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The High Throughput Macromolecular Crystallography beamline P11 at PETRA III

The P11 beamline at PETRA III (DESY, Hamburg) is a versatile instrument dedicated to High Throughput Macromolecular Crystallography [1], which provides variable focus sizes (from 200 x 200 to 5 x 10 μ m2) in an energy range from 6 to 28 keV with a maximum of 1013 ph/s.

Since 2021, an EIGER2 X 16M detector is permanently installed at the beamline, which significantly reduced the data collection time. The beamline is equipped with an automated sample changer (dewar capacity of 23 unipucks ie 368 samples) with a "mounting and un-mounting" cycle of 36s. The total time per sample (including sample changing and full data collection) is less than 2 minutes.

In 2023, we will change our data acquisition software to MXCuBE. The integration to ISPyB, for tracking shipments, importing the sample details to MXCuBE and data archiving, is under progress. The establishment of parallel autoprocessing pipelines in addition to the current one based on XDSAPP [2] and the implementation of strategy calculation including dose estimation are on going. These software developments are synchronizing P11 with the EMBL PETRA III beamlines for MX (P13 and P14) for the future foundation of a uniform structural biology village at PETRA IV.

Serial crystallography can be performed at P11 either with standard mounts or with the TapeDrive [3] developed at the CFEL, specially suited for time resolved experiments using the mix and diffuse method. Real-time processing of serial data using CrystFEL [4] has been recently implemented. The pipeline can successfully perform peak searching, indexation and integration in real time at the maximum data acquisition speed (133Hz).

- 1. Burkhardt A., et al., Status of the crystallography beamlines at PETRA III. Eur. Phys. J. Plus 131, 56 (2016)
- 2. Sparta K.M., et al., XDSAPP2.0. J. Appl. Cryst. 49, 1085-1092 (2016)
- 3. Zielinski K.A., et al., Rapid and efficient room-temperature serial synchrotron crystallography using the CFEL TapeDrive. IUCr J., 9, 778-791 (2022)
- 4. White T. A., et al., Recent developments in CrystFEL. J. Appl. Cryst., 49, 680-689 (2016)

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