

Poster Presentation

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Automated High-Throughput Data Collection at IMCA-CAT

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The Industrial Macromolecular Crystallography Association Collaborative Access Team (IMCA-CAT) operates a data collection facility at the Advanced Photon Source for protein crystallography. IMCA-CAT meets the demands of IMCA member pharmaceutical companies for reliable, high-quality, high-throughput data collection, while ensuring a secure environment for proprietary research. The 17ID micro-focused high-flux insertion device beamline, equipped with a Pilatus 6M pixel array detector, allows for very fast data collection times. The focused beam size (30 μm x 70 μm) can be easily optimized for each sample using a GM/CA-CAT mini-beam quad collimator, with user-selectable beam sizes of 50, 20, 10 and 5 μm . An Alio goniometer has a small (1.2 μm) sphere of confusion, providing stable sample positioning, and X-ray beam position is maintained within 2 μm by custom software in real time. Automated sample mounting is performed with a Rigaku ACTOR robot, accepting both Rigaku and ALS/Unipuck style magazines, providing fast yet reliable sample exchanges and enabling remote access and unattended data collection. Rigaku JDirector software for robot control and data collection has been customized to incorporate additional tools, such as diffraction-based sample centering for both manual and unattended data collection modes, vector data collection and inverse beam anomalous data collection. While targeting the needs of industrial research, the automation and rapid data collection times at 17ID are also ideally suited for structural genomics and other research efforts requiring high-throughput experiments. Access is available to interested researchers through the APS General User Program and through subscription memberships for those needing regular and guaranteed proprietary beamtime.

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