

Towards an automated data collection pipeline

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We are implementing a flexible “pipeline” at the Advanced Light Source allowing the beamline user to automatically collect and process data from dozens of crystals. Components include a robotic mounter to repeatedly transfer cryocooled samples to the goniometer, a database to remotely track high volumes of information, and a facility to autocenter the crystal loop in the beam. Scripted tools orchestrate data collection and reduction. Unattended, the system screens up to 112 crystals, acquiring diffraction snapshots to rank the crystals by quality, and determining the crystal symmetry and optimal collection strategy. It will be possible to collect full MAD/SAD datasets on the best crystals from the initial screen. The pipeline is suitable for either individual users or large-scale structural genomics efforts.