SPACE [1] and beamline control software BSS [2]. For smooth communication with distant users via the Internet, we have newly developed the data management system D-Cha (Database for Crystallography with Home-lab Arrangements) which mediates between the users and SPring-8 beamlines. D-Cha provides the GUI for users to deposit the experimental conditions for samples and to browse / download the collected data on web browser.
The mail-in system has been developed and operated for Structural Genomics Project at RIKEN Structural Genomics II (BL26B2) since September 2005. Then the system has been presented for public users at Structural Biology III (BL38B1) since December 2005 and at RIKEN Structural Genomics I (BL26B1) since December 2006. At BL26B1 and BL26B2, mail-in system has been operated on a daily basis. In addition, the commercial mail-in service has just started in July 2006, as the joint project among JASRI, RIKEN and analysis service companies. The mail-in data collection is our first step of remote beamline access at SPring-8. The next step is to achieve the fully remote control data collection based on the mail-in system.

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MS02 P05

Recent advances in the Crank automated structure solution suite Navraj S. Pannu, Pavol Skubak, Irakli Sikharulidze, Jan Pieter Abrahams, Rudolf A.G. de Graaff. *Biophysical Structural Chemistry, Leiden University, Leiden, The Netherlands.*
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Keywords: automated structure solution, MAD, SAD

For its first release, the CRANK system was shown to effectively detect anomalous scatterers and phase SAD data [1]. Since then, CRANK's speed and robustness has improved, building many structures automatically for SAD, SIRAS, MAD and MAD + native data [2].
One improvement involves using Luzzati parameters refined in the program BP3 to validate the quality and completeness of a substructure obtained. This has proven to be effective and reliable in identifying correct solutions that do not meet the figure of merit levels reported in substructure detection programs necessary to safely assume that a correct solution was found. Thus, this allows for an early termination of substructure detection.
To improve automated model building, an interface to ARP/wARP and REFMAC has been added to also include SAD data directly in model refinement. The multivariate SAD likelihood function, implemented in a modified version of REFMAC has been shown to extend the resolution and phase quality limits required for automated model building with iterative refinement [3]. Recently, the new refinement target was shown to be very effective in combination with the SHELX[C/D/E] pipeline available in CRANK.
The above and other advances are in the latest version of CRANK at http://www.bfsc.leidenuniv.nl/software/crank or the CCP4 pre-release zone.

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MS02 P06

Truncate2 - A Program for Intensity to Amplitude Conversion Norman Stein[a], Charles Ballard[a], [a]*CCP4, Daresbury Laboratory, Warrington, WA4 4AD, UK.*
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Keywords: software, protein structure function, structure solution

Conversion of measured intensities to structure factors in protein crystallography is complicated by the fact that background subtraction can result in negative intensities for weak reflections. Truncate2 is a new CCP4 program, designed to replace the original Truncate program, which uses Bayesian statistics to produce positive structure factor values from negative input intensities. Small positive intensities are also boosted by the conversion process. In addition, Truncate2 calculates a number of statistics from the intensity data, such as moments, cumulative intensity distributions and the Wilson plot. When output in graphical form, these can be used to assess data quality and to check for possible twinning. Truncate2 detects significant anisotropy in the data and performs anisotropy correction. A number of quantitative tests for twinning such as the H test and the Britton test have also been introduced. The prior distribution used in Truncate is the Wilson distribution, which is only appropriate in the absence of twinning and translational NCS. Truncate2 is capable of handling the last two cases in a more accurate manner.

MS02 P07

New developments for a full automation of the FIP beamline at the ESRF Jacquamet L., Bertoni A., Borel F., Charrault P., Israel-Gouy P., Iwema T., Kahn R., Joly J., Ohana J., Pirocchi M., Robin A., Serre L., Vernede X. and Ferrer J. L. *Institut de Biologie Structurale Jean Pierre Ebel, CEA; CNRS; Université Joseph Fourier; 41 rue Jules Horowitz,F-38027 Grenoble, France* .
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Keywords: protein data collection, automatic control, robots

FIP (French beamline for the Investigation of Proteins) at the ESRF (European Synchrotron Radiation Facility) pushed developments in automation to reach a fully automated beamline.
- The energy adjustment and beam optimization are completely automated [1].
- The screening of the different protein crystals is ensured by a robotic system: CATS (Cryogenic Automated Transfer System) [2] now commercialized by IRELEC.
- In addition, this robot offers the possibility to analyze crystals directly as they grow in drops inside crystallization plates [3]. FIP has then developed in collaboration with GREINER Bio-One a new crystallization plate devoted to this new application.
- The centering of the protein crystal is improved using the installed UV-laser [4].
- The automation of the data recording and processing with ADP (Automated Data Processing) [5] has also been achieved.

- The remote access to FIP is available using a nx client.
- The FIP team pushed automation even further and used the robot to replace the goniometer. Ultimately the robot will be able not only to position the crystals in the X-ray beam, but also to rotate the crystals accurately for data recording [6].

Since the beamline was launched in 1999, more than 180 structures have been resolved on FIP.

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MS02 P08

CrystalMation: Capacity, reproducibility and efficiency of a fully integrated automatic high-throughput crystallization platform Conn Mallett[a], Mandel Mickley[b], Rolland Mosko[b], David Robbins[b], Craig Sterling[b], Tom Vondran[b], Michael Willis[b], and Jian Xu[b]
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Keywords: crystallization, automation, high-throughput

CrystalMation is the first fully and seamlessly integrated robotic system commercially available on the market for automating the crystallization process from protein to crystal. It consists of crystallization screen creation, plate setup, reservoir and protein dispense, plate storage and handling, image inspection and scoring, one-click optimization and software applications for experiment management and decision making. We report here a system successfully built and optimized for the Joint Center for Structural Genomics (JCSG) and International AIDS Vaccine Initiative (IAVI), which has been shown to meet the high-throughput criteria. Large scale, systematic and functional tests have been performed on the system, including various volumes, proteins, screens, and plate types. The results indicate the system sets up 96-well SBS format plates at a rate of 4.5 minutes per plate or less. Liquid dispensing was consistent and reproducible, even at low volumes. Inspections of all plates were completed within individually specified schedules and stored in the database. The statistics from this large dataset also suggested that all crystallization conditions that give rise to crystals were repeatable.

MS02 P09

Brighter x-ray sources for the home-laboratory A. Coetzee and A. Schierbeek, *Bruker AXS BV, Oostsingel 209, 2612 HL Delft, The Netherlands*
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Keywords: sources, optics, protein crystallography

With recent developments in microfocus rotating anode technology, such as the MICROSTAR ULTRA, more brilliant X-ray sources are available to evaluate very small protein crystals in-house. The intensity on the sample can be greatly improved, combining these sources with the latest developments in graded multilayer optics [1]; resulting in excellent data being measured at home on samples that were previously only tractable at the synchrotron. These optics can be configured for maximum parallelism of the beam (Göbel mirrors) or in a side-by-side Kirckpartick-Baez scheme as conceived by Montel in the 1950's [2] to optimize flux density. Combining modern powerful X-ray sources with the latest detector technology makes it possible to measure data in a fraction of the time needed for traditional diffraction systems. With the added sensitivity of new generation detectors even smaller crystals and samples with weak scattering power are now routinely measured in the home laboratory. The added accuracy and speed of data collection, opens up many possibilities for High throughput crystal screening and in-house data collection. This study reviews the recent advances in in-house X-ray sources. Typical results obtained on benchmark proteins are presented.

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MS02 P10

Crystal structure of C45S mutant of *Arenicola Marina* peroxiredoxin Aude Smeets[a], Bernard Knoops,[b] and Jean-Paul Declercq[a] [a]Unit of Structural Chemistry (CSTR), UCL, 1 place L. Pasteur, B-1348 Louvain-la-Neuve [b]*Laboratory of Cell Biology, UCL, 5 place Croix du Sud, B-1348 Louvain-La-Neuve*
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Keywords: Arenicola Marina, peroxiredoxins, crystal structure

Arenicola Marina Peroxiredoxin 6 is a member of an ubiquitous family of peroxidases widely distributed among prokaryotes and eukaryotes. Peroxiredoxins (Prxs) are divided into three classes : typical 2-Cys Prxs; atypical 2-Cys Prxs; and 1-Cys prxs. All Prxs have the same basic catalytic mechanism, in which an active site cysteine (the peroxidatic cysteine) is oxidized to a sulfenic acid by the peroxide substrate. The recycling mechanism of sulfenic acid back to a thiol is different in the three classes [1].

Here, we report the crystal structure of the C45S mutant of the homologue of human peroxiredoxin 6 in the marine worm *Arenicola Marina*.

This annelid lives in intertidal flats with considerable amount of sulphide [2].

The human peroxiredoxin 6 belongs to the 1-Cys subgroup. The subgroup of the *Arenicola Marina* peroxiredoxin 6 is unknown at this time.

The protein was crystallized under reductive conditions.

Two crystal forms of the protein were obtained, a centered monoclinic one (at 1.6 Å resolution) and a primitive orthorhombic one (at 2.4 Å resolution).

Both were solved by molecular replacement (PHASER).

The protein contains two domains: a thioredoxin fold [3] and a C-terminal domain.

In both crystal forms, dimers are formed by involving the C-terminal domains of each monomer. The thioredoxin folds of monomers are associated in the dimer to form a large β sheet.

The crystal structure of this new peroxiredoxin will be compare with structures of other peroxiredoxins.