

Automated data collection at the Swiss Light Source macromolecular crystallography beamlines

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Crystallographic fragment screening, which involves screening small-molecule libraries against crystals of a target protein, is an essential tool in modern drug discovery. The technique relies on the high-throughput generation of cryo-cooled, soaked crystals followed by fast and efficient data collection at a synchrotron beamline. Each campaign may generate hundreds or thousands of samples, and the most efficient strategy for acquiring data is to use unattended data collection followed by automatic data processing.

The macromolecular crystallography (MX) group at the Swiss Light Source operates a fast fragment and compound screening (FFCS) pipeline that uses Smart Digital User (SDU) software to collect data at the beamlines. This presentation will give an overview of SDU, describe how it has been implemented at the MX beamlines and present some recent case studies.

Safety Mount	ALC	DMF	DMSO	Dewar Loc.	Puck ID	Sample #	Prefix	Folder	Priority	# mounts	Comments
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141	👍	👍	👍	👍	A1	CPS-1109 3	0026264_1_1109d	SLS_15-06-20200606hca0026264_1_1109d	3	1	

Figure 1. Screenshot of SDU in action at beamline X06SA

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