



XXIX  
National Meeting on  
Medicinal Chemistry

N P C F 16  
16<sup>th</sup> Young Medicinal Chemistry Symposium  
Nuove Prospettive in Chimica Farmaceutica

14<sup>th</sup> - 17<sup>th</sup> September 2025 | Starhotels Du Parc - Parma (Italy)

SUNDAY 14 <sup>th</sup>	
14:30 – 16:45	REGISTRATION
ROOM VERDI-BODONI-FARNESE	
17:00 – 17:30	<b>OPENING CEREMONY</b> <b>Paolo Martelli</b> , Rector of Università di Parma <b>Stefano Alcaro</b> , President of the Medicinal Chemistry Division <b>Maria Laura Bolognesi</b> , President of the Scientific Committee <b>Marco Mor</b> , President of the Organizing Committee
17:30 – 18:10	Chair: <b>Stefano Alcaro</b> <b>SIGIL OF THE MEDICINAL CHEMISTRY DIVISION OF THE ITALIAN CHEMICAL SOCIETY</b> <b>Maurizio Delcanale</b>  <b>MEDICINAL CHEMISTRY DIVISION OF THE ITALIAN CHEMICAL SOCIETY AWARDS</b> <b>Samuele Cazzamalli</b> , Philochem <b>Rita Maria Concetta Di Martino</b> , Università del Piemonte Orientale  <b>BEST BACHELOR THESIS AWARD “M. BOTTA”</b> <b>Laura Gioiello</b> , Università del Piemonte Orientale  <b>BEST DOCTORAL THESIS AWARDS</b> <b>FC01: Nicolò Bisi</b> , Università di Modena e Reggio Emilia <i>Design, Synthesis and Biological Evaluation of <math>\alpha</math>-Synuclein and Tau Aggregation Inhibitors</i> <b>FC02: Sara Puglioli</b> , Philochem <i>DNA-Encoded Libraries for the Discovery of Potent and Selective Tumor-Targeting Ligands</i>
18:10 – 18:50	<b>MUSAJO MEDAL OF THE MEDICINAL CHEMISTRY DIVISION OF THE ITALIAN CHEMICAL SOCIETY</b> <b>Roberto Di Santo</b> , Università di Roma “La Sapienza”
18:50 – 19:50	<b>OPENING LECTURE</b> <b>PL01: Luc van Hijfte</b> , Novalex and President of EFMC <i>The Pharmaceutical Industry: Riding the Wave of Change</i>
20:00	<b>WELCOME COCKTAIL</b> (Starhotels Du Parc)



**MONDAY 15<sup>th</sup> – Morning Session**

<b>9:00</b>	Room Verdi; chair: <b>Marco Mor</b> <b>PL02: Oliver Koch</b> , University of Münster <i>AI and Data-Driven Drug Development</i>	
	Room Verdi; chairs: <b>Fabio Rancati, Paolo Grieco</b>	Room Bodoni-Farnese; chairs: <b>Marco Mor, Giancarlo Aldini</b>
<b>10:00</b>	<b>KN01: Tracey Pirali</b> , Università del Piemonte Orientale <i>Smart Chemistry against CYP-Mediated Drug Metabolism: a Journey Through Deuteration, Soft Drugs, and Degraders</i>	<b>KN02: Francesco Saverio Di Leva</b> , Università di Napoli “Federico II” <i>Deciphering Binding Selectivity and Kinetics in Class A GPCRs: Insights from Free Energy Simulations on Formyl Peptide Receptors</i>
<b>10:30</b>	<b>OC01: Eleonora Diamanti</b> , Università di Bologna <i>Harnessing PROTAC Methodology Against Emerging Flavivirus Infections</i>	<b>OC02: Antonella Ciancetta</b> , Università di Ferrara <i>Not Quite Folded: Challenges In Predicting the NPS-NPSR Complex with AlphaFold2 Multimer</i>
<b>10:50</b>	<b>FC03: Eleonora Procino</b> , Università di Chieti-Pescara “G. d’Annunzio” <i>Development of Linear <math>\beta</math>-Turn Inducers Containing Peptides as ARC Mimetics with DNA Topological and Sequence Selectivity</i>	<b>FC04: Erika Primavera</b> , Università di Perugia <i>PERUSIA: an Automated Tool for Patent Extraction of Chemical Structures and Bioactivity Data</i>
<b>11:00</b>	COFFEE BREAK	
	Room Verdi; chairs: <b>Fabio Rancati, Paolo Grieco</b>	Room Bodoni-Farnese; chairs: <b>Marco Mor, Giancarlo Aldini</b>
<b>11:20</b>	<b>OC03: Bruno Cerra</b> , Università di Perugia <i>Design and Automated Flow Synthesis of Trans-Tetracyclic Tetrahydroquinolines as Steroid-Mimicking Modulators of the Pregnane X Receptor (PXR)</i>	<b>OC06: Giulia D’arrigo</b> , Schrodinger <i>Accelerating Drug Discovery Through Integrated Physics-Based and Machine Learning Approaches Using Schrödinger's Computational Platform</i>
<b>11:40</b>	<b>OC04: Roberta Mazzucato</b> , Chiesi Farmaceutici <i>Cyclization in DDR Inhibitors: a Pathway to Improved Drug Properties</i>	<b>OC07: Carlos Arroniz</b> , Acellera <i>Quantumbind™: an Integrated Computational Platform for Accelerated Drug Discovery</i>
<b>12:00</b>	<b>OC05: Fabio Francavilla</b> , Università di Bari <i>First-In-Class Photo-Activatable 5-HT<sub>7</sub> Receptor Ligands: Design, Synthesis, and Biological Evaluation</i>	<b>OC08: Michele Roggia</b> , Università della Campania “L. Vanvitelli” <i>From Algorithms to Molecules: the Identification of Riboswitch-Targeting Compounds</i>
<b>12:20 – 13:00</b>	<b>Grazia Rovelli, Giorgio Carbone</b> , Italfarmaco <i>The Transformative Role of AI and Generative Chemistry in Modern Drug Discovery</i> <b>Workshop</b>	
<b>12:20</b>	LUNCH	
<b>13:50</b>	POSTER SESSION I AND EXHIBITION	



XXIX  
National Meeting on  
Medicinal Chemistry

N P C F 16  
16<sup>th</sup> Young Medicinal Chemists' Symposium  
Nuove Prospettive in Chimica Farmaceutica

14<sup>th</sup> - 17<sup>th</sup> September 2025 | Starhotels Du Parc - Parma (Italy)

**MONDAY 15<sup>th</sup> - Afternoon session**

<b>15:00</b>	Room Verdi, chair: <b>Gianluca Sbardella</b> <b>PL03: Helena Danielson</b> , University of Uppsala <i>Lead Discovery Using Biosensors – How to Exploit New Opportunities in an Evolving Field</i>	
	Room Verdi; chairs: <b>Gianluca Sbardella, Silvia Rivara</b>	Room Bodoni-Farnese; chairs: <b>Orazio Nicolotti, Isabella Romeo</b>
<b>16:00</b>	<b>KN03: Clelia Dallanoe</b> , Università di Milano <i>Sulfonium Silent Agonists of the Alpha7 Nicotinic Acetylcholine Receptor: Development of Promising Agents for the treatment of Inflammation and Pain</i>	<b>KN04: Giovanni Spagnoli</b> , Sibylla Biotech <i>From Folding Pathways to Therapeutic Innovation: the Journey of a New Drug Discovery Platform</i>
<b>16:30</b>	<b>OC09: Marco Borgogno</b> , IAMA Therapeutics <i>Discovery of IAMA-6: a Selective Inhibitor of NKCC1 and Clinical Candidate to Treat Brain Disorders</i>	<b>OC12: Davide Sala</b> , Axxam <i>Complementary Tools for Early Drug Discovery Library Design: Combinatorial Enumeration and Generative AI</i>
<b>16:50</b>	<b>OC10: Tania Ciaglia</b> , Università di Salerno <i>Design, Synthesis and in Vitro Preliminary Characterization of Phenylenediamine-Based Derivatives as Receptor Tyrosine Kinase-Like Orphan Receptor 1 (ROR1) inhibitors</i>	<b>OC13: Gian Marco Elisi</b> , Università di Urbino <i>Mechanistic Simulations Rationalize Insertion and Permeation of Pharmaceutically Relevant Peptides</i>
<b>17:10</b>	<b>OC11: Chiara Borsari</b> , Università di Milano <i>Innovative Covalent Targeting of Glycolysis for Oncology Applications</i>	<b>OC14: Giordano Mancini</b> , E4 Computer Engineering <i>Reconfigurable HPC: a Catalyst for Innovation in Molecular Sciences</i>
<b>17:30</b>	<b>FC05: Lorenzo Tagliazucchi</b> , Università di Parma <i>Pyrazole Pyridin-6-one Scaffold for the Development of a Novel Class of YAP:TEAD Interface-3 Molecular Disruptors to Treat Colorectal Carcinoma</i>	<b>FC06: Valeria Cavalloro</b> , Università di Pavia <i>From Pharmacophore Modelling to Natural Product Isolation: Identifying Marine Alkaloids as Proteasome Activators</i>
<b>17:40</b>	COFFEE BREAK	
<b>18:00</b> – <b>19:00</b>	MENTORING PROGRAM DCF (ROOM BODONI-FARNESE)	



XXIX  
National Meeting on  
Medicinal Chemistry

NPCF 16  
16<sup>th</sup> Young Medicinal Chemists' Symposium  
Nuove Prospettive in Chimica Farmaceutica

14<sup>th</sup> - 17<sup>th</sup> September 2025 | Starhotels Du Parc - Parma (Italy)

**TUESDAY 16<sup>th</sup> – Morning Session**

<b>9:00</b>	Room Verdi, chair: <b>Maria Laura Bolognesi</b> <b>PL04: Daniele Piomelli</b> , University of California, Irvine <i>The Lipid Amidase NAAA in Spinal Cord Oligodendrocytes Drives Chronic Pain via Neuronal <math>\beta</math>-Amyloid Release</i>	
	Room Verdi; chairs: <b>Maria Laura Bolognesi, Fabrizio Micheli</b>	Room Bodoni-Farnese; chairs: <b>Gabriele Costantino, Patrizia Diana</b>
<b>10:00</b>	<b>KN05: Stefania Butini</b> , Università di Siena <i>From Selective to Multitarget Directed Ligands: Exploring Endocannabinoids' Catabolism as a Therapeutic Strategy in Epilepsy and Neuroinflammatory Conditions</i>	<b>KN06: Federica Pellati</b> , Università di Modena e Reggio Emilia <i>Managing Neuropathic Pain: New Challenges with Natural and Nature-Inspired Molecules from Cannabis Sativa L</i>
<b>10:30</b>	<b>OC15: Aleksei Smirnov</b> , Università di Camerino <i>Phospholipids as Subtype-Specific Allosteric Regulators of Adenosine Receptors: a New Player on the Scene of Purinergic Signaling</i>	<b>OC16: Agostino Cianciulli</b> , Aptuit – Evotec <i>GPR39 Antagonism: a New Paradigm for the Treatment of Acute Myocardial Infarction and Coronary No Reflow</i>
<b>10:50</b>	<b>FC07: Eva Landucci</b> , Università di Pisa <i>Novel Piperidine-Based Derivatives as Reversible MAGL Inhibitors</i>	<b>FC08: Rebecca Orioli</b> , Università di Bologna <i>Design of Chromone- and Coumarin-Derived Multitarget Inhibitors of the Arachidonic Acid Pathway Enzymes</i>
<b>11:00</b>	COFFEE BREAK	
	Room Verdi; chairs: <b>Maria Laura Bolognesi, Fabrizio Micheli</b>	Room Bodoni-Farnese; chairs: <b>Gabriele Costantino, Patrizia Diana</b>
<b>11:20</b>	<b>OC17: Sara Guariento</b> , Chiesi Farmaceutici <i>Discovery of an Indolizine-Based Inhaled Selective PI3K<math>\delta</math> Preclinical Candidate for Inflammatory Lung Diseases: When Scaffold Hopping Meets "Inhalation by Design"</i>	<b>OC19: Barbara Parrino</b> , Università di Palermo <i>Novel Pyrazolo[1,5-A]Pyrimidine-Indole Hybrids as Potent CDK7 Inhibitors in SCLC and NSCLC Models</i>
<b>11:40</b>	<b>OC18: Valeria Pittalà</b> , Università di Catania <i>Bioisosteric Replacement on Heme Oxygenase Inhibitors Reveals 1,4-Disubstituted 1H-1,2,3-Triazole as Effective Linker Moiety</i>	<b>OC20: Gabriella La Spada</b> , Università di Bari <i>Investigating Inhibition of Metalloproteinases, Histone Deacetylases and Sigma Receptors as a Multimodal Therapeutic Approach to Uveal Melanoma</i>
<b>12:00</b>	<b>FC09: Nicola Tardiolo</b> , Università di Siena <i>New Multi-Target Directed Ligands Integrating Inhibition of Endocannabinoids' Catabolic Enzymes and Antagonism at H3 Receptors</i>	<b>FC11: Greta Bagnolini</b> , Università di Bologna <i>Harnessing Phenylfuran-Carboxyquinoline Scaffold to Develop RAD51-BRCA2 Protein-Protein Interaction Inhibitors and Induce Synthetic Lethality in Pancreatic Cancer</i>
<b>12:10</b>	<b>FC10: Filippo Prencipe</b> , Università di Trieste <i>Design and Synthesis of Novel Inhibitors of Glucosylceramide Synthase for the Treatment of Gaucher Disease</i>	<b>FC12: Chiara Lambona</b> , Università di Roma "La Sapienza" <i>Novel DNMT1/HDACs Inhibitors to Fight Cancer</i>
<b>12:20</b>	LUNCH	
<b>13:50</b>	POSTER SESSION II AND EXHIBITION	



**TUESDAY 16<sup>th</sup> - Afternoon session**

	Room Verdi; chairs: <b>Laura Scalvini, Stefano Moro</b>	Room Bodoni-Farnese; chairs: <b>Giannamaria Annunziato, Rita M. Di Martino</b>
<b>15:00</b>	<b>KN07: Samuele Cazzamalli</b> , Philochem (DCF Prize) <i>From DNA-Encoded Chemistry to Targeted Therapeutics</i>	<b>KN08: Rita M. Concetta Di Martino</b> , Università del Piemonte Orientale (DCF Prize) <i>Strategic Modulation of Store-Operated Calcium Entry: from Single-Target Therapy in Rare Muscular Disorders to a Dual-Target Approach for Multiple Sclerosis</i>
<b>15:30</b>	<b>OC21: Roberta Listro</b> , Università di Pavia <i>Novel Inhibitors of Pseudomonas Aeruginosa Adhesion in Cystic Fibrosis</i>	<b>OC23: Emilia Cassese</b> , Università di Napoli "Federico II" <i>Non-Conventional Degradation of NDM-1 Through PPI-FIT: a New Paradigm to Fight Antibiotic Resistance</i>
<b>15:50</b>	<b>OC22: Zeinab Saedi</b> , Palacky University <i>Towards Precision Oncology: Y220C-P53 Mutant Selective Modifiers</i>	<b>OC24: Tommaso Felicetti</b> , Università di Perugia <i>Nanomolar Anti-Influenza Cycloheptathiophenes Disrupting Polymerase Subunits Interaction</i>
<b>16:10</b>	<b>FC13: Emanuele Fabbri</b> , Università di Roma "La Sapienza" <i>From Crystal Hits to Cellular Impact: Structure-Guided Design of a Potent and Selective SIRT6 inhibitor</i>	<b>FC16: Antonietta Mollo</b> , Università di Napoli "Federico II" <i>Optimization of High-Throughput Screening Hits Targeting SARS-COV-2 Papain-Like Protease</i>
<b>16:20</b>	<b>FC14: Gabriele La Monica</b> , Università di Palermo <i>Covalent Inhibition in Triple-Negative Breast Cancer: Design, Synthesis and Biological Profiling of Acrylamide-Based Quinolines</i>	<b>FC17: Carla Di Chio</b> , Università di Messina <i>Design, Synthesis and Biological Evaluation of Novel Dipeptide Nitriles as Potent Antitrypanosomal Agents</i>
<b>16:30</b>	<b>FC15: Francesco Melfi</b> , Università di Chieti-Pescara "G. d'Annunzio" <i>O-Derivatization of Natural Tropolone and <math>\beta</math>-Thujaplicin Leading to Effective Inhibitors of Cancer-Related Human Carbonic Anhydrases IX and XII: in Vitro and in Silico Investigation of Novel Anti-Proliferative Agents</i>	<b>FC18: Francesca Di Matteo</b> , Università di Salerno <i>Design, Synthesis and Biological Evaluation of New KCNT1 Channel Blockers</i>
<b>16:40</b>	COFFEE BREAK	
<b>17:30 – 19:00</b>	DCF – SCI GENERAL MEETING (Assemblea Generale della Divisione di Chimica Farmaceutica - ROOM VERDI)	
<b>20:30</b>	SOCIAL DINNER (Starhotels Du Parc)	



XXIX  
National Meeting on  
Medicinal Chemistry

N P C F 16  
16<sup>th</sup> Young Medicinal Chemistry Symposium  
Nuove Prospettive in Chimica Farmaceutica

14<sup>th</sup> - 17<sup>th</sup> September 2025 | Starhotels Du Parc - Parma (Italy)

**WEDNESDAY 17<sup>th</sup>**

	Room Verdi; chairs: <b>Stefano Moro, Morena Micciaccia</b>	Room Bodoni-Farnese; chairs: <b>Federica Vacondio, Violetta Cecchetti</b>
<b>9:00</b>	<b>KN09: Stephanie Federico</b> , Università di Trieste <i>CK1δ Inhibitors: May They Help in Fighting Neurodegenerative Diseases</i>	<b>KN10: Federico Riccardi Sirtori</b> , Merck group <i>Improving Pharmacokinetic Bioanalysis of Novel Antibody Drug Conjugates (ADCs) Using Hybrid Immunocapture LC-MS Methods</i>
<b>9:30</b>	<b>OC25: Vincenzo Maria D'Amore</b> , Università di Napoli "Federico II" <i>Advancing RNA Aptamer Therapeutics for Glioblastoma: Structural Characterisation of The A40s Aptamer Targeting EphA2</i>	<b>OC28: Samuele Scurati</b> , DASP <i>The Future of High-Throughput Omics: ZenoTOF 7600 System for Lipidomics and Metabolomics</i>
<b>9:50</b>	<b>OC26: Antonio Curcio</b> , Università della Magna Graecia – Catanzaro <i>A Novel Anticancer Strategy: Disrupting PARP1 Expression Targeting a Non-Canonical G-Quadruplex in HR-Deficient Cancer Cells</i>	<b>OC29: Letizia Trevisan</b> , Università di Trieste <i>Exploring The Pyrazine Scaffold to Develop Inhibitors Towards Casein Kinase 1δ</i>
<b>10:10</b>	<b>OC27: Maria Antonietta La Serra</b> , Istituto Italiano Tecnologia (IIT) <i>Alchemical Free Energy Calculations to Investigate Protein-Protein Interactions</i>	<b>OC30: Simona Musella</b> , Università di Salerno <i>New Indolic Compounds as Potent and Selective Haspin Inhibitors: Design, Synthesis and a Comprehensive in Vitro Pharmacological Characterization</i>
<b>10:30</b>	<b>FC19: Valentina Straniero</b> , Università di Milano <i>Novel Modulators of Synapsin III/Alpha-Synuclein Interaction as Disease-Modifying Agents for Synucleinopathies</i>	<b>FC21: Laura Bertarini</b> , Università di Modena e Reggio Emilia <i>Identifying Lipid Patterns Through Lipidomic Profiling for MASLD Detection and Severity Stratification</i>
<b>10:40</b>	<b>FC20: Ilario Greco</b> , Università della Magna Graecia – Catanzaro <i>In Silico Screening of Phytochemicals from Allium Cepa, Vanilla Planifolia, and Rosmarinus Officinalis as Potential Inhibitors of Human Pancreatic Lipase and α-Amylase</i>	<b>FC22: Salvatore Villani</b> , Università del Piemonte Orientale <i>Integrated Targeted and Semi-Untargeted LC-MS/MS Approaches to Characterize Metabolic Effects of H1D01 Inhibition in Cancer Models</i>
<b>10:50</b>	COFFEE BREAK	
	<i>Session sponsored by Chiesi Farmaceutici</i>	
<b>11:10</b>	Room Verdi, chair: <b>Marco Macchia</b> <b>PL05 Tiina Sikanen</b> , University of Helsinki <i>Environmental Fate and Effects of Pharmaceuticals: Current Knowledge and Future Research Needs</i>	
	Room Verdi; chairs: <b>Marco Macchia, Tracey Pirali</b>	Room Bodoni-Farnese; chairs: <b>Alessio Lodola, Marco Pieroni</b>
<b>12:10</b>	<b>OC31: Margherita Brindisi</b> , Università di Napoli "Federico II" <i>From Repositioning to Drug Development: Sustainable Joullie-Ugi and Continuous Flow Implementation Led to Novel Captopril-Inspired Broad-Spectrum Metallo-Beta-Lactamase Inhibitors</i>	<b>OC34: Vittorio Lembo</b> , Università di Urbino <i>Expanding The Landscape of Dual-Target Drug Design: From Systematic Investigation to in Silico Discovery</i>
<b>12:30</b>	<b>OC32: Daniele Aiello</b> , Università di Modena e Reggio Emilia <i>Ecotoxicological Profiling and Leads Prioritization Through Machine Learning-Based Approach for the Design of Safer Antiparasitic Agents</i>	<b>OC35: Simone Di Micco</b> , European Biomedical Research Institute <i>Insights Into Calcium and Phosphate Binding to Human Annexin A4 Through Structural Investigation</i>
<b>12:50</b>	<b>OC33: Margrate Anyanwu</b> , Università di Brescia <i>In Silico-Driven Discovery of PDE9A-Selective Inhibitors Exhibiting Neuroprotective Effects in an in Vitro Kainate Toxicity Model</i>	<b>OC36: Andrea Giuseppe Cavalli</b> , Università di Milano <i>PEPSCORER::RMSD: an Improved Machine-Learning Scoring Function for Protein-Peptide Docking.</i>
<b>13:10</b>	<b>POSTER PRIZES supported by Chemistry Europe (ROOM VERDI)</b>	
<b>13:30</b>	<b>CLOSING REMARKS (ROOM VERDI)</b>	