



XXX National Meeting on Medicinal Chemistry

17th Young Medicinal Chemists' Symposium
Nuove Prospettive in Chimica Farmaceutica

⁷N ¹⁵P ⁶C ⁹F **17**



Scientific Programme

 **University of Messina**
 **September 13-16, 2026**

■ **SUNDAY 13th Opening Session – Central Building**

Aula Magna Rettorato

14:30	REGISTRATION
17:00	OPENING CEREMONY - Chair: Maria Zappalà
	▪ Giovanna Spatari, Rector of the University of Messina ▪ Giovanni Cuda, Rector of the Magna Graecia University of Catanzaro ▪ Federico Basile, Mayor of Messina ▪ Luigi Mondello, President of the Italian Chemical Society ▪ Robert Nisticò, President of the Agenzia Italiana del Farmaco ▪ Stefano Alcaro, President of the Medicinal Chemistry Division of the Italian Chemical Society and Chair of the Scientific Committee ▪ Maria Zappalà, Chair of the Organizing Committee
17:40	Chair: Stefano Alcaro
	SEAL OF THE MEDICINAL CHEMISTRY DIVISION OF THE ITALIAN CHEMICAL SOCIETY ▪ Lucia Bedini, University of Urbino Carlo Bo
	MEDICINAL CHEMISTRY DIVISION OF THE ITALIAN CHEMICAL SOCIETY AWARDS ▪ Mattia Bernetti, University of Urbino Carlo Bo ▪ Vincenzo Maria D'Amore, University of Naples Federico II
	BEST BACHELOR THESIS AWARD "M. BOTTA" ▪ Martina Corsini, Alma Mater Studiorum University of Bologna
	BEST DOCTORAL THESIS AWARDS ▪ FC01: Simona Barone, University of Naples Federico II <i>Histone Deacetylase 6 at the Crossroads of Cancer and Infectious Diseases</i> ▪ FC02: Roberta Bivacqua, University of Palermo <i>Exploration of Thiazole-Based Scaffolds for the Development of Broad-Spectrum Antiviral Agents</i>
18:20	PRATESI MEDAL OF THE MEDICINAL CHEMISTRY DIVISION OF THE ITALIAN CHEMICAL SOCIETY ▪ Gianluca Sbardella, University of Salerno
18:50	OPENING LECTURE ▪ PL01: Fernando Albericio, University of KwaZulu-Natal, Durban, South Africa <i>The Golden Age of Peptides: Emerging Challenges and Future Opportunities</i>
20:00	WELCOME COCKTAIL (Rettorato Courtyard)

■ MONDAY 14th Morning Session - Papardo Campus

Aula Magna Vittorio Ricevuto

Chair: Maria Laura Bolognesi

9:00

PL02: Werngard Czechtizky, Independent Researcher
Artificial Intelligence–Powered Platforms for Drug Discovery

Aula Magna Vittorio Ricevuto

Lecture Hall A-T-4

Chairs: Maria Laura Bolognesi / Marco De Vivo

Chairs: Laura De Luca / Rosaria Gitto

10:10

KN01: Giuseppe La Regina
Sapienza University of Rome
Tubulin Targeting Drives Ferroptosis in Cancer

KN02: Tiziano Tuccinardi
University of Pisa
Artificial Intelligence in Drug Discovery: Reading the Small Print

10:40

OC01: Maria Paola Costi
University of Modena e Reggio Emilia
The Discovery of the First in Class Thymidylate Synthase Dimer Disrupters from the Binding Mode at the Dimer Interface to in vivo Studies

OC02: Pasquale Linciano
University of Pavia
Quenching Bacterial Communication: Discovery and Profiling of Quorum Sensing Inhibitors with Antibiofilm and Antivirulence Activity

11:00-11:30 COFFEE BREAK

Aula Magna Vittorio Ricevuto

Lecture Hall A-T-4

Chairs: Maria Laura Bolognesi / Marco De Vivo

Chairs: Laura De Luca / Rosaria Gitto

11:30

KN03: Valentina Gandin
University of Padova
Targeting Copper Metabolism in Cancer for Theranostics: from Copper(I)-Based Small Molecules to Self-Assembled Supramolecular Nanoplatfoms

KN04: Laura Mercolini
Alma Mater Studiorum University of Bologna
Miniaturized Sample Preparation to Drive Innovation in Pharmaceutical Analysis

12:00

OC03: Marta Serafini
University of Turin
Imaging and Targeting Low Oxygen Levels in Tumours

OC06: Giovanna Baron
University of Milan
5-(3',4'-Dihydroxyphenyl)- γ -valerolactone-Sulfate as an Inflammation-Triggered Prodrug for Targeted Nrf2 Activation

12:20

OC04: Michele De Franco
Memorial Sloan Kettering Cancer Center, NY
Cu(I)-Based Antibody-Drug Conjugates: a Novel Platform for Cancer Theranostics

OC07: Federica Blua
University of Turin
Development of a Gut-Restricted NLRP3 Inhibitor for IBD: from Design to in vivo Efficacy

12:40

OC05: Valeria Napolitano
University of Salerno
Untargeted Diversity-Oriented Synthesis (UnDOS) for the Identification of Novel Antitumor Agents: An Integrated Approach of IVS, Bioinformatics and Omics for Targets Deconvolution

OC08: Alessandra Altomare
University of Milan
A Tunable Carnosine–HNE Michael Adduct Restores Redox–Inflammatory Balance by Modulating the Nrf2–NF- κ B Axis

13:00-14:00 LUNCH

14:00-15:00 POSTER SESSION I AND EXHIBITION

■ MONDAY 14th - Afternoon Session - Papardo Campus

	Aula Magna Vittorio Ricevuto	Lecture Hall A-T-4
	Chairs: Roberta Ettari / Maria Zappalà	Chairs: Massimo Dondio / Paolo Grieco
15:00	KN05: Francesco Leonetti University of Bari Aldo Moro <i>The Fascinating Story of N-Adamantyl Anthranilamide Derivatives: Design and Development of Selective CB2R</i>	KN06: Francesca Spyraakis University of Turin <i>A Precision Medicine Framework for Targeting DNA Polymerase ϵ in Colorectal Cancer</i>
15:30	OC09: Angela De Simone University of Turin <i>LC-MS Profiling of Histone PTMs in Alzheimer's Disease Mouse Model Astrocytes: toward Early Diagnosis and Targeted Neuroprotection</i>	OC11: Paolo Governa University of Parma <i>Ultrafast Graph Recognition (UGR): a Graph-Based Molecular Similarity Method for Ligand-Based Virtual Screening</i>
15:50	OC10: Alessio Nocentini University of Florence <i>Tuning Multitarget Drug Design Based on Carbonic Anhydrase Modulation for the Treatment of Multifactorial Pathologies</i>	OC12: Bianca Fiorillo University of Naples Federico II <i>Molecular Dynamics Study of ATG13 Ubiquitylation in ULK1 Structural Dynamics and Assembly of Autophagy Initiation Complex</i>
16:15	Excursion to Taormina	

■ TUESDAY 15th - Morning Session - Papardo Campus

Aula Magna Vittorio Ricevuto

Chair: Marco Macchia

9:00

PL03: Elisabetta Chiarparin, Angelini Pharma

Programming Disease Biology with Chemistry: Designing Molecules, Designing Mechanisms

Aula Magna Vittorio Ricevuto

Lecture Hall A-T-4

Chairs: Marco Macchia / Vincenzo Maria D'Amore

Chairs: Tracey Pirali / Mattia Bernetti

10:10

KN07: Vincenzo Maria D'Amore

University of Naples Federico II (DCF prize)
From GPCR Activation to Ligand Binding and Kinetics: Integrated Computational Approaches for Medicinal Chemistry

KN08: Mattia Bernetti

University of Urbino Carlo Bo (DCF prize)
Computational Challenges in Structure-Based Drug Design for RNA Targets

10:40

OC13: Elisa Uliassi

Alma Mater Studiorum University of Bologna
Harnessing Multi-Target Drug Discovery for Circadian Clock Dysfunction in Alzheimer's Disease

OC14: Giacomo Rossino

University of Pavia
Small Molecules Targeting the HUR-RNA Complexes: an Innovative Strategy to Discover Anticancer Agents

11:00-11:30 COFFEE BREAK

Aula Magna Vittorio Ricevuto

Lecture Hall A-T-4

Chairs: Marco Macchia / Vincenzo Maria D'Amore

Chairs: Tracey Pirali / Mattia Bernetti

11:30

OC15: Elisa Patacchini

Sapienza University of Rome
Unlocking Neuroprotection: Rational Design and Synthesis of σ 1R Agonists for Huntington's Disease Treatment

OC17: Luca Piemontese

University of Bari Aldo Moro
From Fungal Metabolites to Multi-Target Ligands: A Nature-Inspired and Green Semi-Synthetic Strategy for Alzheimer's Disease Drug Discovery

11:50

OC16 Emanuele Carosati

University of Trieste
From Phenotypic Screening to Target Networks: A Polypharmacology-Oriented Approach for Rett Syndrome Therapeutics

OC18: Nicoletta Brindani

Italian Institute of Technology, Genoa
Discovery and Development of Novel Polymerase Eta Inhibitors to Overcome Cancer Drug Resistance

Aula Magna Vittorio Ricevuto

Chair: Stefano Alcaro

12:10

Sponsor exhibition (Promega)

12:20

Workshop: Jacopo Gomena, Giorgio Carbone, Matteo Zambra, Italfarmaco

Cutting Through the Hype: Generative Chemistry and Predictive AI Across the Pre-Clinical Drug Discovery Pipeline

13:00-14:00 LUNCH

14:00-15:00 POSTER SESSION II AND EXHIBITION

■ TUESDAY 15th - Afternoon Session - Papardo Campus

	Aula Magna Vittorio Ricevuto	Lecture Hall A-T-4
	Chairs: Roberta Ettari / Nicola Micale	
15:00	OC19: Valeria Francesconi University of Genoa <i>Design, Synthesis, and Biological Evaluation of Dihydrotriazine-Based Antifolates Against Trypanosoma Brucei</i>	MENTORING PROGRAM DCF 15:00-15:40
15:20	OC20: Alessandra Corio IRBM, Pomezia, Rome <i>Discovery of IRBM-Z-2: a Potent Allosteric Inhibitor of Zika Virus NS2B-NS3 Protease with Oral Efficacy in Mouse Models</i>	
15:40-16:00 COFFEE BREAK		
Aula Magna Vittorio Ricevuto		
16:00	YOUNG TALKS – RESEARCH IN FIVE MINUTES Chairs: Marco Franceschin / Morena Miciaccia	
	▪ FC03: Mysoon Al-Ansari , King Saud University, Saudi Arabia <i>Luminal A Breast Cancer Secretome Drives Enterococcus faecalis Toward an Onco-Virulence Phenotype</i>	
	▪ FC04: Giorgia Andreozzi , University of Naples Federico II <i>Design and Synthesis of Small Molecules as MicroRNA Modulators in Ischemic Stroke</i>	
	▪ FC05: Marco Banzato , University of Padova <i>Design, Synthesis, and Pharmacokinetic Profiling of Fluorinated Reversible N-Alkyl Carbamate Derivatives of Psilocin for Sub-Hallucinogenic Brain Exposure</i>	
	▪ FC06: Angela Belcastro , University of Milano Bicocca <i>Synthesis and Biological Evaluation of Novel Covalent Inhibitors of MOK KINASE for the Treatment of Neuroinflammation in Amyotrophic Lateral Sclerosis</i>	
	▪ FC07: Chiara Boero , University of Turin <i>Click Chemistry-Based Strategies for Hypoxia Imaging and Targeted Drug Delivery in Colorectal Cancer Models</i>	
	▪ FC08: Jessica Ceramella , University of Calabria <i>A New Series of Carbazole Derivatives with anti-Breast Cancer Properties</i>	
	▪ FC09: Marco D'Ali , University of Messina <i>Stereospecificity Membrane Impact of Two Catechins on Red Blood Cells</i>	
	▪ FC10: Tommaso Felicetti , University of Perugia <i>Advancing RNA-Targeted Drug Discovery: A Biophysical Platform to Identify MALAT1 Binders as Anti-Melanoma Agents</i>	
	▪ FC11: Aurora Gaza , Alma Mater Studiorum University of Bologna <i>Small-Molecule Degraders for Antiparasitic Drug Discovery and Chemical Biology Application</i>	
	▪ FC12: Alessandro Greco , Italian Institute of Technology, Genoa <i>DNA Polymerase η Inhibitors Against Cancer Chemoresistance</i>	

	▪ FC13: Bianca Martinengo, Alma Mater Studiorum University of Bologna <i>Greening Proteolysis Targeting Chimera Development: Cashew Nutshell Liquid-Based Cereblon Ligands</i>
	▪ FC14: Lorenzo Mattolini, University of Florence <i>Discovery of New Heterocyclic Compounds as Metallo-β-Lactamase Inhibitors to Reverse Antimicrobial Resistance</i>
	▪ FC15: Clara Mocchetti, University of Milan <i>Characterization of Hyaluronic Acid Oligomers by NMR Spectroscopy</i>
	▪ FC16: Matteo Mori, University of Milan <i>Non-Agonist Modulation of PPARγ as a Strategy for Insulin Resistance</i>
	▪ FC17: Alessia Onali, University of Cagliari <i>Novel Thiazolidinone-Isatin Hybrids Potently Inhibit hCA IX and Enhance Doxorubicin-Induced Apoptosis in Hypoxic Glioblastoma Cells</i>
	▪ FC18: Marco Paparella, University of Bari Aldo Moro <i>Multitarget Hybrid Small Molecules for Metal Chelation with Additive Cholinesterase Inhibitory and Antioxidant Properties in Alzheimer's Disease</i>
	▪ FC19: Elena Roggiolani, Alma Mater Studiorum University of Bologna <i>Targeting FYN and GSK-3β to Tackle Neurodegeneration</i>
	▪ FC20: Erica Sanna, University of Cagliari <i>Dual SARS-COV-2 NSP13 Helicase Functions Inhibitors Exhibiting Additive Antiviral Activity as a Proof of Concept for Combination Therapy</i>
	▪ FC21: Rosa Sparaco, University of Naples Federico II <i>Deflazacort-H₂S Donor Hybrids: A Dual Anti-Inflammatory and Antioxidant Approach for Duchenne Muscular Dystrophy</i>
	▪ FC22: José Starvaggi, University of Messina <i>Development of Novel Peptide-Based Michael Acceptors Targeting Rhodesain of Trypanosoma Brucei Rhodesiense</i>
Aula Magna Vittorio Ricevuto	
18:30	DCF - SCI GENERAL MEETING <i>Assemblea Generale della Divisione di Chimica Farmaceutica</i>
19:30	Bus Tour Laghi di Ganzirri
20:30	SOCIAL DINNER (Giardini di Giano)

■ WEDNESDAY 16th Morning Session - Papardo Campus

Aula Magna Vittorio Ricevuto

Chair: Stefano Moro

9:00

PL04: Coral Barbas, Universidad San Pablo CEU, Madrid

From Pathways to Patients: Metabolomics in Modern Drug Discovery

Aula Magna Vittorio Ricevuto

Chairs: Stefano Moro / Orazio Nicolotti

10:10

KN09: Jussara Amato

University of Naples Federico II
Protein-Derived Peptides to Target G-Quadruplex DNA: from Molecular Recognition to Anticancer Activity

10:40

OC21: Michele Coluccia

Sapienza University of Rome
2-Aroyl-5,6-dimethoxybenzofurans and Demethylated Derivatives as Novel Therapeutic Tools Against Glioblastoma

11:00

OC22: Sebastiano Intagliata

University of Catania
Exploiting HO-1 Inhibition Through Mutual Prodrugs Strategy for Improving 5-Fluorouracil Efficacy

Lecture Hall A-T-4

Chairs: Nunzio Iraci / Rosanna Maccari

KN10: Michele De Luca

University of Calabria
From Signals to Knowledge: Machine Learning in Advanced Drug Analysis

OC23: Simone Carradori

G. d'Annunzio University of Chieti-Pescara
Improving the Knowledge of Human Microbiota: Production, Characterization and Modulation of Novel Carbonic Anhydrases from Probiotic Bacteria

OC24: Roberta Rocca

Magna Graecia University of Catanzaro
Beyond the G-Quadruplex: Structure-Based Virtual Screening of the HIV-1 LTR-III Architecture Identifies Novel Antiviral Ligands

11:20-11:50 COFFEE BREAK

Aula Magna Vittorio Ricevuto

Chairs: Morena Miciaccia / Tracey Pirali

11:50

OC25: Vincenzo Mazzarella

University of Campania Luigi Vanvitelli
Expanding The Horizon of Label-Free CTC Detection: Toward a CXCR4-Targeted Plasmonic Optical Fiber Biosensor for Liquid Biopsy Applications

12:10

OC26: Isabella Romeo

Magna Graecia University of Catanzaro
Rational Design, Synthesis and Structural Mechanism of MSP20, a Novel TRPV1 Agonist Endowed with Long-Lasting Analgesic Action

12:30

OC27: Daniela Trisciuzzi

University of Bari Aldo Moro
Exploring ligandable pockets of 3D OncoPPI Networks for improving protein inhibition and degradation strategies

Lecture Hall A-T-4

Chairs: Nicola Micale / Santo Previti

OC28: Giovanna Aquino

AREA Science Park, Salerno
Upcycling Spinach Processing By-Products into High-Value Bioactives: Green Extraction Optimization and in vivo Photoprotective Activity in Zebrafish Models

OC29: Salvatore Mirabile

University of Messina
Designing Dual-Action Luminescent Inhibitors of Tyrosinase: Synthesis and Biological Evaluation

OC30: Federico Paccioia

University of Perugia
Structural Determinants Governing Ligand-Binding Domain Opening of the DAF-12 Receptor

Aula Magna Vittorio Ricevuto

Chairs: Stefano Alcaro / Maria Zappalà

13:00

POSTER PRIZES supported by Chemistry Europe

13:20

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