s1.m2.o1 **Automation of Macromolecular Crystallography Data Collection at the ESRF**. Joanne McCarthy, *European Synchrotron Radiation Facility (ESRF), France. E-mail: mccarthy@esrf.fr*

**Keywords: Automation; Macromolecular Crystallography; Synchrotron Beamlines**

Macromolecular crystallography has proven to be the most effective method of determining the structures of biological macromolecules. Each year thousands of data collections that form the basis for such structure determinations are carried out at the ESRF. To cope with this high demand, it is essential to maximise beamline efficiency and to simplify beamline control procedures. The ESRF, in collaboration with the EMBL Grenoble Outstation, are therefore automating much of the crystallographic experiment which may be divided into two parts : beamline and crystal alignment, and data collection and processing.

Recent progress in automatic crystal mounting and centering [1], crystal characterisation [2], absorption edge scanning and automated alignment procedures for the beamline optical elements will be described, as will the development of databases designed to aid the automation process.

[1] S. Cusack et al, *Nat. Struct. Biol*. (1998) **5** 634 - 637
[2] A.G.W. Leslie et al, *Acta Cryst*. (2002) D**58**, 1924-1928

s1.m2.o2 **Automated Crystal Screening for High-throughput X-ray Crystallography at Stanford Synchrotron Radiation Laboratory**. Ashley M. Deacon, Aina E. Cohen, Paul J. Ellis, Scott McPhillips, Timothy M. McPhillips, Mitchell D. Miller, R. Paul Phizackerley, Jinhu Song, S. Michael Soltis, Irina Tsyba, Henry van den Bedem, Guenter Wolf and Zepu Zhang, *Stanford Synchrotron Radiation Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA, USA. E-mail: adeacon@slac.stanford.edu*

**Keywords: Structural Genomics; High-Throughput; Robotics**

The Joint Center for Structural Genomics (JCSG) has developed a high-throughput structure determination pipeline capable of processing many protein targets in parallel. The protein production and crystallization facilities, at the Crystallomics Core of the JCSG, are capable of generating a large number of crystals. A key step in the subsequent structure determination process is to evaluate the diffraction properties of each crystal, select the best ones for full data collection and provide sufficient feedback to guide further crystallization trials. The Structure Determination Core of the JCSG and the Macromolecular Crystallography group at Stanford Synchrotron Radiation Laboratory have developed an automated crystal screening facility, comprising the Stanford Auto-Mounter (SAM) [1], integrated within the BLU-ICE data collection environment [2]. A compact cassette is used for shipping and storing up to 96 crystals, mounted on regular Hampton-style pins. Three of these cassettes can be loaded in a dispensing dewar on the beam line at any time. A 4-axis industrial pick-and-place robot is capable of mounting any of these crystals onto the goniometer. The crystal is automatically aligned with the X-ray beam. Diffraction images are collected at several crystal orientations, before the crystal is returned to its storage cassette and the next crystal is mounted. A computer program, DISTL, has been developed to evaluate the diffraction images, identify the most promising ones in terms of diffraction resolution and spot quality and provide a reliable set of diffraction spots for use by standard auto-indexing programs. One hundred crystals can be screened in approximately 5 hours of beam time. The system has been used by the JCSG to screen over 5000 crystals from more than 300 different proteins. Recently, the screening system has been installed on all the protein crystallography beam lines at SSRL, where it is now available to the general user community.

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[1] McPhillips, T. M., McPhillips, S. E., Chiu, H. J., Cohen, A. E., Deacon, A. M., Ellis, P. J., Garman, E., Gonzalez, A., Sauter, N. K., Phizackerley, R. P., Soltis, S. M., Kuhn, P., *J. Synch. Rad.* (2002) **9**, 401-406.
[2] Cohen, A. E., Ellis, P. J., Miller, M. D., Deacon, A. M., Phizackerley, R. P., *J. Appl. Cryst.* (2002). **35**, 720-726.