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MX3: A new macromolecular crystallography beamline at the Australian Synchrotron

The High-Performance Macromolecular Crystallography beamline (MX3) will be capable of providing high-flux, microfocus X-rays for small and weakly diffracting protein crystals. The beamline has an energy range from 10-15 keV with beam sizes at sample from 2x2 to 40x40 microns with flux up to 1.3e14 ph/s (at 13 keV). The beamline will provide three modes of data collection: goniometer (standard pin-mounted experiments), serial crystallography (fixed target and injector), and in-tray collection. The optical design allows users to rapidly change beam size by a combination of a secondary source aperture and compound refractive lenses.

The major endstation components are comprised of an Eiger2 XE 16M detector (Dectris), an ISARA sample changing robot (Irelec), and a MD3-up diffractometer (Arinax). This allows for data collection in excess of 500 Hz via the Dectris Stream2 interface, rapid automated pin and tray exchange, and automated pin centering with a sub-micron sphere of confusion.

A high degree of automation will support unattended data collection of entire projects. Given a set of expected outcomes, all samples attached to an experiment can go through screening, data collection and merging without user interaction. Results are entered in a database for easy comparisons across multiple experiments.

In-tray screening and in-tray data collection are related but separate. In-tray screening will be achieved through a program aimed at synchrotron users and non-users alike. “Tray Tuesdays” will set aside beamtime for automated screening and evaluation of plate wells. The ScreenShot user interface developed in-house will serve as a portal for sending trays and evaluating the results. Early X-ray diffraction screening of crystalline material can direct researchers’ efforts towards the most promising conditions, guiding optimisation and minimising wasted synchrotron time.

In-tray data collection in contrast, aims to collect entire datasets without harvesting of crystals. This will be performed at room temperature and will merge data from multiple crystals to form a complete dataset. While screening can be done with most standard tray types, colleting full datasets requires special low-background trays that are commercially available.

Primary authors: Dr ERIKSSON, Daniel (Australian Synchrotron - ANSTO); Dr CARADOC-DAVIES, Tom (Australian Synchrotron - ANSTO); Mr BARROW, Graham (Australian Synchrotron - ANSTO); Dr CAIN, Nicole (Australian Synchrotron - ANSTO); Dr CAMPBELL, Eleanor (Australian Synchrotron - ANSTO); Dr CHEN, Simin (Australian Synchrotron - ANSTO); Mr CHERUKUVADA, Hima (Australian Synchrotron); Dr HERNANDEZ VIVANCO, Francisco (Australian Synchrotron - ANSTO); Mr KHEMARAM, Rakesh (Australian Synchrotron - ANSTO); Mr OLDFIELD, Jacob (Australian Synchrotron - ANSTO); Mr QUINTON, Joe (Australian Synchrotron - ANSTO)

Presenter: Dr ERIKSSON, Daniel (Australian Synchrotron - ANSTO)