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The FragMAX facility for structure-based drug discovery at MAX IV Laboratory

The FragMAX facility supports structure-based drug and chemical tool compound discovery at MAX IV Laboratory. It was designed as a platform for crystal-based fragment screening, but the underlying workflows are applicable to all medium- to large-scale protein-ligand studies. The platform is comprised of three primary elements: (i) a medium-throughput crystal preparation facility, (ii) diffraction data collection at the BioMAX beamline, and (iii) FragMAXapp, an intuitive web-based tool for large-scale data processing. In 2019, the FragMAX platform began providing services to external users and has since established an international user program that is accessible to academic and industrial research organizations. Access can be requested through the MAX IV user program, the MAX IV Industrial Relations Office and iNEXT Discovery.

The FragMAX crystal preparation facility is co-located with the Lund Protein Production Platform (LP3) and provides the complete set of instruments for protein crystallization and crystal optimization. In addition, it offers workflows that include liquid handling systems for automated crystal soaking and robot-assisted crystal mounting. The facility provides free access to multiple fragment libraries, including the in-house developed FragMAXlib, and allows users to send their own compound collections or screening sets. FragMAX personnel can help with sample preparation, and users are also welcome on-site. Data collection is performed at the BioMAX beamline which offers a high-intensity X-ray beam, fast and reliable sample changer (464 crystals), state-of-the-art X-ray detector (Eiger 16M) and, as of spring 2023, fully unattended operation. All steps of the experiment, from crystal preparation to structure refinement, are recorded in a transferable database system. In addition, FragMAX provides several freely accessible tools for accelerated structure modeling and refinement as well as PDB deposition support. FragMAX provides customized experiments and a modular experimental design, allowing users of varying levels of expertise to routinely obtain actionable screening hits for their targets. All workflows are continuously evolving, and we intend to increase cooperation with other Swedish research infrastructures in the future.

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