

The Independent Investigator Program at the IMCA-CAT 17-ID Beamline at the APS

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The Industrial Macromolecular Crystallography Association Collaborative Access Team (IMCA-CAT) operates an experimental facility for macromolecular crystallography at the Advanced Photon Source (APS) at Argonne National Laboratory. Comprising Illinois Institute of Technology (IIT) staff and IMCA member companies, the CAT is committed to providing a high-throughput and highly reliable facility for macromolecular crystallographic data collection and processing. Currently, IMCA is fully subscribed at twelve memberships, representing ten pharmaceutical companies: Abbott Laboratories, Bristol-Myers Squibb, Eli Lilly, GlaxoSmithKline, Merck, Pfizer, Pharmacia, Procter & Gamble, Schering-Plough, and 3-Dimensional Pharmaceuticals. Research programs include *de novo* protein structures, structures of protein-ligand complexes, and crystallographic methods development.

Located at sector 17 at the APS, the IMCA-CAT facility includes an insertion device beamline, a bending magnet beamline, computing resources, and a biochemistry laboratory with a cold room. The bending magnet beamline, 17-BM, is approaching the end of its commissioning phase, whereas the insertion device beamline, 17-ID, is fully operational and accommodating researchers through the Independent Investigator Program. The insertion device beamline is fully tunable in the energy range of 6.5 keV to 14.8 keV and the x-ray beam is focused in the vertical direction. The experiment end station is equipped with a Mar 16.5 cm CCD detector mounted on a Mar goniostat, an Oxford Cryosystems cryostream cooler for maintaining the sample crystal at a temperature of 100 Kelvin, and a Bicron fluorescence detector. User-friendly, GUI-driven software enables full user control to change energy and align the x-ray beam, measure absorption edges from energy scans and subsequently calculate the anomalous scattering factors, f' and f'' , for heavy atoms in the sample, and collect and process experimental diffraction data. Thus, the facility is fully suited to performing multiwavelength

anomalous diffraction (MAD) experiments, single-wavelength anomalous diffraction (SAD) experiments, single isomorphous replacement with anomalous scattering (SIRAS) experiments, or conventional isomorphous replacement, molecular replacement, and difference fourier experiments.

The IMCA-CAT facility satisfies the demands of the IMCA member companies to perform macromolecular crystallography experiments in a high-throughput mode for drug discovery and product development. This also makes the IMCA-CAT facility suitable to structural genomics efforts. In collaboration with the Center for Advanced Research and Biotechnology, IMCA-CAT is engaged in the large-scale structure determination of proteins of unknown function from the *Haemophilus influenzae* genome.¹ Researchers are invited to submit proposals to our Independent Investigator Program for the insertion device beamline.

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Reference

¹ E. Eisenstein, G.L. Gilliland, O. Herzberg, J. Moulton, J. Orban, R.J. Poljak, L. Banerjee, D. Richardson, and A.J. Howard, *Curr. Opin. Biotech.* **11**, 25-30 (2000).