

XXVI  
National Meeting  
in Medicinal  
Chemistry



<sup>7</sup>N <sup>15</sup>P <sup>6</sup>C <sup>9</sup>F <sup>12</sup>

XII Young  
Medicinal  
Chemists'  
Symposium

Milan, Ca' Granda, July 16-19, 2019

Tuesday 16<sup>th</sup> July 2019, Ca' Granda - University of Milan, Aula Magna

14.30-17.00	<b>REGISTRATION</b>
17.00-17.30	<p><b>OPENING CEREMONY</b> Rector (<b>Prof. Elio Franzini</b>) and Pro-Rector (<b>Prof. Mariapia Abbracchio</b>) <b>Gabriele Costantino</b> - <i>Chairman of the Scientific Committee</i> <b>Gianluca Sbardella</b> - <i>President of the Medicinal Chemistry Division</i> <b>Marina Carini</b> - <i>Co-chair of the Organizing Committee</i> <b>Marco De Amici</b> - <i>Co-chair of the Organizing Committee</i></p>
17.30-18.00	<p><b>Medicinal Chemistry Division of the Italian Chemical Society's Awards</b> <b>Alberto Massarotti</b>, <i>University of Piemonte Orientale, Novara</i> <b>Salvatore Di Maro</b>, <i>University "Luigi Vanvitelli", Caserta</i> <b>Best Doctoral Thesis Awards</b> Quinoline-based efflux inhibitors as antimicrobial resistance breakers (ARBs) <b>Tommaso Felicetti</b>, <i>University of Perugia</i> Development of new antiprotozoal agents: design, synthesis and biological evaluation <b>Francesco Saccoliti</b>, <i>IIT, Genoa, and La Sapienza University, Rome</i></p>
18.00-18.30	<p><b>Musajo Medal of the Medicinal Chemistry Division of the Italian Chemical Society</b> Recipient: <b>Federico Da Settimo</b>, <i>University of Pisa</i> <b>Seal of the Medicinal Chemistry Division of the Italian Chemical Society</b> Recipient: <b>Daniele Donati</b>, <i>Nerviano Medical Sciences S.r.l., Nerviano (MI)</i></p>
18.30-19.30 <b>OL</b>	<p>Chair: <b>Gianluca Sbardella</b>, <i>University of Salerno</i> Breakthroughs in GPCR structural biology and their impact on computer-aided drug design <b>Kenneth A. Jacobson</b>, <i>National Institutes of Health, Bethesda, USA</i></p>
19.45	<p><b>WELCOME BUFFET</b> Loggiato del Rettorato</p>

CL = Closing Lecture  
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## Wednesday 17<sup>th</sup> July 2019, Ca' Granda

NMMC - Aula Magna - Chair: Marco De Amici, *University of Milan*

9:00-9:40 PL	(ChemMedChem lecture): Inducing protein degradation with small molecules: how Protacs work Alessio Ciulli, <i>University of Dundee, UK</i>	
	NMMC1 - Aula Magna	NMMC2 - Room 201
	Chairs: <b>Gianluca Sbardella</b> , <i>University of Salerno</i> <b>Cosimo Damiano Altomare</b>	Chairs: <b>Marco De Amici</b> <b>Marco L. Lolli</b>
9:50-10:20 KN	Annelated medium-sized azaheterocycles as attractive scaffolds or CNS targeted leads <b>Cosimo Damiano Altomare</b> , <i>University of Bari</i>	Hydroxyazoles as carboxylate bioisosteres: an efficient tool for designing active compounds with added intellectual property value <b>Marco L. Lolli</b> , <i>University of Turin</i>
10:20-10:40 OC	Alkylphospholipid cures canine leishmaniasis. Discovery, pharmacological characterization and mechanism of action through genomic approach <b>Maria Paola Costi</b> , <i>University of Modena and Reggio Emilia</i>	Indole-based privileged structures via multicomponent reactions <b>Sveva Pelliccia</b> , <i>Federico II University, Naples</i>
10:40-11:00 OC	Benzoylpiperidine-based compounds as reversible, potent and selective MAGL inhibitors <b>Carlotta Granchi</b> , <i>University of Pisa</i>	Nanotechnological approaches for biomedical applications <b>Tatiana Da Ros</b> , <i>University of Trieste</i>
11:00-11:30	<b>COFFEE BREAK</b>	
11:30-11:50 OC	Scouting sigma receptor ligands as new tools for the treatment of neurodegenerative diseases and cancer <b>Silvia Franchini</b> , <i>University of Modena and Reggio Emilia</i>	Discovery of first-in-class inhibitors of APOBEC DNA cytosine deaminases <b>Daniel Harki</b> , <i>University of Minnesota, USA</i>
11:50-12:10 OC	5-(1H-imidazol-2-yl)-4-methyl-4H-thieno[3,2-b]pyrrole derivatives as new potent reversible inhibitors of histone lysine demethylase (KDM1A/LSD1) <b>Alessia Romussi</b> , <i>The FIRCO Institute of Molecular Oncology Foundation (IFOM), Milan</i>	Acyclic boronic acids mimic $\beta$ -lactamases tetrahedral intermediates leading to broad spectrum inhibitors <b>Donatella Tondi</b> , <i>University of Modena and Reggio Emilia</i>
12:10-12:30 OC	New stilbene-ammonium based nicotinic ligands: insights into alpha9-10 and alpha7 nAChR responses <b>Francesco Bavo</b> , <i>University of Milan</i>	Unexpected activity of bromiphen against prokaryotic and eukaryotic infectious agents <b>Laura Fumagalli</b> , <i>University of Milan</i>
12:30-14:00	<b>LUNCH</b>	
14:00-15:00	<b>POSTER SESSION (P1 – P53)</b>	
	NPCF1 - Aula Magna	NPCF2 - Room 201
	Chairs: <b>Girolamo Cirrincione</b> , <i>University of Palermo</i> <b>Alberto Massarotti</b>	Chairs: <b>Roberto Di Santo</b> , <i>La Sapienza University, Rome</i> <b>Salvatore Di Maro</b>
15:00-15:30 KN	From ZINC to ZINClick: our way to explore the chemical space <b>Alberto Massarotti</b> , <i>University of Piemonte Orientale, Novara</i>	How we turned a weak and metabolically unstable CXCL12-mimic peptide into a stable, potent and selective CXCR4 antagonist: a successful peptide optimization story <b>Salvatore Di Maro</b> , <i>University "Luigi Vanvitelli", Caserta</i>
15:30-15:50 OC	Unveiling target associations for polypharmacology from analysis of crystallographic ligands in the protein data bank <b>Luca Pinzi</b> , <i>University of Modena and Reggio Emilia</i>	The understanding of the mechanism of action of pyridobenzothiazolones reveals mutations in the 3'-UTR: identification of a compound protecting mice from dengue-2 lethal infection <b>Giuseppe Manfroni</b> , <i>University of Perugia</i>
15:50-16:10 OC	Design and receptor interactions of A1 adenosine receptor agonists in the native ribose and conformationally-constrained (N)-methanocarba series <b>Veronica Salmaso</b> , <i>National Institutes of Health, USA</i>	TRPM8 channel modulators: identification of a selective superantagonist by structural simplification and hit refinement approaches <b>Carmine Ostacolo</b> , <i>Federico II University, Naples</i>
16:10-16:20 FC	Exploring the 1-(4-fluorobenzyl) piperazine scaffold for the development of new potent tyrosinase inhibitors <b>Serena Vittorio</b> , <i>University of Messina</i>	Design, synthesis and interaction studies of new compounds targeting the RNA-binding protein HuR <b>Serena Della Volpe</b> , <i>University of Pavia</i>
16:20-16:50	<b>COFFEE BREAK</b>	

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16:50-17:10 OC	Identification of a novel quinoline-based DNA demethylating compound highly potent in cancer cells <b>Clemens Zwergel</b> , <i>La Sapienza University, Rome</i>	Preclinical studies on the antitumor activity induced by novel oxadiazole Topsisin analogs against pancreatic cancer cells <b>Daniela Carbone</b> , <i>University of Palermo</i> , and <i>VU University Medical Center, Amsterdam, The Netherlands</i>
17:10-17:20 FC	A novel NO-photoresponsive polymeric platform as an enhancer of doxorubicin delivery <b>Federica Sodano</b> , <i>University of Turin</i>	Identification of RAD51-BRCA2 disruptors to inhibit homologous recombination and synergize with Olaparib as new anticancer drug discovery concept <b>Greta Bagnolini</b> , <i>Italian Institute of Technology (IIT) and University of Bologna</i>
17:20-17:30 FC	Multiscale approach to predict the binding mode of metallo $\beta$ -lactamase inhibitors <b>Silvia Gervasoni</b> , <i>University of Milan</i>	Lead optimization of [1,2]oxazole[5,4-e]isoindoles as tubulin polymerization inhibitors <b>Marilia Barreca</b> , <i>University of Palermo</i>
17:30-17:40 FC	The mechanism of N-palmitoylethanolamine hydrolysis catalysed by N-acylethanolamine elucidated by QM/MM simulations <b>Laura Scalvini</b> , <i>University of Parma</i>	New enantiopure hydroxyethyl-piperazines as carbonic anhydrase inhibitors <b>Niccolò Chieramonte</b> , <i>University of Florence and University of Münster, Germany</i>
18:00-19:30	<b>DCF-SCI General Meeting (ASSEMBLEA DELLA DIVISIONE DI CHIMICA FARMACEUTICA)</b>	

## Thursday 18<sup>th</sup> July 2019, Ca' Granda

NMMC - Aula Magna - Chair: Marina Carini, *University of Milan*

8:40-9:20 PL	Implementing molecular interaction kinetic analysis for drug discovery <b>Helena Danielson</b> , <i>Uppsala University, Sweden</i>	
	<b>NMMC3 - Aula Magna</b>	<b>NMMC4 - Room 201</b>
	Chairs: <b>Marina Carini</b> <b>Claudio Dalvit</b>	Chairs: <b>Tiziano Bandiera</b> , <i>IIT, Genoa</i> <b>Barbara Gatto</b>
9:30-10:00 KN	Ligand-based fluorine NMR screening: principles and applications in drug discovery <b>Claudio Dalvit</b> , <i>Lavis (TN)</i>	Druggable targets in nucleic acids <b>Barbara Gatto</b> , <i>University of Padua</i>
10:00-10:20 OC	Targeting Transient Receptor Potential Vanilloid 1 (TRPV1) for topical treatment of inflammatory skin disorders <b>Silvio Aprile</b> , <i>University of Piemonte Orientale, Novara</i>	Bio-inspired G-Quadruplex binders powered by multicomponent reactions <b>Mariateresa Giustiniano</b> , <i>Federico II University, Naples</i>
10:20-10:40 OC	Targeting Chagas disease using fragment-based lead discovery: validation and screening of FPPS enzyme <b>Giulia Opassi</b> , <i>Uppsala University, Sweden</i>	Targeting DNA G-Quadruplex structures: toward the development of new anticancer agents <b>Rita Morigi</b> , <i>University of Bologna</i>
10:40-11:10	<b>COFFEE BREAK</b>	
11:10-11:30 OC	Anopheles Gambiae 3-hydroxykynurenine transaminase: LC-MS/MS and inhibition study of new potential inhibitors <b>Erika Del Grosso</b> , <i>University of Piemonte Orientale, Novara</i>	First asymmetric synthesis of NMS-P528, a new highly promising agent for antibody-drug conjugates generation <b>Paolo Orsini</b> , <i>Nerviano Medical Sciences S.r.l., Nerviano (MI)</i>
11:30-11:50 OC	Chemical characterization and evaluation of the antibacterial activity of essential oils from fibre-type Cannabis sativa L. (HEMP) <b>Federica Pellati</b> , <i>University of Modena and Reggio Emilia</i>	Integrins & p53: dual-targeting peptidomimetics to challenge glioblastoma multiforme <b>Francesco Merlino</b> , <i>Federico II University</i>
11:50-12:10 OC	Delving into Spirulina platensis peptidome: discovery of a novel decameric peptide with potent in vivo antihypertensive activity <b>Eduardo Sommella</b> , <i>Federico II University, Naples</i>	Direct preparation of melatonin derivatives via C-H activation/functionalization protocol, a useful tool in synthetic medicinal chemistry <b>Michele Mari</b> , <i>University of Urbino</i>
12:10-12:30 OC	Substituted acetamide as a cysteine trap for the development of novel irreversible tyrosine kinase inhibitors with antiproliferative activity <b>Riccardo Castelli</b> , <i>University of Parma</i>	Targeting the opioid receptors: biphalin analogues design <b>Adriano Mollica</b> , <i>University "G. d'Annunzio" of Chieti-Pescara</i>
12:30-14:00	<b>LUNCH</b>	

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14:00-15:00	POSTER SESSION (P54 – P110)	
	NPCF - Aula Magna - Chair: Giulio Vistoli, <i>University of Milan</i>	
15:00-15:30 KN	Toward the computational design of nanoreceptors with intelligent recognition abilities Marco De Vivo, <i>Istituto Italiano di Tecnologia (IIT), Genoa</i>	
	NPCF3 - Aula Magna	NPCF4 - Room 201
	Chairs: <b>Federico Corelli</b> , <i>University of Siena</i> <b>Andrea Milelli</b>	Chairs: <b>Vincenzo Summa</b> , <i>Federico II University, Naples</i> <b>Roberta Costi</b>
15:30-16:00 KN	Histone deacetylase inhibitors as multitarget ligands: new players in Alzheimer's disease drug discovery? <b>Andrea Milelli</b> , <i>University of Bologna</i>	The new era against neglected tropical diseases: fighting protozoa striking known and innovative targets <b>Roberta Costi</b> , <i>La Sapienza University, Rome</i>
16:00-16:20 OC	A fluorescent mitochondria-targeted NO photodonor activable with highly biocompatible green light <b>Mariacristina Failla</b> , <i>University of Catania</i>	Plasmodium falciparum dihydroorotate dehydrogenase inhibitors with hydroxypyrazole core: new scaffolds against malaria disease <b>Agnese Pippione</b> , <i>University of Turin</i>
16:20-16:40 OC	Design, synthesis and pharmacological characterization of selective blockers of 2- arachidonoylglycerol degradation <b>Samuele Maramai</b> , <i>University of Siena and Sussex Drug Discovery Centre, UK</i>	Structural insights for the development of novel antituberculars targeting the iron uptake pathway <b>Matteo Mori</b> , <i>University of Milan</i>
16:40-17:10	COFFEE BREAK	
17:10-17:30 OC	Predicting resistance of clinical Abl mutations using computational methods <b>Davide Branduardi</b> , <i>Schrödinger, Cambridge, UK</i>	Your manuscript through the Editor's eyes <b>Joseph Unsay</b> , <i>Associate Editor, Chemistry - a European Journal, Wiley-VCH, Germany</i>
17:30-17:50 OC	Development of a screening platform for the identification of small-molecule ligands for the reader protein PHF20 <b>Alessandra Feoli</b> , <i>University of Salerno</i>	Enriching the tool-box of NorA inhibitors by computer-aided scaffold hopping approach <b>Rolando Cannalire</b> , <i>University of Perugia</i>
17:50-18:00 FC	Memantine-ferulic acid hybrids as molecular probes for the study of Alzheimer's disease <b>Filippo Basagni</b> , <i>University of Bologna</i>	Discovery of a novel class of potent and non cytotoxic Trypanosoma brucei growth inhibitors <b>Federica Ferrigno</b> , <i>IRBM S.p.A., Pomezia (Rome)</i>
18:00-18:10 FC	Buffalo ricotta peptide reduces oxidative stress in intestinal epithelial cells and angiotensin II-induced vasoconstriction on mice mesenteric arteries by induction of Nrf2 translocation <b>Giacomo Pepe</b> , <i>University of Salerno</i>	Halogenated phenothiazines with anti-TB activity through the NDH-II inhibition <b>Maria Giulia Nizi</b> , <i>University of Perugia</i>
18:15-19:15	CELEBRATION OF THE 40 <sup>th</sup> ANNIVERSARY OF THE DIVISION OF MEDICINAL CHEMISTRY AND OF THE 100 <sup>th</sup> ANNIVERSARY OF "LA CHIMICA E L'INDUSTRIA"	
20:30	GALA DINNER - Villa Necchi Campiglio	

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# Friday 19<sup>th</sup> July 2019, Ca' Granda

NMMC - Aula Magna - Chair: Gabriele Costantino, <i>University of Parma</i>		
9:00-9:40 PL	Artificial Intelligence. Not just another Tool in the Toolbox David E. Leahy, <i>The Discovery Bus Ltd, Macclesfield, UK</i>	
9:40-10:10 KN	Unveiling uncharted pockets of IDO1 for novel therapeutic opportunities Antonio Macchiarulo, <i>University of Perugia</i>	
	NMMCS - Aula Magna	NMMCS6 - Room 201
	Chairs: <b>Gabriele Costantino</b> <b>Antonio Macchiarulo</b>	Chairs: <b>Vincenza Andrisano</b> , <i>University of Bologna</i> <b>Stefano Alcaro</b> , <i>Magna Græcia University, Catanzaro</i>
10:20-10:40 OC	Novel strategies to iron-starve <i>Staphylococcus aureus</i> : structural and dynamic characterization of the hemophore-Hb interaction <b>Francesca Spyraakis</b> , <i>University of Turin</i>	A new CXCL12/HMGB1 heterocomplex inhibitor <b>Jacopo Sgrignani</b> , <i>Istituto di Ricerca in Biomedicina (IRB) - Università della Svizzera Italiana, Bellinzona (USI), Switzerland</i>
10:40-11:00 OC	Rescuing defective CFTR applying a drug repositioning strategy <b>Paola Fossa</b> , <i>University of Genoa</i>	Developing glycoproteins as potential vaccines against tuberculosis <b>Teodora Bavaro</b> , <i>University of Pavia</i>
11:00-11:30	COFFEE BREAK	
11:30-11:50 OC	Can we improve drug design by illuminating druggable targets with BDDCS? <b>Giovanni Bocci</b> , <i>University of New Mexico, Albuquerque, USA</i>	Kinase inhibitors as potential neuroprotective agents: playing with the triazolotriazine scaffold on GSK-3 $\beta$ and CK-1 $\delta$ <b>Stephanie Federico</b> , <i>University of Trieste</i>
11:50-12:10 OC	Flow nanoprecipitation of size-controlled D-leucine nanoparticles as excipient for spray-drying formulations <b>Bruno Cerra</b> , <i>University of Perugia</i>	Identification of chromeno[3,2-c]pyridine as suitable scaffold of novel multitarget-directed ligands for the treatment of Alzheimer's disease <b>Rosa Purgatorio</b> , <i>University of Bari</i>
12:10-13:10 CL	Integrated structural biology: approaching infectious and degenerative diseases Martino Bolognesi, <i>University of Milan</i> - Chair: Gabriele Costantino	
13:10-13:30	CLOSING REMARKS and POSTER PRIZES	
13:30	LUNCH	

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