

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.



	Experiment title: A Number of Proteins from Bacteria to Eukarya and from Antarctic to Volcanic Areas	Experiment number: MX-342
Beamline:	Date of experiment: from: 01-10-2004 to: 02-10-2004	Date of report: 04-04-2005
Shifts: 2	Local contact(s): Bill Shepard	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): Stefano Mangani Vito Calderone Rosalida Leone		

Report:

Matrix metalloproteinases (MMPs) are a class of extracellular zinc-containing peptidases that are involved in a variety of tissue-remodelling activities, and whose misfunction/misregulation is implicated in several pathologies ranging from arthritis rheumatoides to metastatic processes.

We have solved several MMP-12 structures (1OS2, 1OS9, 1Q3A, 1RMZ); now we have managed to get atomic resolution crystals of MMP12 on which we perform several soakings with inhibitors designed in our group.

We have determined the structure of MMP-12 at 1.02 Å resolution (1Y93) (1) in the presence of hydroxamic acid which is a weak inhibitor of MMPs.

This high resolution scaffold allows to soak the crystal with stronger inhibitors which can displace hydroxamate and make it possible to determine the structure of the protein in the presence of various inhibitors; this can in turn give more accurate basis for a rational drug design.

The table 1 shows the data collection statistics while Table 2 shows the refinement statistics.

References

1) Conformational variability of matrix metalloproteinases: Beyond a single 3D structure. (2005).

I. Bertini, V. Calderone, M. Cosenza, M. Fragai, Y.-M. Lee, C. Luchinat, S. Mangani, B. Terni, and P. Turano.

Proc Natl Acad Sci USA (In press)

Table 1. Data collection statistics.

	MMP12-AHA
Space group	C2
Cell dimensions	a= 50.92 b= 59.59 c= 53.49 Å, $\alpha = \gamma = 90^\circ$ $\beta = 115.14^\circ$
Resolution (Å)	48.4 – 1.0
Total reflections	263803 (27281)
Unique reflections	70833 (8671)
Overall completeness (%)	97.6 (84.9)
R _{sym} (%)	5.7 (25.1)
Multiplicity	3.7 (3.1)
I/σ(I)	5.5 (2.7)
B-factor from Wilson plot (Å ²)	6.63

Table 2. Refinement statistics.

	MMP12-AHA
Space group	C2
Cell dimensions	a= 50.92 b= 59.59 c= 53.49 Å, $\alpha = \gamma = 90^\circ$ $\beta = 115.14^\circ$
Resolution (Å)	48.4 – 1.0
Total reflections	263803 (27281)
Unique reflections	70833 (8671)
Overall completeness (%)	97.6 (84.9)
R _{sym} (%)	5.7 (25.1)
Multiplicity	3.7 (3.1)
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