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Keywords: X-ray Source, Diamond, Instrument Development

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Integrated crystallographic services at EMBL-Hamburg

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EMBL Hamburg is operating three beamlines (P12 for small-angle X-ray scattering ‘SAXS’, P13 and P14 for macromolecular crystallography ‘MX’) on the PETRA III storage ring at DESY (Hamburg, Germany). The beamlines are embedded in the Integrated Facility for Structural Biology which - in addition to the X-ray experiments on the beamlines - offers facilities and services for sample preparation and characterization and for data analysis.

By using the highly brilliant X-ray beam produced by PETRA III, beamlines P13 and P14 enable X-ray diffraction experiments on the most challenging crystals:

- small (< 100 μm^3) crystals can be exploited using micro-focused X-ray beams and serial crystallography strategies
- optimum data can be extracted from large crystals with a highly parallel large beam.
- phasing is facilitated by a high photon flux at low X-ray energies
- diffraction from large unit cells (> 1000 Å) can be resolved
- data from fragile crystals can be collected *in situ* in CrystalDirect™ plates
- For pump-probe experiments, a dedicated endstation is under construction on P14.

For less challenging cases, a highly automated and integrated environment is in place for high-throughput data collection.

The Sample Preparation and Characterization facility (SPC) provides an entry point for protein samples which still need to be tested and prepared for use in SAXS and/or MX. A suite of biophysical protocols is available to evaluate the suitability of user-supplied samples; preparative techniques can then be applied to optimize samples for crystallization. For crystallization, high-end equipment is in place that can be accessed remotely via the web-based CRIMS system. A CrystalDirect system has been installed for automated crystal harvesting and a dedicated derivative lab is available for users for derivatization experiments.

Various modes of access are available (For details, please visit: www.embl-hamburg.de):

- competitive: P13 / 14
- collaborative: P13 / P14
- EU-supported (iNext): P13 / P14 / SPC
- fee for service (academic / industrial): P13 / P14 / SPC

We will describe the user-accessible facilities, examples of projects ‘from protein to structure’, experimental highlights, and the available access modes.

Keywords: beam lines, micro crystallography, integrated facility