# **Proposed Microsymposia**

#### 1) Membrane proteins: from monomeric proteins to super-assemblies and in situ studies.

**Proposed Chair: Beatrice Vallone** <u>beatrice.vallone@uniroma1.it</u> (Department of Biochemistry Science "A. Rossi Fanelli" Sapienza University of Rome)

The last decade has seen an increase in deposition of membrane proteins (150000 structures and about 1500 unique structures). This is opening new avenues in the understanding of physiopathology and in drug design. The "in situ" analysis by cryo-tomographic methods is likely to unveil the molecular determinants of complex biological phenomena. The microsymposium will aim at presenting some of the most relevant and recent advancements in membrane protein structural biology at different levels of complexity also attempting to select cases that involve methodological innovations of interest for the bio-structure community.

#### 2) Crystallographic structures versus AlphaFold models

**Proposed Chair: Luigi Vitagliano** <u>luigi.vitagliano@cnr.it</u> (Institute of Biostructures and Bioimaging CNR Naples)

Protein structure prediction based on machine learning is revolutionizing structure biology. Although these approaches very frequently provide accurate three-dimensional models, in some cases, significant discrepancies with the experimental structures have been detected. In this scenario, the micro-symposium aims at highlighting differences between newly determined structures and the corresponding predicted models to clarify the limitations of these innovative approaches and to suggest possible interventions needed to improved them.

## 3) SAXS applied to structural biology

## Proposed chair: Dritan Siliqi dritan.siliqi@ic.cnr.it (Institute of Crystallography CNR Bari)

This microsymposium is focused on the present progress of SAXS, which has become an essential tool to structurally characterize biomolecules in solution, as well as in response to variations in external conditions (temperature, pH, salinity, ligands).

- methods and/or software on SAXS

- novel experimental setup at the synchrotrons SAXS beamlines

- SAXS applied on the protein/complex structure determination

- combination of SAXS with other techniques like : crystallography, Cryo-EM and, Molecular Dynamic simulations and ab-initio modelling (especially with AlphaFold),

## 4) Mineral sciences for sustainable development

**Proposed chairs: Allan Pring** allan.pring@flinders.edu.au (Flinders University, Australia); **Carlotta Giacobbe** carlotta.giacobbe@esrf.fr (ESRF, France)

The proposed microsymposium aims at gathering persons who are using approaches based on the structural knowledge of minerals and related materials to find new methods (or to improve present expertise) when dealing with problems related to pollution, public health, sustainable resources, waste disposal, recycling of materials, CO2 capture and any other issue relevant to sustainable development.

# Plenary

Title: A divisive affair: the structural biology of chromosome partition in eukaryote

Andrea Musacchio <u>andrea.musacchio@mpi-dortmund.mpg.de</u> Max-Planck Institute of Molecular Physiology Dept. of Mechanistic Cell Biology, Germany

## Keynotes

**Title** Multidisciplinary approach for the study of the proteins involved in the molecular mechanism of a rare disease such as Schwachman Diamond Syndrome

Dritan Siliqi dritan.siliqi@ic.cnr.it Institute of Crystallography CNR Bari, Italy

Title: Non-covalent interactions in cyclic peptoids: macrocycle conformation and solid state assembly

**Consiglia Tedesco** <u>ctedesco@unisa.it</u> Department of Chemistry and Biology University of Salerno, Italy

**Title:** Innovative approach for a classic target: fragment screening on trypanothione reductase reveals new opportunities for drug design

Andrea Ilari andrea.ilari@cnr.it Institute of Molecular Biology and Pathology CNR Rome, Italy

Title: Les liaisons dangereuses: structural analysis of B-cell receptor self-recognition in leukaemias

Massimo Degano degano.massimo@hsr.it Ospedale San Raffaele – Milano, Italy

**Title:** Integrative structural biology studies of trans-synaptic contacts between mammalian photoreceptors and bipolar cells

**Federico Forneris** <u>federico.forneris@unipv.it</u> Department of Biology and Biotechnology University of Pavia, Pavia, Italy