MS02 P01

Embedding the ESRF into the High-Throughput Gene-to-Structure Pipeline Joanne McCarthy[a] [a]*European Synchrotron Radiation Facility (ESRF), Grenoble, France.* E-mail: mccarthy@esrf.fr

Keywords: macromolecular crystallography; high-throughput; automation

Macromolecular crystallography (MX) is the most effective method of determining the high resolution structures of biological macromolecules. Each year many thousands of data collections that form the basis for such structure determinations are carried out at the ESRF. The nature of these data collections at synchrotron-based MX facilities is, in routine cases, rather repetitive. Indeed, it has become something of a cliché to describe the process of macromolecular crystal structure determination as a pipeline which can be broken down into a series of discrete steps with the completion of one step triggering the start of the next. At the ESRF these have been automated and linked together to produce a fully automatic data collection pipeline (DCP), a prototype of which is available on all the ESRF MX end-stations. The DCP begins with the scanning of the unique 2D datamatrices on SPINE standard sample holders contained in the SC3 sample changer robot [1]. These unique identifiers provide a means of tracking individual samples through the pipeline. For a set of samples chosen (up to 50), the DCP then carries out automatic screening, characterisation and ranking of crystal quality using the DNA software [2, 3, http://www.dna.ac.uk]. For the best or most appropriate samples, automatic collection, integration and scaling of data can then be carried out via the DCP. Results are stored in, and are accessible via, the ISPyB database (http://ispyb.esrf.fr) which allows the two-way communication of information between users' home labs and the ESRF beam-lines and has paved the way for remote access experiments.

[1] Cipriani, F. *et al*, *Acta Cryst.* 2006, *D***62**, 1251.
[2] Leslie, A. *et al*, *Acta Cryst.* 2002 *D***58**, 1924.
[3] Popov, A. N. and Bourenkov, G. P. *Acta Cryst.* 2003, *D***59**, 1145.

MS02 P02

Gene Composer, a Gene and Expression Construct Design Project Management Tool Peter Nollert, John Walchli, Mark Mixon, Alex Burgin. *Emerald BioSystems, Bainbridge Island, WA, USA*
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Keywords: whole gene synthesis, expression construct design, software

With the goal of improving success rates for eukaryotic protein expression and crystallization, we are developing Gene Composer software to facilitate the information-rich design of protein constructs, their respective nucleic acid coding sequences and expression vectors. The Protein Design Module distills protein structure information from PDB files and comparative sequence information into an interactive alignment viewer. This graphical user interface allows the researcher to simultaneously visualize sequence conservation in the context of known protein secondary structure, ligand contacts, water contacts, crystal contacts, B-factors, solvent accessible area, residue property type and several other property views. The Gene Design Module automates the back-translation of a protein amino acid sequence into a codon-optimized nucleic acid sequence, which can be handed off to be synthesized. The Construct Design Module allows the user to define termini, make insertions or deletions, change residues, add tags, define cloning sites and finally permute those constructs and virtually clone them into one or multiple expression vectors of choice. Using this procedure, Gene Composer will generate all primers and mutagenic oligonucleotides necessary to perform all corresponding wet-lab procedures. We will present each of the Gene Composer modules and a detailed protocol for PCR-based gene synthesis from designed oligonucleotides.

MS02 P03

The Matrix Maker: A Liquid Handling Robot for High-Throughput Protein Crystallization Peter Nollert, Laurelin Ward, Natalie Duncan, Lance Stewart, Mark Mixon. *Emerald BioSystems, Bainbridge Island, WA, USA*
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Keywords: high-throughput optimization, crystallization reagents, formulation

The Matrix Maker liquid handling robot has been developed to produce primary and secondary reagent matrices for protein crystallization. Controlled via customized database software, the Matrix Maker assists in the design of any formulation matrix and dispenses matrices from stock solutions. The system consists of positive displacement pumps capable of dispensing any formulation from up to 60 simultaneous stock solutions. Solutions can be dispensed into virtually any kind of vessel, from tubes to multichamber plates. Interchangeable pumps allow accurate dispensing of volumes from 10 ul to 50 ml. In its original application of making solutions for protein crystallization screening, the Matrix Maker allows a substantial reduction in liquid handling time compared with manual solution preparation. Formulation accuracy is still maintained, as shown by pH measurements and protein crystallization results. The performance and ease-of-use of the Matrix Maker make this instrument an essential component in modern high-throughput protein crystallization laboratories.

MS02 P04

Mail-in data collection at SPring-8 protein crystallography beamlines Nobuo Okazaki[a], Kazuya Hasegawa[a], Go Ueno[b], Hironomi Murakami[b], Masaki Yamamoto[a, b], [a]*SPring-8/JASRI,* [b]*RIKEN SPring-8 Center*
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Keywords: mail-in data collection, remote operation, web based application

The mail-in data collection system at SPring-8 makes it possible that distant users collect diffraction data without visiting SPring-8. The mail-in users only send samples to SPring-8 via home-delivery services as the first step. Then they can request measurement conditions and check results at their laboratory on the Web. The data collection for delivered samples are carried out with the automated beamline operation system using sample auto-changer