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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 a proteolytically resistant core from the severe acute respiratory syndrome (SARS) coronavirus S2 fusion protein	**Experiment number**: MX-267
Beamline: ID14-4 ID14-1	**Date of experiment**: from: July 28th to: July 30th from: Octobr 30th 2004 to: Novemebr 1st	**Date of report**: 26/07/05
Shifts: 6 6	**Local contact(s)**: Dr. Elspeth Gordon Dr. Joanna Timmins	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Vinit M. Supekar*, Chiara Bruckmann and Andrea Carfí*

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

Report:

Abstract

A new Coronavirus (CoV) has recently been identified as the causative agent of the severe acute respiratory syndrome (SARS) in humans. CoVs enter target cells through fusion of viral and cellular membranes mediated by the viral envelope glycoprotein S. We have determined by X-ray crystallography the structure of a proteolytically stable core fragment from the heptad repeat regions HR1 and HR2 of the SARS-CoV S protein. We have also determined the structure of an HR1-HR2 S core fragment containing a shorter HR1 peptide and a C-terminally longer HR2 peptide that extends up to the transmembrane region. In these structures, three HR1 helices form a parallel coiled-coil trimer, while three HR2 peptides pack in an oblique and anti-parallel fashion into the coiled-coil hydrophobic grooves, adopting mixed extended and α-helical conformations as in post-fusion paramyxoviruses F proteins structures. Our structure positions a previously proposed internal fusion peptide adjacent to the N-terminus of HR1. Peptides from the HR2 region of SARS-CoV S have been shown to inhibit viral entry and infection *in vitro*. The structures presented here can thus open the path to the design of small-molecule inhibitors of viral entry and candidate vaccine antigens against this new virus.

Data Collected

We collected data from crystals from two different constructs at high resolution. For both molecules we collected data from mercury derivatized crystals. The two structures were solved at 1.6Å resolution by the SIR method. The crystals largest dimension were 50 μm and the use of a small and well focused beam was essential for the success of our experiments.

PDB deposition

PDB ID codes 2BEQ and 2BEZ

Publication

Supekar *et al.* PNAS 101, 17958-63 (2004)