

## NEWSLETTER n. 14, Giugno 2022



Cari Colleghi ed Amici della Sezione AIC-BMM,

vi proponiamo un aggiornamento sulle attività della Sezione dell'ultimo semestre.

Il 23 e 24 Maggio 2022 si è svolto il 3<sup>rd</sup> AIC-BMM Meeting finalmente in presenza. È stata adottata la formula consolidata di due mezze giornate intense, suddivise in cinque sessioni. Tutte le presentazioni sono state di altissima qualità e hanno stimolato il dibattito sugli aspetti più recenti della biologia strutturale. Una menzione speciale va ai giovani cristallografi, che hanno mostrato lavori esaustivi e rilevanti, dimostrando la vitalità della nostra sezione BMM. Un report della conferenza è allegato alla presente ed è disponibile, insieme al libro degli abstract, nel sito della nostra sezione (<https://cristallografia.org/en/biological-macromolecules-section/>).

Il sito web dell'AIC è stato recentemente rinnovato. La pagina della nostra sezione è ora raggiungibile dal menù a tendina in alto a destra, selezionando Association → AIC sessions and commissions → Biological Macromolecules Section. Il layout è cambiato, ma le informazioni sono pressoché inalterate. A destra della pagina troverete il riquadro relativo alle newsletters BMM.

I prossimi eventi di interesse per la sezione sono riportati nel seguito, in ordine cronologico:

- Scuola AIC a Trieste dal titolo "Protein structure models, biophysical data and high-performance computing for drug design" che si terrà in presenza dal 7 al 10 Settembre 2022. La scuola sarà di indubbio interesse per i giovani biocristallografi. Maggiori informazioni nel sito <http://school2022.cristallografia.org/>.

- Congresso AIC-SILS che si terrà in presenza a Trieste dal 12 al 15 Settembre 2022. Tutte le informazioni sono sul sito <https://eventi.mlib.ic.cnr.it/event/33/>. La scadenza per l'invio degli abstract è stata prorogata al 20 Giugno. Sottolineiamo la rilevanza dell'evento, sia per l'alto profilo scientifico del programma che per la possibilità di far interagire la comunità cristallografica con quella attiva nel campo delle sorgenti di radiazione. Segnaliamo in particolare i microsposi di diretto interesse per la comunità BMM:

MS-01 Modern Integrative Structural Biology

MS-09 Current Approaches in Structural Biology

*Il Coordinamento*

*Stefano Mangani*

*Rocco Caliendo*

*Andrea Ilari*

*Marina Mapelli*

## **ALLEGATO: Report del 3<sup>rd</sup> Meeting of the Biological Macromolecules Section**

The **3<sup>rd</sup> Meeting of the Biological Macromolecules Section** of the Italian Crystallographic Association was finally held as an in-person event, 23-24 May 2022, hosted by the beautiful location of the Centro Studi CISL in San Domenico, Florence (<http://www.congressi.unisi.it/aicbmm/>). The already established formula of a two-half days meeting divided in five sessions has been adopted. All presentations were of very high quality and stimulated debate over up-to-date aspects of structural biology. A special mention is due to the young scientists that showed important pieces of work, demonstrating the vitality of our BMM section.

**Monday, May 23, 2022**

### **Afternoon session I**

The first session of the 3<sup>rd</sup> AIC – BMM meeting was chaired by Giusy Tassone and was centered on the application of structural techniques to molecular aspects of pathogenesis. The first invited lecture was delivered by Mariarita Bertoldi, from the University of Verona, who presented an important study about human aromatic amino acid decarboxylase (AADC), responsible for the synthesis of the essential neurotransmitters dopamine and serotonin and its variants associated with AADC deficiency, a rare autosomal recessive disease that leads to neurotransmitter imbalance. The talk prompted a wide discussion pointing to the relevance of structural studies to understand the molecular aspects of disease.

The session continued with five selected talks given, in the order, by Cecile Exertier, from the Institute of Molecular Biology and Pathology (IMBP) – CNR, Rome; Stefano Morasso from the Protein Facility, Elettra Sincrotrone, Trieste; Annarita Fiorillo, from the Department of Biochemical Sciences, Sapienza University of Rome; Romualdo Troisi from the Department of Chemical Sciences, University of Naples Federico II; Lucia Dello Iacono – Biochemistry Function, GSK Vaccines, Siena.

The five speakers presented studies on different systems going from leishmanial, SARS-Cov2 proteins, DNA and vaccines, all having the common denominator of being directed towards the discovery of new treatments of important pathologies through the structural and biochemical characterization of the macromolecules involved.

### **Afternoon Session II**

The second session of the meeting was chaired by Adele Di Matteo from IMBP – CNR, Rome and consisted of four talks given, in the order, by Elisa Costanzi from the Center for Structural Studies Heinrich Heine - University of Düsseldorf; Simona Fermani from the Department of Chemistry G. Ciamician - University of Bologna; Francesca Troilo from IMBP – CNR, Rome and Cristina Visentin from the Department of Bioscience, University of Milan.

The presentations covered structural and biochemical characterization of proteins and enzymes from diverse organisms and aimed to different goals. From environmental remediation and potential industrial applications in the case of the alpha/beta hydrolase Pet46 presented by Costanzi and the characterization of the fungal 1,3- $\beta$ -transglucanase by Troilo, to a thorough interdisciplinary study about the molecular mechanism of the essential plant enzyme AB-GAPDH by Fermani and the study about modulation of the RidA proteins by specific mutations presented by Visentin.

The afternoon ended with an enjoyable “apericena” in the outside garden of the convention center where the attendees had to occasion to familiarize and further discuss scientific topics eased by some glasses of prosecco.

**Tuesday, May 24, 2022**

### **Morning session I**

The second day first morning session was chaired by Marina Mapelli from the European Institute of Oncology in Milan and started with the second invited lecture given by Enrico Ravera from the CERM center of the University of Florence.

Ravera, as a NMR expert, provided a stimulating talk about the complementarity of the different techniques: X-ray diffraction, Cryo-EM and NMR spectroscopy and about the advantages of an integrative approach to tackle complex biochemical systems. He also illustrated the possibility to couple X-ray data and NMR long-range structural information to achieve a better refinement of a protein structure.

The session continued with three talks given by Rocco Caliandro from the Institute of Crystallography, CNR, Bari, Marco Mazzorana from the Diamond Light Source, Didcot, UK and Annie Heroux from the Elettra Sincrotrone, Trieste. Caliandro presented results about an interdisciplinary study on the structure of Rituximab, a therapeutic monoclonal antibody targeting the CD20 protein, while Mazzorana and Heroux talks showed important improvements on data collection efficiency on their respective synchrotron sources. A final presentation was given by Alphatest, one of the Meeting sponsors showing the capabilities of Gating-Coupled Interferometry to provide accurate estimates of ligand binding affinity and protein kinetic parameters.

## **Morning Session II**

The final session was chaired by Luigi Scietti from the European Institute of Oncology who introduced six talks dedicated to protein-protein and protein-ligand interactions.

Cecilia Pozzi, from the University of Siena, presented new advances into the structure of the interface between human YAP and TEAD4 proteins that regulate the activity of the TEAD transcription factor.

Emanuele Fornasier from the University of Padova illustrated new inactive conformation of the SARS-CoV-2 Main Protease highlighting the relevance of the conformational variability presented by the enzyme both for its function and druggability.

Gianpiero Garau from the Istituto Italiano di Tecnologia in Pisa talked about the caveats of using virtual predictions of membrane protein structures as exemplified by the case of the FAAH and NAPE-PLD proteins whose structures conflict with the computational results.

Lorenzo Antonelli from the IMBP-CNR in Rome talked about a project for repositioning FDA-approved drugs as agonists of the sigma-1 receptor present in human central nervous system (CNS).

Marta Semrau from the Protein Facility of the Elettra Sincrotrone in Trieste presented the first crystal structures of essential proteins from the CNS, namely the complexes between of the CBM21 domain of human protein targeting for glycogen (PTG) and  $\beta$ -cyclodextrin, the whole Protein Phosphatase 1 (PP1)-PTG holoenzyme and PP1 in complex with PTG N-terminal peptide.

The final lecture was given by Dorian Lamba from the Institute of Crystallography, Trieste Outstation who provided a thorough overview of nerve growth factor (NGF) activity and of its precursor proNGF and presented stimulating new results about the role of small molecules like ATP, carbohydrates and lipids in regulating the neurotrophin factors activity.

The Meeting was concluded by the announcement by the Scientific Committee of the three prizes given to the best presentations by young crystallographers consisting in 100 € and a certificate. The prizes were awarded to:

Cecile Exertier

Emanuele Fornasier

Francesca Troilo.

A final remark about the extremely good quality of the presented scientific work was done by the Committee, with the wish to meet again next year with intact will to pursue excellence in our science.