EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

http://193.49.43.2:8080/smis/servlet/UserUtils?start

Reports supporting requests for additional beam time

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** Insight of Molecular Mechanisms of Flavoproteins and Glycosyltransferases	**Experiment number**: MX-1381
Beamline: ID23-1	**Date of experiment**: from: 23th to: 24th November	**Date of report**: 23-11-2011
Shifts: 2	**Local contact(s)**: Dr. Christoph Mueller Dieckmann	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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BIFI - Edificio I + D

Report:

We are going to summarize the results obtained in experiment

Results:

- Ferredoxin NADP(H) reductase (FNR) from *Anabaena* in reduced state: We managed to get diffraction data at 2 Å from a FNR monocrystal, previously reduced under anaerobic conditions with DTT . X data images have been processed by XDS and MR and refinement is taking place at home. Soon, we plan to solve the structure of the reduced enzyme. FNR crystals belonged to the $P6_5$ hexagonal space group. At present we are carrying out new trials of crystallisation of FNR in semiquinone and reduced state in order to get more insights into the conformation changes that must take place during redox reactions. Also, another Xray data collection was obtained from a mutant of FNR at 1.5 Å and then processed by XDS.

- FAD synthetase: Crystals of FAD synthetase from *Streptococcus pneumoniae* complexed with the cofactor FAD did not diffract well and no good datasets could be obtained. Crystals seem not to be good enough for getting high resolution. More screenings have been proved in presence of reducing agents in order to decrease the oligomerization degree that has been observed in this FAD synthase.

- Apoptosis Induction Factor (AIF): X diffraction data from crystals of human AIF in complex with NADH were collected up to 2.85 Å of resolution. They were processed and the solved structure shows the position of the coenzyme NADH in the active site. The structure is going to be included in a manuscript that is being writing. This structure is going to increase the knowledge of complex formation and residues that are critical in the enzyme activity. A AIF mutant crystal was also diffracted up to 2 Å and processed by XDS.

- POFUT1

We tested crystals of POFUT1 with EGF12 but unfortunately for us we could not get any complexes of the crystals. We only got the apo POFUT1 structure in all the diffracted crystals. We are currently trying to get new conditions.
We could not test all the different crystals we brought because we had problems with the sample changer and therefore we will need to go to the ESRF with the same crystals and hopefully with new crystal forms.