



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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XXX National Meeting on Medicinal Chemistry

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

N¹ P¹ C¹ F¹ 17

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



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The **XXX National Meeting on Medicinal Chemistry**, together with the **17th Young Medicinal Chemists' Symposium "Nuove Prospettive in Chimica Farmaceutica" (NPCF17)**, represents the best opportunity to share the progress of research and to favor collaborations among medicinal chemists from both academia and industry. The participants will have the chance to present the results of their studies in the highly stimulating environment of the meeting that will cover the most recent advances belonging to one or more of our peculiar Analytical, Computational and Synthetic Medicinal Chemistry topics, listed in research and therapeutic areas.



TOPICS

- Advanced methodologies in synthetic chemistry
- Advanced therapeutic tools
- Bioactive peptides and peptidomimetics
- Innovative targets in Medicinal Chemistry
- Nutraceuticals
- Artificial intelligence-powered platforms for drug discovery and predictive toxicology
- Pharmaceutical analysis
- Recent advances in protein inhibition and degradation
- Theranostic approaches in Medicinal Chemistry



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