

Poster Presentation

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MxDC & MxLIVE: Software for Macromolecular Crystallography Experiments at the CLS

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The Canadian Macromolecular Crystallography Facility (CMCF) is a suite of two beamlines 08ID-1 and 08B1-1. Beamline 08B1-1 is a bending-magnet beamline for high-throughput macromolecular crystallography enabling Multiple-Wavelength Anomalous Dispersion (MAD) and Single-Wavelength Anomalous Dispersion (SAD) experiments with a high level of automation. We have developed an integrated software system with modules for beamline control, experiment management, and automated data processing for both on-side and remote users. The experiment management module, also known as MxLIVE (Macromolecular Crystallography Laboratory Information Virtual Environment) is responsible for managing the storage of information about samples, sample shipments, experiment requests, experiment results and data sets. It provides a web-based interface for users to submit sample information and experiment requests, track shipments en route to the CLS and review experiment results and data sets as they are completed on site, and for beamline staff to manage Mail-In data acquisition sessions, reducing the need for user travel to the synchrotron. The beamline control module includes a user-friendly interface for data collection, MxDC (Macromolecular Crystallography Data Collector). MxDC is fully integrated with beamline hardware as well as software applications such as MxLIVE and AutoProcess, an innovative data processing pipeline. This makes MxDC a hub for all experiment-focused activities at CMCF beamlines, including sample auto-mounting, centering and screening crystals, diffraction experiments, and automated data reduction.

Keywords: data collection software, macromolecular crystallography, laboratory information management