BEAMLINE SCIENTIST:
Pawel Grochulski
pawel.grochulski@lightsource.ca
306-657-3538

BEAMLINE LEADER:
Mirek Cygler
mirek@BRI.NRC.CA
514-496-6321

SCIENCE ASSOCIATE:
James Gorin
james.gorin@lightsource.ca
306-657-3776

RESEARCH ASSOCIATE
Shaun Labiuk
shaun.labiuk@lightsource.ca
306-657-3541

Canadian Macromolecular Crystallography Facility 08ID-1 Beamline

Pawel Grochulski (1, 2)
(1) Canadian Light Source
(2) College of Pharmacy and Nutrition, University of Saskatchewan

Beamline Overview

Status	Operational-accepting proposals
Source	Small-gap in-vacuum undulator
Monochromator Mirror	DCM, Si(111) cryo-cooled first crystal and sagittally bent second 1.1 m ULE with 3 stripes
Spectral range	6.0 – 18.0 keV (2.07 – 0.69 Å)
Measured flux @12 keV	>1 x 10^{12} ph/s (100 mA)
Flux density @12 keV	> 1 x 10^{14} ph/s/mm^2 (100 mA)
Beam crossfire at the sample @12keV (FWHM)	0.9 mrad x 0.2 mrad
Measured focal spot size at 12 keV (FWHM)	170 µm x 50 µm (H x V)

Figure 1: A geographical distribution of the CMCF Users in 2009.

Introduction

The CMCF 08ID-1 beamline is serving protein crystallographers as a primary beamline designed for small crystals and crystals with large cell dimensions. Together with CMCF 08B1-1, which is designed to be fully automated, both beamlines constitute the Canadian Macromolecular Crystallography Facility.

The 2009 activity period saw an increase in the user community to 30 laboratories across the country and 4 from the US (Figure 1). The 08ID-1 beamline was open to general users by the peer review process on August 1, 2009. During the last year. purchased access reached 4.5% of total available beamtime and mail-in crystallography accounted for 4.5%. The deposition of protein structures originating from the 08ID-1 beamline in the Protein Data Bank increased to fifty-five compared to fifteen at the end of the last activity period. The 2009 activity period resulted in 20 high impact publications in which data were collected at the 08ID-1 beamline.

Science

The Canadian Macromolecular Crystallography Facility facilitates high-resolution structural studies of macromolecules. The data obtained at the CMCF 08ID-1 beamline are used to model detailed three dimensional structures of macromolecules which are used to increase understanding of the structural basis of basic biology and biochemistry, to develop and improve the design of ligands that bind to macromolecules in order to use these ligands as pharmaceuticals, and to develop a basis for modifying the structures of macromolecules themselves in order to alter their functions.

Instrumentation and Software

During the 2009 activity period, several improvements were made to the beamline hardware and software to enable more productive operation. The Stanford automounter (SAM) has been installed in the experimental hutch and it is being tested (Figure 2). Its full implementation will allow remote access to the beamline in 2010. The robot accepts universal pucks as well as SSRL cassettes and can hold up to 192 samples.

In order to implement remote access to the beamline, software development is as important as the development of hardware and they both need to be done at the same time. Part of this is development of an interactive GUI for data collection, called MXDC. It has been in development for several years and is now fully tested and implemented at the beamline.

The automatic data processing software, Autoprocess, is being developed using primarily the XDS [1] package, with POINTLESS [2] and BEST [3] also used. The goal of this development is to collect and process data without human intervention. The system has been tested and debugged on almost all data collected at the 08ID-1 beamline either by the users or by the staff. Some users chose to use different packages such as HKL2000 [4] or MOSFLM [5] which are also available at the beamline.

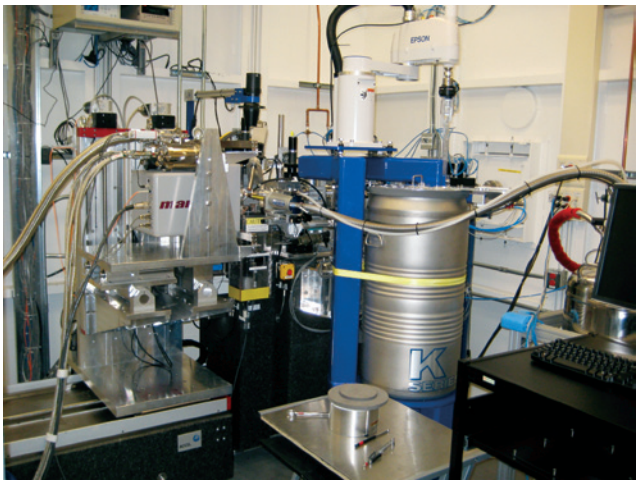

Figure 2: The SAM robot installed in the 08ID-1 end-station.

Performance

To reduce scattering from slits and air a pinhole was introduced which is located in the nozzle just before the sample and it collimates the beam in combination with a 170 µm x 50 µm focus. So far 100µm and 200 µm pinholes were tested. Significant decrease in the background noise was observed as well as increase in the signal to noise level using the 100 µm pinhole. These very encouraging results will allow introduction of the 'mini-beam" apparatus together with the upgrade of the crystal visualization system in 2010. The aim is to obtain a beam size of 50 µm or less with flux of more than 10^{11} ph/sec.

Conclusion

The last year was very productive for the CMCF community. The peer review system was introduced; the community has grown to 34 laboratories in Canada and the US. Beamtime used by commercial access reached 4.5 % of available beamtime and the mail-crystallography has grown to 4.5% of available beamtime. The SAM automounter was installed and is being tested. Finally, the number of publications in 2009 reached 20.

CMCF Beamline Team

Name	Institution	Role
Mirek Cygler	BRI/NRC	Leader
Natalie Strynadka	University of British Columbia	08B1-1 Leader
Mark Glover	U of Alberta	Member
Brian Mark	U of Manitoba	Member
Pawel Grochulski	CLSI/ U of Saskatchewan	Member
Bart Hazes	U of Alberta	Member
Stanley Moore	U of Saskatchewan	Member
Emil Pai	U of Toronto	Member
James Rini	U of Toronto	Member
Joe Schrag	BRI/NRC	Member
Michel Fodje	CLSI	Member

Associated Staff

Name	Role
Russ Berg	Lead Controls Software Engineer
Peter Thorpe	Lead Mechanical Engineer
Shawn Carriere	Mechanical Engineer, Robotics
Gillian Black	Software Engineer

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