIBITION**		

Tuesday, September 13th, 2022

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

Wednesday September 14th, 2022

	Aldo Moro Hall		Vincenzo Starace Hall
	Chair: **Marcello Leopoldo**		
9.00-9.50	**PL4**: Targeting chemokine receptor CCR2 - From insurmountable antagonists to affinity-based probes **Laura Heitman,** *Leiden University, The Netherlands*		
	Aldo Moro Hall		**Vincenzo Starace Hall**
	Chairs: **Marco Catto**, **Marcello Leopoldo**		Chairs: **Gianluca Sbardella**, **Cosimo D. Altomare**
10.00-10.30	**KN9:** Development and hands-on application of PyRMD: a new AI-powered virtual screening tool **Sandro Cosconati,** *Luigi Vanvitelli University, Naples, Italy*		**KN10:** The discovery of potent and selective agonists of human transient receptor potential Cation Channel Subfamily M member 5: from HTS to early hit validation **Alessio Barilli,** *Aptuit, an Evotec Company, Verona, Italy*
10.30-10.50	**OC26:** Exploring CCRL2 Chemeerin binding using accelerated molecular dynamics **Antonio Coluccia**, *Sapienza University of Rome, Italy*		**OC28:** 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 **Margherita Brindisi**, *University of Naples Federico II, Italy*
10.50-11.10	**OC27:** Functionalized ligands targeting G protein-coupled adenosine receptors **Stephanie Federico**, *University of Trieste, Italy*		**OC29:** New insights in the development of cannabinoid receptor subtype 2 (CB_2R) ligands **Marialessandra Contino,** *University of Bari, Italy*
11.10-11.30	**COFFEE BREAK**		
11.30-11.50	**OC30:** Optimizing the choice of 3D query structures in ligand-based virtual screenings with PharmScreen® **Giorgia Zaetta,** *Parc Científic de Pharmacelera, Barcelona, Spain*		**OC32:** Novel cyclic uPA-derived decapeptides reduce in vivo lung dissemination and re-educate CAF phenotype by acting through integrin αvβ5 **Alfonso Carotenuto**, *University of Naples Federico II, Italy*
11.50-12.10	**OC31:** A computational grid-based analysis to map drug-like peptide binding pockets of peptide-protein interactions systems **Daniela Trisciuzzi,** *University of Bari, Italy*		**OC33:** Screening of amino-acid-anthraquinone click chemistry conjugates targeting human telomeric G-quadruplexes **Giovanni Ribaudo,** *University of Brescia, Italy*
	Aldo Moro Hall		
	Chair: **Gianluca Sbardella**		
12.10-13.10	**PL5**: COVID-19 pandemic: what we learnt in antiviral drug discovery, successes, and failures **Vincenzo Summa,** *University of Naples Federico II, Italy*		
13.10-13.30	**CLOSING REMARKS and POSTER PRIZES**		
13.30	**LUNCH**		

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