



6th AIC-BMM Meeting – Schedule and Scientific Program

Thursday, Feb 20th 2025

13.00 Participant registration and accommodation check-in. Appetizers & light lunch

14.30 Welcome by Rita Berisio, Coordinator of AIC-BMM

Afternoon Session I – Chair: Marco Mazzorana

Molecular mechanisms in biological processes

14.40 Invited speaker **Daniele Narzi**. *Department of Physical and Chemical Sciences, University of L'Aquila, Italy.*

Title: From Structure to Function: Integrating Theoretical Approaches to Elucidate the Catalytic Mechanism of Oxygen Evolution in Photosystem".

15.10 **Noemi Destefani**. *Biocrystallography Unit, Division of Immunology, IRCCS San Raffaele Scientific Institute, Milan, Italy.*

Title: Antigen-mediated and cell-autonomous B-cell receptor signalling in chronic lymphocytic leukaemia.

15.30 **Lorenzo Antonelli**. *Institute of Molecular Biology and Pathology (IBPM-CNR) and Department of Biochemical Sciences, University La Sapienza, Rome, Italy.*

Title: Deciphering the activation mechanism of Sigma 1 Receptor and the nature of its endogenous ligands.

15.50 **Alessandro Borsellini**. *Human Technopole, Milan, Italy.*

Title: Molecular mechanisms of condensin II activity.

16.10 *Coffee Break & Snack*

Afternoon Session II – Chair: Veronica Morea

Macromolecular structures as a strategy against infectious pathogens

16.40 Invited speaker: **Adele Di Matteo**. *Institute of Molecular Biology and Pathology (IBPM-CNR), Rome, Italy.*

Title: Tackling Signaling Pathways in *Pseudomonas aeruginosa* to Unveil Druggable Targets.

17:10 **Cécile Exertier**. *Institute of Molecular Biology and Pathology (IBPM-CNR), Rome, Italy.*



Title: A proof-of-concept study for the design of PROTACs (PROteolysis TARgeting Chimeras) to tackle Leishmaniasis.

17.30 **Mario Privitera.** *Institute of Biostructures and Bioimaging (IBB-CNR) and University of Campania Luigi Vanvitelli, Caserta, Italy.*

Title: Structural features of KP32 phage portal attacking *Klebsiella pneumoniae* cell wall. Integrating structural biology and AI to unravel a complex biological problem

17.50 **Valeria Napolitano.** *Institute of Biostructures and Bioimaging (IBB-CNR), Naples, Italy.*

Title: Structural basis of protein encapsulation in *Klebsiella pneumoniae* and applications against multi-drug resistant pathogens.

18.10 **Filippo Vascon.** *Department of Biology, University of Padua, Italy.*

Title: Deciphering the Bacterial SOS Response: From Structural Insights to Inhibitor Development.

18.30 Poster flash presentations. Chair: Stefano Mangani

18.30 **Bianca Braggiotti.** *Institute of Biophysics (IBF-CNR), Milan, Italy.*

Title: TRAF2 in TNF Signaling and Immune Regulation: Structural Insights and Therapeutic Potential in Cancer.

18.35 **Vittorio Brufani.** *Institute of Molecular Biology and Pathology (IBPM-CNR) and Department of Biochemical Sciences, University La Sapienza, Rome, Italy.*

Title: Investigating BiP's Function in the Regulation of S1R Activity.

18.40 **Viviana Perrotta.** *Institute of Biostructures and Bioimaging (IBB-CNR), Naples, Italy.*

Title: Understanding PE_PGERS, cell wall proteins promoting mycobacterial survival in TB.

18.45 **Chiara Marella D'Aprile.** *Institute of Crystallography (IC-CNR), Bari, Italy.*

Title: Bacteriorhodopsin/Perovskite adducts for Next-Generation of in-crystal lab-on-chip Solar Cells.

18.50 **Martina D'Auria.** *Department of Chemical Sciences, University of Naples Federico II, Italy.*

Title: A novel PET hydrolase derived from thermophilic microorganism.

18.55 **Ornella Ghilardi.** *Institute of Biostructures and Bioimaging (IBB-CNR) and Department of Medical Biotechnologies, University of Siena, Italy.*

Title: Crystal structure and biophysical characterisation of the enterococcal foldase PpiC, a cross-opsonic antigen against Gram-positive nosocomial pathogens.

19.00 **Federica Sonzini.** *Department of Biosciences, University of Milan, Italy.*

Italian Crystallographic Association

6th Meeting of the Biological Macromolecules Section

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Title: The open dimeric conformation of cardiotoxic light chains: a key feature underlying soluble toxicity in cardiac AL amyloidosis.

19.05 **Doriano Lamba.** *Institute of Crystallography, National Research Council, Trieste Outstation, Trieste, Italy.*

Title: Disentangling the mechanism underlying the covalent methanesulfonyl fluoride acetylcholinesterase adduct formation and evolvement: structural and mechanistic insights into an aged-like inactive complex susceptible to reactivation by a combination of nucleophiles

19.10 **Arianna Lardieri.** *Department of Biochemical Sciences, University La Sapienza, Rome, Italy.*

Title: Cryo-EM structure of Apo-PdxR from *Bacillus clausii* in complex with its target DNA.

19.15 **Louiza Moudoud.** *Biocrystallography Group, IRCCS San Raffaele Scientific Institute, Milan, Italy.*

Title: Thermal and Structural Characterization of Rv0678: Insights into Multidrug Resistance in Tuberculosis.

19.20 **Patrizio Di Micco.** *Institute of Molecular Biology and Pathology (IBPM-CNR), Rome, Italy.*

Title: Face2Face: A simple tool for macromolecule interfaces analysis.

19.25 **Gianmarco Pascarella.** *Institute of Molecular Biology and Pathology (IBPM-CNR), Rome, Italy.*

Title: Consensus3D. A comprehensive pipeline for accurate detection of conserved protein regions based on structure alignment programs consensus.

19.30 **Veronica Morea.** *Institute of Molecular Biology and Pathology (IBPM), National Research Council of Italy (CNR), Rome*

Title: Structure-based design of peptides for biomedical applications

Conclusions of Day I

19.40 *Aperitif & appetizers*

20.30 *Social Dinner @ Ristorante Pizzeria San Domenico, Piazza S. Domenico, 11, 50014 Fiesole FI, Italia (www.pizzeriasandomenico.it/)*

Friday, Feb 21st 2025

Morning Session I – Chair: Massimiliano Perduca

Drug development

9.00 Invited speaker: **Grzegorz Popowicz.** *Helmholtz Zentrum München – German Research Center*

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for Environmental Health (GmbH), Munich, Germany.

Title: From AI crystallographer to AI drug designer? Where advanced computational tools can help us understand molecules.

9.30 **Luisa Napolitano.** *Structural Biology Laboratory, Elettra Sincrotrone Trieste and Institute of Crystallography (IC-CNR), Trieste, Italy.*

Title: High Resolution Structure of StARD3 protein in complex with VS1 inhibitor.

9.50 **Elisa Fagnani.** *Institute of Biophysics (IBF-CNR), Milan, Italy.*

Title: Development of BIR1-targeting compounds for cancer treatment: study of IAPs modulation in NF-KB pathway.

10.10 **Andrea Dalle Vedove.** *AREA Science Park and Protein Targets for Drug Discovery Lab, Elettra-Sincrotrone Trieste, Italy.*

Title: What's new in Elettra's Structural Biology Laboratory.

10.30 **James Parry.** *Unchained Labs*

Title: Meet the Aunty - Queen of Protein Stability

10.40 *Coffee Break & Snacks*

Morning Session II – Chair: Silvia Onesti

Large macromolecular complexes by integrated structural biology

11.00 Invited speaker: **Philipp Sebastian Herdmann.** *Human Technopole, Milan, Italy.*
Title: Towards a Biopsy at the Nanoscale.

11.30 **Luca Mazzei.** *Department of Pharmacy and Biotechnology, University of Bologna, Italy.*
Title: Structural characterization of urease activity and inhibition: an integrated X-ray crystallography and cryo-EM study.

11.50 **Christian Buratto.** *Department of Chemical Sciences, University of Padua, Italy.*
Title: Ruthenium-based polyoxometalates as a possible chaperone in cryo-EM structure determination: a case study.

12.10 **Luca Broggin.** *Department of Biosciences, University of Milan, Italy.*
Title: Structural characterization of Atrial Natriuretic Peptide amyloid fibrils from Isolated Atrial Amyloidosis patients.

12.30 **Sofia De Felice.** *Department of Biology, University of Padua, Italy.*
Title: Structural and functional characterization of hyper-stable human serum albumin variants.



13.00 Announcement of the AIC Prizes for six oral young participants

13.15 Closing remarks & light lunch

Timing: Invited talks: 25 min. + 5 min. for discussion

Selected talks: 15 min. + 5 min. for discussion

Flash poster presentations: 5 min. Discussions over coffee breaks and in any other occasion.