

Poster Sessions

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CrysAlis^{Pro}, the software for controlling data collection and data reduction Agilent's single crystal X-ray diffractometers, contains easy to use features for variable temperature and variable wavelength studies.

The results presented here show how the many multi-temperature experiments identify a clear phase transition of a spin crossover compound during the ramping. The Cryojet (manufactured by Oxford Instruments) was used to study the compound at 5° intervals and controlled to within ±0.1° from room temperature to 100K.

An example of the variable temperature software is shown in the figure below.



Temperature	Slit	Sample	Heater	On/Off	Auto Vent	Motor
295.0	5.0	7.0	ON	YES	YES	YES
292.0	5.0	7.0	ON	YES	YES	YES
289.0	5.0	7.0	ON	YES	YES	YES
286.0	7.0	9.0	ON	YES	YES	YES
283.0	5.0	7.0	ON	YES	YES	YES

During the poster session, further information and a demo of the software will be available.

Keywords: Variable Temperature, Small Molecule, CrysAlisPro

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I04-1, a fixed wavelength protein crystallography station in its first year of operations

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Diamond Light Source is the third generation synchrotron light source in the UK, producing an electron beam energy of 3 GeV aiming at a beam current of 300 mA. Four macromolecular crystallography (MX) beamlines I02, I03, I04 and I24, tunable in the energy range of 5 to 25 keV, are already operational and I23, the long wavelength MX beamline is in design stage.

I04-1, the last phase II macromolecular crystallography beamline, entered its user operation program at the beginning of April 2010 and is fully operational since April 2011. The beamline was designed to be highly reliable and the very stable beam is producing high quality data with structures starting to be deposited in the protein databank (PDB). The experimental end-station is equipped with the MD2 diffractometer and a single-photon counting Pilatus 2M detector, running at 30Hz, which allows high throughput data collection and features such as fast grid and helical X-ray scanning of the samples. In combination with the CATS sample changer robot, an average of ten datasets per hour can be routinely achieved. Further developments of the robot involve speeding

up the exchange process and *in-situ* plate screening capability. A set of software pipelines ranging from data collection strategy, diffraction image visualization, streamlined data processing, structure solution and difference map calculation is in place to meet the high throughput needs of academic and industrial researchers studying ligand binding. Finally, with the wavelength fixed to 0.92 Å (bromine K-edge), selenium (Se-) and bromine (Br-) single anomalous diffraction (SAD) experiments were also successfully performed.

Keywords: high_throughput_crystallography, Pilatus_2M, SAD_experiment

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In-situ Crystallisation Screening and Data Collection on Microfocus Beamline I24

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Despite significant progress in high-throughput methods within macromolecular crystallography, the production of diffraction quality crystals remains a major bottleneck. Effort in a crystallization trial can be guided with feedback on the nature and quality of early crystallisation 'hits'. Using a dedicated goniometer installed on the Diamond beamline I24, crystals can be studied directly in their crystallization plates. Valuable time is saved and manual intervention minimised with the removal of the requirement to loop and freeze samples individually. The intense and flexible microfocus beam of I24 allows weakly diffracting samples, such as membrane proteins and complexes, to be assessed with maximal signal-to-noise against the background scatter from the plate medium. In combination with novel methods in data merging, we demonstrate the ability to solve structures entirely *in-situ*, illustrating the potential of the technique to facilitate the sequence to structure pipeline.

Keywords: crystallization, screening, microbeam

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Rapid shutterless data acquisition with a frame transfer CCD

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For CCD detectors, the speed of synchrotron single crystal data acquisition is usually limited by the readout time of the detector and the mechanical synchronization of shutter with rotation motor. To avoid these complexities and obtain faster data collection rates we have tried using a shutterless acquisition with continuous rotation of the crystal. This method is already used with Pilatus detectors and we have developed a version for a frame transfer CCD camera [1] at beamline ID11 at the ESRF. In this mode the camera reads out one image of x-ray data while the next is exposed. The frame transfer is a rapid image shift (4.2 ms) which switches buffers to allow the process to continue. During the continuous rotation fast electronic hardware is used to record the angular encoder positions and times when frame transfers begin and end. Our Frelon2K [1] camera can provide up to 26 images per second at full resolution with 1024x2048 pixels in this mode, and