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Automated Crystal Screening at the Advanced Light Source

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ABSTRACT

We have implemented a macromolecular crystal screening environment at the Advanced Light Source allowing the beamline user to assess the diffraction quality automatically from dozens of samples. This assessment enables the user to collect full datasets on the best crystals from the initial screen. Oscillation images are analyzed in real time to determine the feasibility of autoindexing. Bragg reflections are chosen with the program DISTL (Z. Zhang & A. Deacon, SSRL), and autoindexing is accomplished with the new LABELIT package. Crystals are ranked with a quality score that includes factors such as resolution limit, mosaicity, and residual fit. Plans for the future include a script to determine the optimal data collection strategy for the sample, and automated collection and analysis of full datasets once the strategy is decided upon.

Components of the system include a robotic mounter to repeatedly transfer cryocooled samples to the goniometer, a database to track high volumes of information, a facility to autocenter the crystal loop in the beam, and a graphical user interface (Fig. 1) to orchestrate the entire process. Minimal input is required, as the process is automatically handled using scripted tools. Unattended, the system can screen up to 112 crystals. The prototype is installed on branchlines 5.0.1, 5.0.2, and 5.0.3 of the ALS, and is suitable for either individual users or large-scale structural genomics efforts.

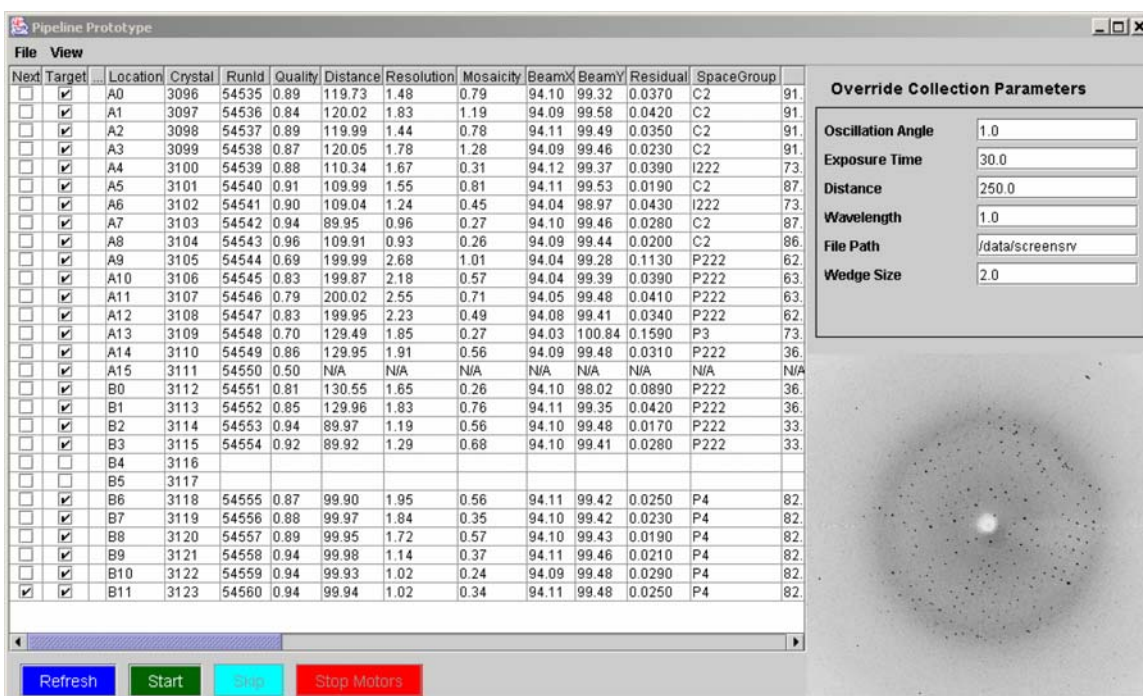


Fig. 1. Java-based GUI for controlling the automated screen.