Poster Presentation

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AutoProcess:Automated strategy calculation, data processing & structure solution

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Two critical aspect of macromolecular crystallography experiments are (1) Determining the optimal parameters and strategy for collecting good quality data and (2) Optimal processing of the collected data to obtain to facilitate structure determination. These tasks can be daunting to inexperienced crystallographers and often lead to inefficiencies as valuable beam-time is used up. To support automation, remote access and high-throughput crystallography, we have developed a software system for automation of all data processing tasks required at the synchrotron. AutoProcess, is layered on the XDS data processing package and makes use of other utilities such as BEST from the European Molecular Biology Laboratory (EMBL), CCP4 utilities and SHELX. The software can be used from the command line as a standalone application but can also be run as a service on a high-performance computing cluster, and integrated into beamline control and information management systems such as MxDC and MxLIVE to allows users to determine the optimal strategy for data collection, and/or process full datasets with the click of a button. Users are presented with a graphical data processing report as well as reflection output files in popular formats automatically. For small molecule and peptide structures, an unrefined initial structure with an electron density map is automatically generated using only the raw diffraction images and the chemical composition of the molecule. Future developments will include sub-structure solution for MAD/SAD/SIRAS data. The software is freely available under an open-source license from the authors. The Canadian Light Source is supported by the Natural Sciences and Engineering Research Council of Canada, the National Research Council Canada, the Canadian Institutes of Health Research, the Province of Saskatchewan, Western Economic Diversification Canada, and the University of Saskatchewan.

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