ChemBioStruct26

Scientific Program

MONDAY, 26 OCTOBER 2026

12:30-13:15 Participant registration

13:15-13-30 **Welcome address — Rita Berisio (Chair and Coordinator of the Biomacromolecular section of the Italian Crystallographic Association)**

Molecular Tools for Probing Protein and Oligonucleotide Structure and Dynamics in Biology – Chair Marina Mapelli

13:30–14:00 **Invited Lecture · Massimo Degano** — Bridging crystallography and chemistry towards a dual-action ClpP-targeted multiple myeloma therapy

14:00–14:15 **Marta Palerma** — Crystal Structures of Human Histone Deacetylase 8 Reveal Stereoselective Binding of Novel Hydroxamic Acid Inhibitors

14:15–14:30 **M. Giovanna E. Papadopoulos** — Comparative Molecular Dynamics Study of MPS I-Associated Mutations in α-L-Iduronidase

14:30–14:45 **Humberto Fernandes** — From Molecular Motion to Clinical Insight: Structural Biology of PDE6-Associated Optoretinography and Retinal cGMP Restoration

14:45–15:00 **Giovanni Barra** —Structural and binding studies of the mycobacterial heat shock protein reveal a silent state and offer insights into dendritic cell activation

15:00-15:30 **Coffee Break**

AFTERNOON SESSION II

Chemical Interrogation of Interactions Shaping Molecules: From Metals and Carbohydrates to Metabolites and Protein Partners – Chair Francesco Peri

15:30–16:00 **Invited Lecture · Rachel Hevey** — Using structural information to improve the drug-like properties and target selectivity of carbohydrate-based therapeutics

16:00–16:15 **Vittorio Brufani** — Oligomerization Dynamics of Sigma-1 Receptor: Trimer, Hexamer and Nonamer Revealed by Cryo-EM and Mass Photometry

16:15–16:30 **Maria della Valle** — Atomic-level characterization of protein/nano-plastics interactions in living cells

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16:30–16:45 **Ilaria Di Donato** — Dissecting zinc recognition by AdcA from *Enterococcus faecium*: an integrated structural and biophysical approach

16:45–17:00 **Giuseppe Ghibellini** — From an Unexpected Crystallization Outcome to PDB Data Mining: Uncovering the ligand-protein interaction of the NADH Derived Metabolite NADHX

FLASH PRESENTATIONS · 17:00–18:16 – Chair Giancarlo Tria

17:00–17:04 **Margherita Antonelli** — Genetic manipulation of *Chlamydia trachomatis* to investigate immune escaping strategies

17:04–17:08 **Elena Bianchi** — Ellagitannins as Potent Inhibitors of SGK1: New Insights for Therapeutic Applications

17:08–17:12 **Claudia Binda** — Monoamine Oxidases across evolution: from drug targets to biocatalysts

17:12–17:16 **Elisa Bruni** — Development of a virus-free cell assay for the evaluation of viral protease inhibitors

17:16–17:20 **Eleonora Comparini** — Targeting diadenosine tetraphosphate hydrolase in *Pseudomonas aeruginosa*: A structural path to antivirulence drug discovery

17:20–17:24 **Ionela Raluca Comnea-Stancu** — Selective Electrochemical Recognition of L- and D-Citrulline at a Poly-erythrosine/TiO2@S-Doped Graphene Interface

17:24–17:28 **Martina D'Auria** — Structural characterization of a thermophilic PETase isolated from a geothermal environment

17:28–17:32 **Andrea Dalle Vedove** — A Structural Biology Facility at Elettra 2.0

17:32–17:36 **Emily Freeman** — Capturing protein dynamics through room temperature and time-resolved serial crystallography on ID29 at the ESRF

17:36–17:40 **Luca Gessa** — Structural Insights into RBP3 and Its Potential Interaction with GLUT1

FLASH PRESENTATIONS · CONTINUED

17:40–17:44 **Ramona Georgescu-State** — Green-engineered nanostructured electrochemical interface for stochastic recognition of IL-6 and IL-8 in complex biological matrices

17:44–17:48 **Ornella Ghilardi** — Structural and functional insights into peptidoglycan hydrolases involved in Gram-positive cell division

17:48–17:52 **Wawrzyniec Haberek** — NAT2 mediated acetylation of vorinostat

17:52–17:56 **Zbigniew Kaczynski** — Structural diversity of O-polysaccharides from plant-pathogenic bacteria

17:56–18:00 **Shangkun Li** — Bio-Inspired Stable {Co4O4} Molecular Catalyst for the Oxygen Evolution Reaction

18:00–18:04 **Viviana Perrotta** — AI-guided identification of novel phosphoethanolamine transferase inhibitors as potential colistin adjuvants against antimicrobial resistance

18:04–18:08 **Filippo Piazza** — Harnessing Cashew NutShell Liquid for Target-Based Sustainable Antiviral Drug Discovery via Ugi 4-C reaction

18:08–18:12 **Mario Privitera** — Deciphering the KP32 Phage Architecture: Implications for Antimicrobial Strategies against *Klebsiella pneumoniae*

18:12–18:16 **Alessia Ruggiero** — The dual role of Rv3463 in *Mycobacterium tuberculosis*: bridging redox metabolism to host immune response

TUESDAY, 27 OCTOBER 2026

MORNING SESSION I

Precision Chemistry: Antibodies, Chemical Probes and Beyond as Next-Generation Therapeutics – Chair Cecilia Pozzi

09:00–09:30 **Invited Lecture · Johannes Huebner** — Monoclonal Antibodies and Beyond: Novel Anti-Infective Strategies Targeting Bacterial Surface Structures of multidrug-resistant pathogens

09:30–09:45 **Prabhanshu Tripathi** — Dual Homotypic Antibody Interfaces Enable Broad Recognition of the Malaria Circumsporozoite Protein

09:45–10:00 **Karthik Ramanadane** — Integrative structural analysis of the LRP2-LRPAP1 complex reveals multiple regulatory sites

10:00–10:15 **Md Saiful Islam** — Structural Basis of ATM Activation by MRN and DNA multiple regulatory sites

10:15–10:45 **Coffee Break**

MORNING SESSION II

Integrating Chemical Biology and Structural Analysis to Accelerate Drug and Vaccine Discovery – Chair Rita Berisio

10:45–11:15 **Invited Lecture · Maria Grazia Pizza** — Shaping Immunity: Structural Vaccinology for Next-Generation Vaccine Antigens

11:15–11:45 **Invited Lecture · Juan Hermoso** — From Antibiotic Sensing to Cell Envelope Protection: Structural Biology of Bacterial Resistance Mechanisms

11:45–12:00 **Michelle Fornasier** — Structure-Guided Development of Selective Pyrazine-Based CK1δ Inhibitors

12:00–12:15 **Federica Gabriele** — Site-Selective Targeting of Cryptosporidium parvum Thioredoxin Reductase by Gold Compounds: Structural and Mechanistic Insights

12:15–12:30 **Laura Nagy** — Looking for the next target: The story of a 70-year-old *Shigella sonnei* mutant

12:30–12:45 **Renata Ceragno** — A Modular Synthetic Strategy for Late-Stage Functionalisation of *Staphylococcus aureus* Capsular Polysaccharide Type 1 Oligosaccharides

12:45–13:00 **Rita Berisio** — Conclusions and Announcement of AIC, SCI and Elsevier Young Researcher Awards