1st Italian Crystallographic Association
Biological MacroMolecules Group Meeting
Scientific Program and Book of Abstracts

Centro Studi Ricerca e Formazione Cisl
Fiesole, 20-21 February 2020
Welcome to the 1st Italian Crystallographic Association – Biological MacroMolecules (AIC-BMM) Group Meeting

We are delighted to welcome you to Fiesole for the 1st Italian Crystallographic Association – Biological MacroMolecules Group Meeting.

This booklet contains the scientific program, the logistic information you may find useful for your stay at the Centro Studi Ricerca e Formazione Cisl and the collection of the received contributions.

We are grateful to Diego Gatta (AIC-President), for promoting and supporting this new 'intensive' format of AIC-Group Meeting.

We hope this “experiment” might become a reference for the Macromolecular Crystallography and Structural Biology scientific communities in Italy.

The junior researchers, PostDocs and PhD students will benefit from the significant opportunities for cultivating new collaborations and for advancing their professional career.

We thank Simona Galli (AIC- Treasurer) for her continuous assistance in the financial operations.

We kindly acknowledge BiKi Technologies Srl, Central European Research Infrastructure Consortium, ELETTRA-Sincrotrone Trieste, iXTAL Srl, and Molecular Horizon Srl for generously sponsoring this event.

Please do not hesitate to get in touch with the AIC-BMM Committee in case of special needs.

We wish you a scientifically profitable and pleasant stay in Fiesole!

The AIC-BMM Committee

Coordinator: Martino Bolognesi

Members: Rocco Caliandro, Doriano Lamba, Stefano Mangani
1st AIC-BMM Group Meeting - Scientific Program

Thursday, Feb 20th 2020

14:00–15:00  Participant registration and accommodation check-in
15:15–15:30  Welcome by AIC-BMM Committee

Afternoon Session I – Chair: M. Ferraroni (University of Firenze)

15:30–15:50  Gabriele Cruciani (University of Perugia & Molecular Horizon Srl)
PROTACs: from rational design to characterization and biological functions
15:50–16:10  Marco Patrone (IRCCS Ospedale San Raffaele, Milano)
Combinatorial allosteric modulation of agonist response in a self-interacting
G-protein coupled receptor
16:10–16:30  Elisa Costanzi (University of Padova)
Calmodulin binds to the STAS domain of SLC26A5 prestin with a calcium-
dependent, one-lobe, binding mode
16:30–16:50  Nicole Balasco (Institute of Biostructure and Bioimaging - CNR, Napoli)
The analysis of protein fine structure is a valuable tool for quality assessment

16:50–17:30  Coffee Break & Snacks

Afternoon Session II – Chair: R. Berisio (Institute of Biostructure and Bioimaging - CNR, Napoli)

17:30–17:50  Lucia Dello Iacono (GSK Vaccines, Siena)
X-ray structure of a Neisseria meningitidis serogroup A capsular polysaccharide
epitope
17:50–18:10  Maria Romano (Institute of Biostructure and Bioimaging - CNR, Napoli)
Structural basis for carbapenem resistance mediated by bacterial porins
18:10–18:30  Castrese Morrone (University of Piemonte Orientale, Novara)
Biochemical and structural studies on Mycobacterium tuberculosis DNA replication
and repair pathways
18:30–18:50  Matteo Mori (University of Milano)
Structural and biochemical investigations into the binding mode of furan-based
inhibitors of MbtI from M. tuberculosis

19:00–20:30  Aperitive & Buffet Dinner
**Evening Session** – *Chair: M. Mapelli (European Institute of Oncology IRCCS, Milano)*

20:30–20:50  **Davide M. Ferraris** (University of Piemonte Orientale, Novara & iXTAL Srl)
Bringing proteins into orbit: the opportunities of space research for protein science and structural biology

20:50–21:10  **Gabriele Giachin** (CIBIO - University of Trento)
Deflavination Prompts Transitioning from Fatty Acid Oxidation to Mitochondrial Complex I Assembly: Unveiling Amyloid Toxicity

21:10–21:30  **Antonio Chaves-Sanjuan** (University of Milano)
Structural based inhibition of the NF-Y transcription factor

21:30–21:50  **Daniele Santorelli** (University "La Sapienza", Roma)
Structural and biochemical characterization of the ribosome biogenesis factor RsgA from Pseudomonas aeruginosa

22:00–23:00  **AIC-BMM LOGO Vote Context, Open Discussions, Refreshing Senses & Memories**
Friday, Feb 21st 2020

Morning Session I – Chair: P. Storici (ELETTRA-Sincrotrone Trieste)

09:00–09:20 Walter Rocchia (Italian Institute of Technology, Genova & Biki Technologies Srl)
Molecular Dynamics-based Computational Solutions for Drug Design and Structural Biology

09:20–09:40 Alessandro Grinzato (University of Padova)
Effects of light on paired PSII supercomplex structural arrangement

09:40–10:00 Giusy Tassone (University of Siena)
Structural characterization of a synthetic mimic of the Photoactive Yellow Protein

10:00–10:20 Marta Semrau (ELETTRA-Sincrotrone Trieste & CIBIO - University of Trento)
Towards structural characterisation of ULK1 autophagy initiation complex and PTG/PP1 complex

10:20–11:00 Coffee Break & Snacks

Morning Session II – Chair: A. Di Matteo (Institute of Molecular Biology and Pathology-CNR, Roma)

11:00–11:20 Alejandra Angela Carriles Linares (IRCCS Ospedale San Raffaele, Milano)
Targeting BcRs: A Structural Approach To Personalized Treatments in Chronic Lymphocytic Leukemia

11:20–11:40 Davide Capelli (Institute of Crystallography-CNR, Roma)
Surface Plasmon Resonance as a tool for ligand binding investigation of engineered GPR17 receptor, a G protein coupled receptor involved in myelination

11:40–12:00 Annarita Fiorillo (University "La Sapienza", Roma)
Structure of PA4063, a zinc-binding protein from Pseudomonas aeruginosa

12:00–12:20 Luca Mazzei (University of Bologna)
Structural studies on the reactivity and inhibition of urease, a nickel-enzyme involved in human pathogenesis and environmental issues

12:20–12:40 Prizes & Awards, LOGO AIC-BMM – Chair: B. Vallone (University "La Sapienza", Roma)

12:40–13:00 Concluding remarks by the AIC-BMM Committee

13:00–14:00 Buffet Lunch

14:00 Farewell & Departure