IMCA-CAT Advanced Photon Source Facility for Structure-Based Drug Discovery. Anne M. Mulichak, Kevin P. Battaile, Joe Digilio, Erica Duguid, J. Lewis Muir, Eric Zoellner and Lisa J. Keefe. IMCA-CAT/Hauptman-Woodward Medical Research Institute @Advanced Photon Source, Argonne, IL.

The Industrial Macromolecular Crystallography Association Collaborative Access Team operates a macromolecular crystallography facility at Sector 17 of the Advanced Photon Source that serves the needs of the IMCA member pharmaceutical companies for guaranteed, high-throughput, high-quality diffraction data in support of structure-based drug design, while assuring the security of proprietary research. The 17ID micro-focused high-flux insertion device beamline is equipped with a Pilatus 6M pixel array detector, and a mini-beam quad collimator allows user-selectable beam sizes down to 5 microns for each sample. An Alio goniometer has a small 1.2 micron sphere of confusion, providing stable sample positioning, and the X-ray beam position is maintained by real-time positional feedback within 2 microns. These features, along with flexible diffraction rastering and vector data collection capabilities, enable experiments with very small crystals and other challenging systems. Automated sample mounting is performed with a highly reliable Rigaku ACTOR robot which is compatible with both Rigaku and ALS/Unipuck style magazines, enabling remote access and unattended data collection. Mail-in service is the predominant access mode for IMCA members, utilizing fully automated data collection for routine systems, as well as manual collection by experienced staff for more challenging samples. The mail-in model allows the most efficient and flexible use of beamtime, with most samples examined within one day of arrival. Puck bar coding integrated with custom software protocols ensure the security and confidentiality of proprietary experiments. Beamtime at IMCA-CAT is available to outside industrial users via subscription agreements and to academic users via the APS General User Program.