

TOWARDS FULL AUTOMATION AT THE CANADIAN MACROMOLECULAR CRYSTALLOGRAPHY FACILITY

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The Canadian Macromolecular Crystallography Facility (CMCF) which serves more than 60 protein crystallographers located across Canada consists of two beamlines [1]. The first, an insertion device beamline (08ID-1) is capable of satisfying the requirements of the most challenging and diverse crystallographic experiments, *i.e.* physically small crystals with large unit cell dimensions. The second, the 08B1 bending magnet beamline is being constructed and has been designed for high-throughput data collection, capable of being accessed remotely.

The primary method of access to CMCF beamlines will be remotely via the CA•Net research network. In what is commonly referred to in the field as 'Mail-in Crystallography', scientists will be able to send prefrozen crystals to the facility and be able to setup experimental parameters as well as inspect, evaluate and download their data from their home laboratories via the internet. To facilitate remote access the SAM robots [2] are being built for both beamlines (Fig. 1). The robot is used in combination with Universal Puck (Uni-Puck), a single sample holding cassette standard among facilities in North America. With the Uni-Puck, the robot can hold 192 samples, sufficient for a shift of screening and data collection.

Features of the final software will include automatic alignment and configuration of the beamline hardware, automatic crystal mounting and centering of crystals in

the X-ray beam, automatic measurement of fluorescence spectra for MAD experiments, automatic screening and analysis of crystals in order to assess crystal quality and determine optimum parameters and strategies for data collection, automatic data collection and data processing. Centering of the crystals, automatic performance of MAD experiments and automatic data processing from raw images to processed reflection files, including automated indexing, space group selection, integration and file format conversion with minimal user's input has been implemented at the 08ID-1 beamline (Fig. 2). All software development is focused on the XDS package [3] however other popular data processing software is also available at the beamlines (HKL2000, CCP4).

References

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Figure 1. SAM robot at the CMCF.

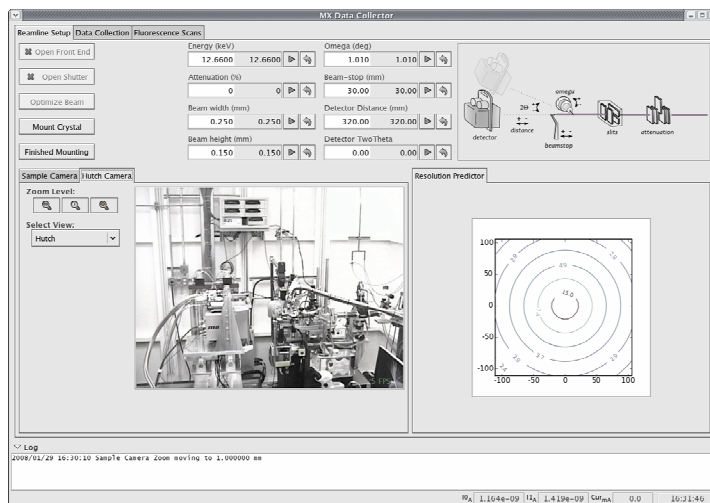


Figure 2. CMCF Users' software.