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 via the User Portal:
https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Deadlines for submission of Experimental Reports

Experimental reports must be submitted within the period of 3 months after the end of the experiment.

Experiment Report supporting a new proposal ("relevant report")

If you are submitting a proposal for a new project, or to continue a project for which you have previously been allocated beam time, you must submit a report on each of your previous measurement(s):

- even on those carried out close to the proposal submission deadline (it can be a *"preliminary report"),*
- even for experiments whose scientific area is different form the scientific area of the new proposal,
- carried out on CRG beamlines.

You must then register the report(s) as "relevant report(s)" in the new application form for beam time.

Deadlines for submitting a report supporting a new proposal

- 1st March Proposal Round - **5th March**
- 10th September Proposal Round - **13th September**

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.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report in English.
- include the experiment number 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:** Structural studies on SUMO proteases	**Experiment number**: MX-1556
Beamline: ID23-1	**Date of experiment**: from: 27 June 2013 to: 28 June 2013	**Date of report**:
Shifts: 2	**Local contact(s)**:	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

David Reverter, Universitat Autònoma de Barcelona. Principal investigator.

Pablo Gallego, Universitat Autònoma de Barcelona. Postdoctoral associate.

Report:

Crystals measured at the ID23-1 beamline at the ESRF from june 27th to june 28th in the context of the MX-1556 project. Several crystals from different projects were checked at the ID23-1 beamline, for most of them it was the first time diffraction and it was uncertain whether they were crystals of protein or salt. Unfortunately all projects from the MX-1556 visit at the ESRF synchroton did not result in data good enough to prepare a publication.

- Crystals of Nek9 kinase protein (Nek9). 13 crystals were checked and they were either salt or they did not display any diffraction.

- Crystals of LC8 in complex with the C-terminal domain of Nek9 kinase protein (Nek9-CC). 6 crystals were checked and they did not display any diffraction spot.

- Crystals of tri-domain procarboxypeptidase D (triCPD). 7 crystal were checked. 2 crystals diffracted beyond 3.5 Å resolution. We were able to collect a data set at a final resolution of 4.4 Å and the crystal displayed an hexagonal space group (sg 168 or P6) with unit cell values (207, 207, 81 Å). We were unable to solve the structure.

- Crystals of the Smc5-Nse2 complex. 10 crystals were checked. They were either salt or did not display any measurable diffraction.

- Crystals of Senp5-preSUMO2 complex. 5 crystals were checked. Only one crystal was suitable for data collection but diffracted at low resolution (5.3 Å). The crystal displayed a trigonal space group (sg 144) with unit cell values (132, 132, 97 Å). Unfortunately the collected data set was not good enough to solve the structure.

- Crystals of diSUMO2 linkage. 5 crystals were checked. All of them diffracted at high resolution (1.2 Å). The crystal displayed a trigonal space group (H3) with unit cell values but after solving the structure by molecular replacement, it turn out to be only a SUMO alone.

- Crystals of OCT with norvaline. 7 crystals were checked of Ornithine Transcarbamylase in complex with a substrate norvaline. Only one crystal diffracted beyond 4 A resolution, P321 space group with a unit cell (180, 180, 116 Å), but the data set collected was not good.

- Crystals of the transthyretine domain of CPD (TTL). 2 crystals were checked. A very high resolution data set at 0.9 Å was collected. The crystal displayed a $P2_1$ space group with unit cell values (37, 47, 42 Å and 90, 90.17, 90 º) and the final statistics were excellent. The final structure was solved by molecular replacement. The structure has not been deposited yet.

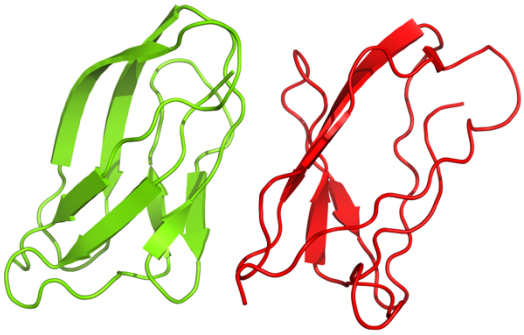

Figure1 : Final cartoon representation of the dimer of the transthyretine domain of CPD at 0.9 Å resolution.