EUROPEAN **S**YNCHROTRON **R**ADIATION **F**ACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

ESRF

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:** Structure of *Pseudomonas aeruginosa* quorum sensing protein LasR bound to the autoinducer C_{12}-HSL	**Experiment number**: MX-394
Beamline: ID14-4 BM30A	**Date of experiment**: from: May 16th to: May 17th from: June 30th to: July 1st	**Date of report**: July 25th 2005
Shifts: 1 2	**Local contact(s)**: Dr Xavier THIBAULT Dr Sonia FIEULAINE	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Matt Bottomley* and Andrea Carfí*

Dept. of Biochemistry, IRBM P. Angeletti, Pomezia (RM) 00040, Italy

Report:

Introduction

Pseudomonas aeruginosa is an opportunistic human pathogen responsible for the death of most cystic fibrosis sufferers and many other immunocompromised patients. Fatality is caused by numerous virulence factors, whose production follows activation of the *Pseudomonas aeruginosa* quorum sensing protein LasR by the autoinducer (AI) C_{12}-HSL. In order to understand the basis for ligand binding and specificity and to obtain atomic level information for rational design of small molecules inhibitors of LasR activation we have expressed and crystallized its ligand binding domain.

Data Collected

The LasR ligand binding domain-AI complex has been crystallized in the monoclinic $P2_1$ space group with unit cell parameters a = 53.88 Å, b = 85.16 Å, c = 75.67 Å and $\beta = 95.81^{?}$. The structure of the LasR-C_{12}-HSL complex has been now determined by the SAD method using crystals from a selenomethionine substituted protein. A 1.8Å resolution native data set has also been collected and the structure has now been refined to that resolution.

This structure provides a structural platform for the design of inhibitors of LasR activation. A manuscript describing the structure is in preparation.