

ADVANCED PHOTON SOURCE

Mail-in PX for General Users at SGX-CAT



The SGX-CAT control room at APS sector 31.

Greyhounds of both the canine and vehicular varieties serve as apt metaphors for the SGX collaborative access team (CAT) beamline at sector 31 of the Argonne Advanced Photon Source (APS). Like the elegant greyhounds themselves, the SGX-CAT mail-in protein crystallography (PX) program is designed for maximum speed and efficiency. And like the famed catch-phrase for the cross-continental U.S. bus company—Greyhound Lines, Inc.—the SGX-CAT byword for mail-in PX by both general users and strategic partners is, “Leave the driving to us.” The beamline staff prides itself on providing the best possible x-ray diffraction data to its user community. The SGX-CAT facility was constructed and is operated by SGX Pharmaceuticals, Inc., located in San Diego, California. From the outset of operations, SGX-CAT has functioned as a 100% mail-in protein crystallography facility. This approach has resulted in the development of unique tools for automated sample handling, data collection, and information management. While total automation may prove elusive, SGX-CAT is currently at 90% hands-off sample handling and data collection. The last piece of the beamline’s automation, a robot for changing sample carousels, is now in its final testing phase.

The automation focuses on three main components: sample placement, sample evaluation, and information manage-

ment. SGX-CAT-developed software for automatic sample centering was brought on line in February 2005, and has to date been used for over 20,000 crystals. Crystal-evaluation software, which has looked at more than 14,000 samples to date, is in general superior to humans for this task. Data collection throughput has been equally impressive, with more than 4,000 datasets measured annually. In a 2004 time study, SGX-CAT on average required approximately 13 minutes to screen each crystal. Most of this time was devoted to evaluation of the quality of diffraction, rather than to mounting the crystal and acquiring the diffraction images. This cycle time is now down to an average of four minutes per sample.

Information management, which is the glue that holds the SGX-CAT system together, is accomplished using an Oracle® database. A Web-based interface to the database is updated automatically every 15 minutes and tracks some 40 pieces of information about each crystalline sample from time of arrival at SGX-CAT to return of data (screening images from each crystal and raw data-collection images) to the user. The system links related samples and, based on the results of automated sample evaluation, identifies (highlighted on the display by a color code) superior samples as optimal candidates for data collection, helping the beamline staff to make correct decisions rapidly. All information about crystals is linked to the actual crystals through bar-codes on the samples (SGX-CAT supplies the bar codes), ensuring the highest accuracy in data entry and sample tracking.

Because its automation tools give users the greatest likelihood of success in data collection, SGX-CAT has developed a strong level of trust between beamline staff and users (both general users and strategic partners). The benefits of these tools, which were initially developed for proprietary use of SGX-CAT by the company, are now available to general users, who can access up to 25% of the beam time available at SGX-CAT.

Prospective general users wishing to avail themselves of the SGX-CAT mail-in crystallography program must first submit a proposal to the Advanced Photon Source, following the process detailed at http://www.aps.anl.gov/Users/Scientific_Access/General_User/index.html. A PDF file detailing the SGX-CAT “Express Crystallography General User Program” can be downloaded from <http://www.sgxcata.com>.

CALL FOR PROPOSALS

At the Advanced Photon Source, our door is open to experimenters from all scientific disciplines whose research requires the highest brilliance hard x-ray beams in the Western Hemisphere.

General-user proposals for beam time during Run 2008-1 are due by November 2, 2007.

Information on access to beam time at the APS is at http://www.aps.anl.gov/user/beamtime/get_beam.html or contact Dr. Dennis Mills, DMM@aps.anl.gov, 630/252-5680.

Argonne is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC

The Advanced Photon Source is funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences