Oral presentation

Structural Biology at Elettra Sincrotrone – the present and the future

Raghurama P Hegde¹, Nicola Demitri¹, Maurizio Polentarutti¹, Giorgio Bais¹, Paola Storici¹, Silvia Onesti¹, Michele Cianci², Lisa Vaccari¹, Annie Heroux³, B Gopal⁴, D D Sarma⁴, Giorgio Paolucci¹

¹ Elettra-Sincrotrone Trieste S.C.p.A. Strada Statale 14 - km 163,5, 34149 Basovizza, Trieste Italy, ²Department of Agricultural, Food and Environmental Sciences, Università Politecnica delle Marche, Via Brecce Bianche, 60131 Ancona, Italy, ³Former Elettra- Sincrotrone Trieste S.C.p.A. Strada Statale 14 - km 163,5, 34149 Basovizza, Trieste Italy, ⁴Indian Institute of Science, CV Raman Rd, Bengaluru, Karnataka 560012, India

sengaturu, Kurnataka 500012, Inat

raghurama.hegde@elettra.eu

Elettra Sincrotrone Trieste is a multidisciplinary research center, based on a third generation source, for materials and life sciences and includes 28 beamlines. Among those XRD2 is dedicated to high throughput <u>macromolecular crystallography</u> (MX) experiments; it has been in operation since 2018, and it caters to the structural biology community worldwide, operating in partnership with Department of Science and Technology/Indian Institute of Science, India. The beamline has a native beam size of ~100 μ m x 300 μ m with apertures to reduce the beam size at the crystal, a large tuneable energy range for SAD/MAD experiments (8 to 20 keV), automated sample mounting in cryogenic environment and a DECTRIS PILATUS 6M area detector. On site and remote access for data collection, as well as monitoring and automatic data analysis pipelines are in place. The post processing pipeline enables users to quickly analyse data from protein-ligand complexes which could be a useful tool for structure-based drug design. Project proposals can be submitted through the year and are evaluated monthly, to ensure a fast allocation mechanism, with typical scheduling times of one to two weeks.

The structural biology laboratory at Elettra comprises research groups working on the structural analysis of protein-nucleic acid interactions and protein targets for drug discovery. Protein production, characterization and crystallization facilities, which have been recently empowered, complements the beamline operations, providing a complete structural biology workflow at Elettra.

A major upgrade to Elettra, Elettra 2.0, envisages an upgrade to the entire structural biology platform at Elettra. The MX beamline, to be housed at a new location and to be christened μ XRD, will feature an in vacuum undulator source providing a beam size at the sample of ~5 μ m x 5 μ m expandable up to 50 μ m x 50 μ m, an energy range of 5-17 keV, a flux of ~ 8 x 10¹² ph/s at Se K edge, coupled with a fast detector. The high flux with a microfocus beam would provide opportunities for working with small crystals and will open the door for new data collection methods such as serial crystallography. In parallel, the structural biology laboratory will be upgraded with new crystallization robots, protein purification and characterization facilities within the framework of the NextGeneration EU project (PNRR funds) PRP@CERIC, coordinated by Area Science Park.

A brand new cryo-EM facility is being set up in collaboration with Istituto Officina dei Materiali (IOM) of the National Research Council of Italy (Consiglio Nazionale delle Ricerche, CNR), funded by PRP@CERIC and will offer access to users. A tight integration between the cryo-EM centre, the laboratory facilities and the beamline will provide a more complete platform for structural biologists from all over the world.