BioMAX & FragMAX: Trends and developments at a 4th generation Macromolecular Crystallography Beamline

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Keywords: Macromolecular Crystallography, Beamline, fragment screening

The MAX IV laboratory operates two Macromolecular Crystallography (MX) beamlines, namely BioMAX and MicroMAX. BioMAX is a highly versatile beamline that became operational in 2017. It offers beam sizes ranging from 20 x 5 μm^2 FWHM (focused) to 100 x 100 μm^2 (defocused) with a maximum photon flux of 7 x 10^{12} photons/s and energies between 6 and 24 keV. The experimental hutch contains an MD3 microdiffractometer, an IRELEC Isara sample changer, and a 16M Eiger detector. The beamline is easily operated with the MXCuBE data acquisition software and offers a wide range of experiments, including fully remote data collection at cryogenic temperatures, collection of small crystals with large unit cells, experimental phasing, and state-of-the-art synchrotron serial crystallography (SSX) setups. In addition, all collected data sets are immediately processed by multiple auto-processing pipelines, and the results and metadata are stored in the ISPyB/EXI laboratory information management system [1].

BioMAX is able to collect almost 500 datasets per day and this exceptional throughput has prompted the development of the FragMAX platform for crystal-based fragment screening [2]. The platform consists of three primary components: (i) a crystal preparation facility, (ii) *automated* diffraction data collection at the BioMAX beamline, and (iii) FragMAXapp, an intuitive web application for large-scale data processing [3]. The crystal preparation facility is co-located with the Lund Protein Production Platform (LP3) and offers a comprehensive set of tools for protein crystallization, fragment libraries, pucks and pins, automated crystal soaking, and robot-assisted crystal mounting.

BioMAX and FragMAX are accessible via the MAX IV user program, the MAX IV Industrial Relations Office (IRO), and the iNEXT Discovery program. Both are continuously evolving and will soon include in-situ data collection, remote data collection for room temperature experiments, new sample delivery instruments, and software tools for accelerated structure refinement and deposition.

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