



April 2011 - issue n°03

We are pleased to send you the third issue of our twice yearly 'ESRF MX Update' newsletter. Its aim is to keep industrial MX clients up to date with developments at the ESRF.

## NEWS FROM THE INDUSTRIAL & COMMERCIAL UNIT

### WOULD YOU LIKE TO BE TRAINED IN HOW TO OPTIMISE YOUR USE OF OUR BEAMLINES?

**Contact us** to organise training at your home laboratory, at the ESRF or over the phone. Last December, 4 industrial clients came to Grenoble to participate in a training session despite the heavy snow covering Europe! They really appreciated the 'real beamline experience' that is to some extent lost through remote access or is lost at the beginning of an experiment when samples need screening.

### NEW PRICES WITH THE PILATUS ON ID29

As previously announced, the price of a shift on ID29 will be increased in run4 2011, starting 23 August 2011.

A Pilatus 6M pixel detector was installed on ID29 in July 2010. This detector has yielded an increased throughput for protein crystallography experiments: typically, data sets are now collected two to three times faster than is possible on our other high-intensity MX beamlines (ID14-4 and ID23-1). As a result, ID29 is increasingly popular with our industrial clients.

During a 'grace period' used to fine-tune the surroundings of the detector so that it works at its highest speed and is compatible with all the MX software we routinely use on the other beamlines at the ESRF, our industrial clients have been able to benefit from this enhanced throughput at no extra charge. The cost of this beamtime will now be increased to reflect the improved throughput. Feel free to **contact us** for more details

### SMALL MOLECULES STUDIES ON MX BEAMLINES

We see more and more small molecule crystals coming along with macromolecule crystals. The use of small beams, high energies, mini-kappa goniometers and/or the Pilatus detector allow us to perform this kind of experiment easily. We also propose a structure determination service for these small molecules for laboratories which are not familiar with the technique. Don't hesitate to **contact us** for more details.

## HEADLINES

### HERCULES FOR INDUSTRY

2-4 May 2011 in Grenoble

### FIRST BIOSAXS

experiments performed for industrial clients on ID14-3

### FIRST SULFUR-SAD

experiment performed by an industrial client on ID29

### BEAMLINE NEWS

Keep an eye on the MX beamline **changes**

## UPGRADE NEWS

You can find here all the most recent news on the status of ID30 and the expected impact of the upgrade programme on the Structural Biology beam-lines during 2011-2012.

### **ID30:**

After the BM29 (bioSAXS beamline) hutch (cf. last [upgrade news](#)), the construction of the optics hutches has now started at ID30 and first radiation tests are foreseen for mid-Sept 2011 before ID30 goes canted.



*Optics hutch of ID30A as of March 2011*

### **Predicted impact of the ESRF Upgrade on the beam lines usage for 2011 & 2012:**

Two major shutdowns are scheduled during which the machine will be upgraded:

- Winter shutdown 2011-2012: The machine will not deliver beam between 05/12/2011 and 03/05/2012.
- Summer shutdown 2012, slightly longer than usual: The machine will not deliver beam between 25/07/2012 (as usual) and the 09/09/2012.

ID23-1, ID23-2, ID29, ID14-1, ID14-4 will be available to users during all of 2011 and 2012 (except during the shutdowns).

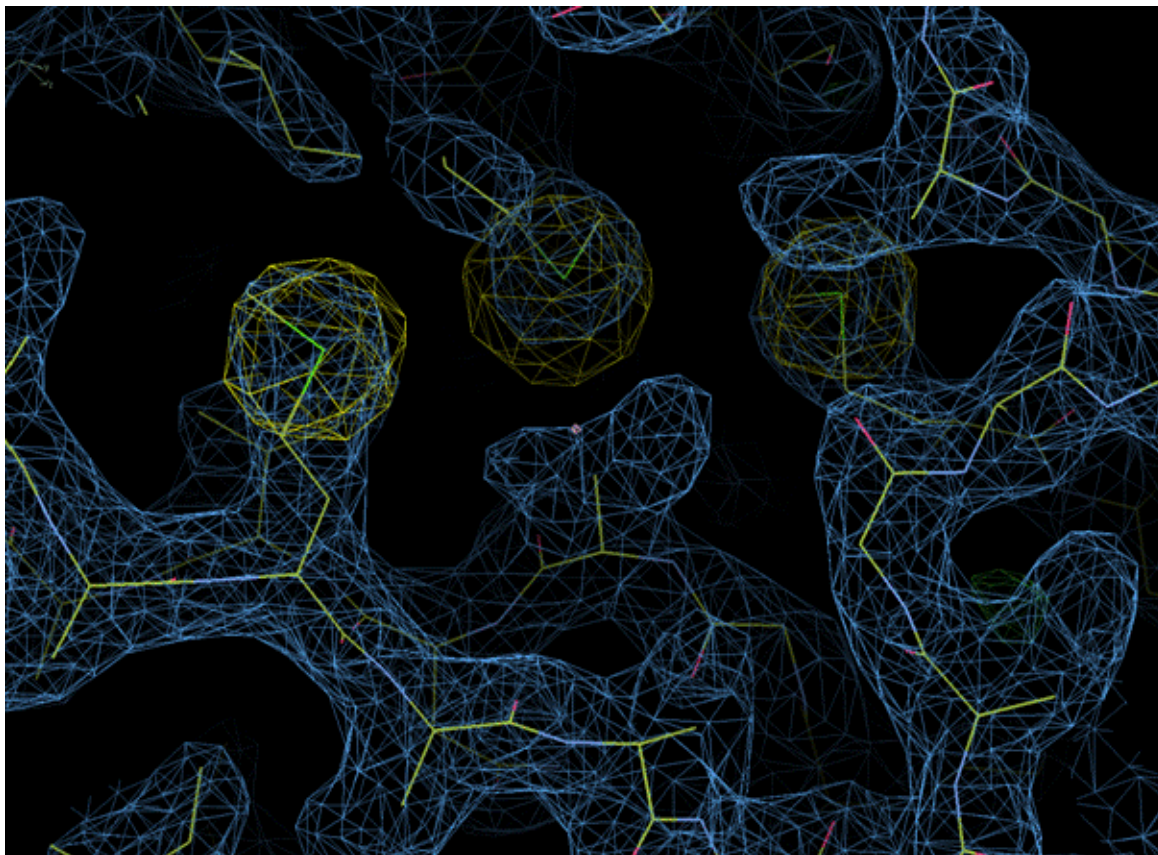
ID14-3 (BIOSAXS beamline) will stay operational until December 2011 (not until summer 2011 as initially planned).

## NEWS FROM THE BEAMLINES

### FIRST S-SAD EXPERIMENT PERFORMED BY INDUSTRIAL CLIENTS WITH THE PILATUS ON ID29

Despite the success of sulphur SAD phasing on home sources, the use of 3<sup>rd</sup> generation synchrotron undulator beamlines for S-SAD phasing remains challenging, due to both the intrinsic nature of many of the samples available but also the challenge of radiation damage. Recently however, AstraZeneca Sweden solved a structure using S-SAD phasing techniques on ID29 using the PILATUS 6M detector – the first industrial group to do so since the installation of the detector in July 2010.

This *de-novo* phasing strategy was applied by AstraZeneca because the production of Seleno-Methione variants was still on-going and experience with this phasing method was desired in-house. A strategy to minimize radiation damage was provided by EDNA that allowed for two datasets to be collected from a single crystal. Despite the fact that usable anomalous signal did not extend beyond 4.5Å, the sulphur substructure could be solved through careful crosschecking and cyclic re-refinement using DM phase restraints. The initial phase estimates were subsequently used for stepwise phase extension to 2.4Å.



*Electron density map of the S-SAD structure with an anomalous difference map showing three methionine sulphurs (yellow).*

## REMOTE ACCESS MADE EASIER

Tired of launching all the software necessary to run your ESRF experiment from home in remote access? You can now double-click on the desktop icon for the beamline on which you are scheduled and everything will open automatically. More details can be found [here](#).

## IS RADIATION DAMAGE A CONCERN FOR YOUR PROJECT?

Have you sometimes observed signs of radiation damage during your experiment but you don't know how to quantify it or how to get the best data collection strategy which would take that information in account?

EDNA can determine your crystal sensitivity through a preliminary experiment, called 'burning', sacrificing a whole or part of a crystal. This sensitivity can then be fed back to EDNA for the study of another part of the same crystal or another sample of the same kind to calculate the BEST strategy for your data collection. See this [webpage](#) for more details.

## YOUR SYSTEM DOESN'T DIFFRACT AS WELL AS YOU WISH?

The diffraction properties of crystals can often be improved by controlled dehydration. The EMBL and ESRF have developed, and now operate as standard, a novel device for controlling crystal dehydration while mounted on a standard macromolecular crystallography beamline. This allows the fine-tuning of the dehydration protocol and enhances the possibility to fully characterise a given system, thus increasing the chances of finding a suitable dehydration protocol. The device can also be used for room temperature data collection. For more details you can read this [document](#) and/or [contact us](#).

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