11:00 Invited oral

Status and the future of structural biology at the Canadian Light Source

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The Canadian Macromolecular Crystallography Facility (CMCF) together with the Biological X-ray Absorption Spectroscopy (BioXAS) facility form a suite of beamlines allowing Canadian researchers to conduct cutting edge research in structural biology at the Canadian Light Source (CLS). The CLS is a 2.9 GeV national synchrotron radiation facility located at the University of Saskatchewan in Saskatoon. The CMCF consists of 08ID-1 and 08B1-1 beamlines and it provides service to more than 60 Principal Investigators in Canada and the United States [1]. Up to 25% of the beam time is devoted to commercial users and the general user program is guaranteed up to 55% of the useful beam time and is run under a peer-review proposal system. The CMCF staff provides "Mail-In" crystallography service to the users with the highest scored proposals. Beamlines are equipped with very robust end-stations including on-axis visualization systems and Rayonix 300 CCD series detectors. They are each complemented with a Stanford automounter (SAM) allowing remote control of the beamlines. *MxDC*, an in-house developed beamline control system, is integrated with a data processing module, *AutoProcess*, allowing full automation of data collection and data processing with minimal human intervention [2]. It also allows remote control of experiments through interaction with a Laboratory Information Management System (LIMS) that was developed at the facility. The number of scientific papers for which data were collected at the 08ID-1 beamline exceeds 70 at present, and the number of PDB entries exceeds 160 structures.

X-ray spectroscopy (XAS) contributes to structural biology in two ways. It can provide information on species for which crystal structures are not available and it can also provide supplemental information on systems for which crystal structures are available. Since about 30% of the human genome is made up of genes encoding metalloproteins, XAS, but in particular the extended X-ray absorption fine structure (EXAFS), is extremely useful to study the geometry of the metal's vicinity within a radius of 5 Å. Its major strength is that very accurate values for bond lengths can be obtained, typically to better than ± 0.02 Å, which is comparable to accuracies obtained for small-molecule structures. These values are about ten times more accurate than those obtained from a typical protein crystallography experiment at a moderate resolution [3]. In EXAFS experiments multiple scattering (MS) occurs when multiple atoms backscatter photoelectrons. In this case, interference between the different backscattered waves can make the EXAFS sensitive to the relative arrangement of the atoms including some information on bond angles. Therefore the CMCF 08B1-1 beamline has been recently equipped with a four-element solid state detector, VORTEX-ME4, to perform EXAFS studies on protein crystals. Additionally, the BioXAS facility has been designed and is being built. It will be composed of two beamlines allowing the study of biological and health-related metals. These are important in diseases such as Alzheimer's, environmental toxins, in metal-containing drugs, and as essential constituents of living systems.

1. Grochulski, P., Fodje, M.N., Gorin, J., Labiuk, S.L., and Berg, R. (2011) 08ID-1Beamline, the Prime Beamline at the Canadian Macromolecular Crystallography Facility. *J. Appl. Cryst*. In press.
2. Fodje, M. N., Berg, R., Black, G., Grochulski, P., & Janzen, K. (2010). Automation of the Macromolecular Crystallography Beamlines at the Canadian Light Source. *PCaPAC*, (pp. 130-132). Saskatoon.
3. DePristo, M.A., de Bakker, P.I.W. and Blundell, T.L. (2004) Heterogeneity and Inaccuracy in Protein Structures Solved by X-ray Crystallography. *Structure***12**, 831–838.