

How MXPress workflows use automated decision-making to get the best possible data from your samples

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Abstract

Complex workflows have been developed for the ESRF MX beamlines that are designed to extract the best possible data from all samples. In order to remove manual intervention in the most repetitive steps of structural biology projects, initial screening and data collection, a fully automatic system has been developed to mount, locate, centre to the optimal diffraction volume, characterize and, if possible, collect data from multiple cryocooled crystals. Using a fast X-ray-based routine, samples are located and centred systematically at the position of highest diffraction signal and important parameters for sample characterization, such as flux, beam size and crystal volume, are automatically taken into account, ensuring the calculation of optimal data-collection strategies. The workflows use the information gathered during characterization to optimise the most complex data collection strategies; this includes adapting the beam diameter dynamically to match the diffraction volume within the crystal and collecting multi-wedge data sets at different orientations to maximise completeness with low symmetry space groups. Complex multi-position and multi-crystal data collections have now also been integrated into the selection of experiments available. This has led to increased data quality and throughput, allowing even the most challenging samples to be treated automatically.