

Workshop Report:

High Throughput Screening/Macromolecular Crystallography

Workshop held in conjunction with SSRL 31st Annual Users' Meeting, October 20, 2004

A High Throughput Screening/Macromolecular Crystallography workshop was held on October 20, 2004 in conjunction with the Annual SSRL Users' Meeting. The aim of the workshop was to provide the participants with an overview of the latest developments at SSRL involving the Stanford Automated Sample Mounting (SAM) robot, crystal screening software, and new options for data backup and data analysis.

The workshop was divided in two sessions. The first session focused on the SAM system while the second session covered new developments in computing facilities and software. Each session was followed by an open discussion and anonymous voting on the importance of points raised by both the SSRL staff and users.

In the first session, Paul Ellis (SSRL) talked about the SAM robot and summarized the improvements carried out on the system after the last user run. The system was very reliable during the 2004 run, with a system failure rate of about 3 in 1,000 samples. Aina Cohen (SSRL, workshop co-organizer) followed with instructions on sample preparation for use with the SAM system. She described how to flash freeze the samples, and also how to transfer them from cryovials and ALS pucks into cassettes avoiding ice formation using new tools designed for this purpose. Dan Harrington (SSRL) talked about how to store the sample information in a spreadsheet and how to import this information into the Crystal Screening data base either through a web browser or using a new option in the **Blu-Ice** data acquisition software screening tab. He finished by explaining how to prepare the cassettes for shipping to SSRL. Robert Thorne (Cornell University) described the development of the Micromount, a new Kapton-based tool for mounting crystals. He explained the advantages over nylon loops: less liquid around the crystal improves the cooling rate and decreases the scattering background; reproducible shape and size provides a good match to the sample size and makes it easier to center by automated algorithms.

The second session was opened by Ana González (SSRL, workshop co-organizer). She introduced **WebIce**, a new web-based tool for image analysis, autoindexing and strategy calculation. In the future, this tool will provide a portal to all SSRL macromolecular crystallography resources including data collection. She gave an interactive tutorial to illustrate the usage of the current version. Thomas Eriksson (SSRL) gave an overview of the computer environment, with an emphasis on the description of new facilities: Linux computers to replace SGI Octanes at the beam lines, development on a new Linux based desktop for remote access to the SSRL computers, and new DVD and Fire Wire options for data backup.

Follow-up discussions indicated that a high priority should be given to developing a system to robustly rank the diffraction quality of samples and to store the results together with other user-supplied sample information. Standardization across synchrotrons is also a largely shared concern. Although increased automation is welcomed by the users, they wish to be able to override automated decisions; this requirement will be considered in future software developments at SSRL.

The organizers thank the DOE Office of Biological and Environmental Research, and the National Institutes of Health, National Center for Research Resources' Biomedical Technology Program, and the National Institute of General Medical Science for supporting the well-received workshop.

Ana González and Aina Cohen
SSRL
Menlo Park, CA

