



## 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.

	<b>Experiment title:</b> Structural analysis of the SUMO protease family	<b>Experiment number:</b> MX-1322
<b>Beamline:</b> ID23-2	<b>Date of experiment:</b> from: 20.06.2011 to: 21.06.2011	<b>Date of report:</b> 13.11.2011.
<b>Shifts:</b> 17.00-08.00	<b>Local contact(s):</b> Ricardo Ferraz Leal	<i>Received at ESRF:</i>

**Names and affiliations of applicants (\* indicates experimentalists):**

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**Report:**

Crystals from different projects were collected during these experiments.

**Projects:**

1. Structure of SENP6 catalytic domain, Two crystals diffracted beyond 1.8 Å, they belonged to the P3 space group (sg 143) with a very small unit cell (61 – 61 - 28 Å). Unfortunately, Matthews coefficient calculations indicate that the crystal is formed by a small peptide, not more than 10 kDa, which does not correspond to the expected SENP6 protein (45 kDa).
2. Structure of novel class of metallo-carboxypeptidase structure from *Pseudomonas aureginosa* at 1.6 Å resolution, alone and in complex with two different inhibitors. Three different data sets were collected, WT and complexes, that belonged to the P21 space group (dimensions 42 -83 -107 Å, b=96°). Data has been correctly processed and the results are in preparation for publication soon.
3. Structure of the complex between human carboxypeptidase A4 and a novel protein inhibitor from a marine organism. Two data sets at 1.8 Å resolution were collected from the complex NvCI-CPA4. Crystals belonged to P21 space group (dimensions 69 - 72 - 80 Å, b=108°) The structure of the complex and of the novel inhibitor has been solved by molecular replacement using the structure of CPA4 as a model. Results are in preparation to be published soon.
4. The last project is related to the biosynthesis and degradation of the amino acid arginine in *Mycoplama penetrans*. The first enzyme of the pathway is **Carbamate kinase**, three data sets at 2.4 Å resolution were collected. Crystals belonged to P321 space group (dimensions 51 - 51 - 174 Å). We also have crystals from the second step-enzyme from the *Mycoplama penetrans* arginine

degradation pathway, a protein called **Ornithine carbamoyltransferase**. Two data sets at 2.3 Å resolution were collected. Crystals belonged to P321 space group (dimensions 183 - 183 - 117 Å) with 4 molecules per asymmetric unit. The last enzyme of the pathway is **Arginine deiminase**, three data sets at 2.3 Å resolution were collected. Crystals belonged to P21 space group (dimensions 120 - 128 - 220 Å,  $\beta = 91^\circ$ ). Matthews coefficient indicates that there are 12 molecules per asymmetric unit. These three projects are still in the refinement process, as soon as the structures are finished, the results will be deposited and published elsewhere.