

WORKSHOP

Integrating BIOSAXS and High-Performance Computing: Advancements in Structural Biology and Nanoscience

Dates: April 2–4, 2025

Location: Villa Romanazzi Carducci – Bari

Chairs: Dr. Cinzia Giannini and Dr. Dritan Siliqi

April 2nd

13:00 – 13:15 **Participants arrival**

13:15 – 13:50 **Institutional greetings**

13:50 – 14:00 **Workshop Introduction**
Dr. C. Giannini & Dr. D. Siliqi

14:00 – 18:00 **Contributions from Guest Speakers**

14:00 – 14:45 **Dr. Thibaud Stoll**, Excelsus Structural Solutions (Swiss) AG, Villigen, Switzerland
Title: Exploring the Power of SAXS for the Advanced Characterization of Biopharmaceuticals

14:45 – 15:30 **Dr. Helio Cesar Nogueira Tolentino**, Heterogeneous and Hierarchical Matter Division, Brazilian Synchrotron Light Laboratory, Campinas, Brazil
Title: SIRIUS Synchrotron Beamlines: New Tools to Investigate Heterogeneous and Biological Materials

15:30 - 16:00 **Coffee Break**

16:00 – 17:15 **Dr. Nuria Sanchez Puig**, Department of Biomacromolecular Chemistry, Institute of Chemistry, UNAM, Mexico City, Mexico
Title: Exploring the Conformational Dynamics of the SBDS and EFL1 Proteins: Understanding the Molecular Mechanisms in Shwachman-Diamond Syndrome

17:15 – 18:00 **Dr. Abril Gijbbers Alejandro**, Department of Biochemistry, Faculty of Medicine, UNAM, Mexico City, Mexico
Title: Shedding light on ESX-1 substrates: An integrated structural approach to the mycobacterial secretion system

19:00 **Welcome cocktail**

April 3rd

09:00 – 13:00 **Session 1: BIOSAXS a valid and powerful technique for Structural Biology and Nanoscience**

Chair Dr. Cinzia Giannini

09:00 – 09:40 **Prof. Ulf Olsson**, Division of Physical Chemistry, Lund, Sweden

Title: Chaperone protein self-assembly and suppression of amyloid formation

09:40 – 10:20 **Dr. Nathan Cowieson**, BioSAXS beamline B21. Diamond Light Source Ltd, UK

Title: SAXS in the context of a structural biology project

10:20 – 11:00 **Dr. Narayanan Theyencheri**, European Synchrotron Radiation Facility, Grenoble, France

Title: Advances in SAXS methods for probing the structure and dynamics with fourth generation synchrotron sources

11:00 - 11:30 **Coffee break**

11:30 – 12:10 **Dr. Cy Jeffries**, EMBL c/o DESY, Hamburg, Germany

Title: The Small Angle Scattering Biological Data Bank – SASBDB

12:10 – 12:30 **Dr. Gemma Newby**, Xenocs, Grenoble, France

Title: SAXS WAXS – Xenocs, Your Access To The Nanoscale In The Lab

12:30 – 14:00 **Lunch break**

14:00 – 18:00 **Session2: Hight Performance Computing (HPC) applied on Structural Biology and Drug Design**

Chair Dr. Dritan Siliqi

14:00 – 14:40 **Dr. Eugene Krissinel**, Research Complex at Harwell (RCaH), Oxon, UK

Title: CCP4: From Legacy to the Cloud – A High-Throughput Evolution

- 14:40 – 15:20** **Dr. Johannes Schwab**, MRC Laboratory of Molecular Biology, Cambridge, UK
Title: Estimating molecular motions from cryo-EM images with DynaMight
- 15:20 - 16:00** **Dr. Milot Mirdita**, Steinegger Lab, Seoul National University, Seoul, South Korea
Title: Protein Analysis in the AlphaFold Era
- 16:00 – 16:30** **Coffee break**
- 16:30 – 17:10** **Dr. Alessandra Magistrato**, Istituto Officina dei Materiali (IOM) – SISSA, Trieste
Title: Exploring Biomolecular Mechanisms through All-Atom Simulations: from RNA Metabolism to Metal Ion Transport
- 17:10 – 17:50** **Prof. Alexander Varnek**, UNISTRA Laboratory of Chemoinformatics, University of Strasbourg, Strasbourg, France
Title: Chemography approach to (ultra)big chemical space analysis
- 20:00** **Social dinner**

April 4th

Visit to IC laboratories
Guided tour

Scientific Committee

Dr. Cinzia Giannini
Dr. Dritan Siliqi
Dr. Michele Saviano
Dr. Giancarlo Tria
Dr. Giuseppe Felice Mangiatordi
Dr. Teresa Sibillano
Dr. Davide Altamura
Dr. Liberato De Caro

Organizing Committee

Dr. Francesco Scattarella
Dr. Domenico Alberga
Dr. Vincenzo Mangini
Dr. Daniela Malerba
Sig. Rocco Lassandro
Dr. Francesco Baldassarre
Dr. Erika Manicone

Workshop Secretary

Dr. Caterina Chiarella
Dr. Brunella Maria Aresta
Dr. Giovanni Filograsso
Dr. Lucrezia Cassano