- 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.

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MS02 P11

Towards a better understanding of DNA repair in Deinococcus radiodurans Joanna Timmins[a], Ingar Leiros,[b] Elspeth Gordon[a], Gordon Leonard[a] and Sean McSweeney[a] [a]*ESRFs, Grenoble, France.* [b]*NorStruct, University of Tromsø, Norway.* E-mail: timmins@esrf.fr

Keywords: Crystal structure, DNA repair, Protein-DNA interactions.

Our team is interested in the structural biology of *Deinococcus radiodurans*, a Gram-positive eubacterium that displays an extraordinary resistance to a wide-range of DNA-damaging agents, such as ionising radiation and desiccation. Ionising radiation induces the most lethal form of DNA damage, namely DNA double-strand breaks (DSBs). Whilst in most species only a few DSBs can be tolerated and repaired, *D. radiodurans* can withstand and repair over 100 DSBs in its genomic DNA. Initial investigations support the view that the extreme radiation resistance of *D. radiodurans* is complex and is most likely determined by a combination of factors such as efficient DNA repair machinery, genome packing and cell structure. To improve our understanding of this unusual phenotype, we are studying the proteins involved in the three major DNA repair pathways. Two of these, the nucleotide-excision and recombinational repair pathways, have been the focus of our recent work. We have determined the three-dimensional structures of RecO alone and in complex with its cellular partner RecR, both of which are involved in recombinational repair. More recently, we obtained the structure of a key protein involved in nucleotide-excision repair. These three novel structures together with extensive biochemical studies have largely contributed to our improved understanding of the molecular mechanisms underlying DNA repair