EUROPEAN SYNCHROTRON RADIATION FACILITY

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:** Solution structures of SCR domains in medically-important regulators of complement	**Experiment number**: MD-199
Beamline: ID02	**Date of experiment**: 24 May 2006 (1 day)	**Date of report**: 28th Feb 2007
Shifts: 6	**Local contact(s)**: Dr Stephanie Finet	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Gilbert, H. E.* & Perkins, S. J.* (UCL)

Asokan, R. & Holers, V. M. (Colorado Health Sciences Center, Denver, USA)

Report:

The 15 SCR Flexible Extracellular Domains of Human Complement Receptor Type 2 can Mediate Multiple Ligand and Antigen Interactions. (2006) *J. Mol. Biol.* 362, 1132–1147. Gilbert, H. E., Asokan, R., Holers, V. M. & Perkins, S. J.

Abstract: Complement receptor type 2 (CR2, CD21) is a cell surface protein that links the innate and adaptive immune response during the activation of B cells. The extracellular portion of CR2 comprises 15 or 16 short complement regulator (SCR) domains, for which the overall arrangement in solution is unknown. This was determined by constrained scattering and ultracentrifugation modelling. The radius of gyration of CR2 SCR 1-15 was determined to be 11.5 nm by both X-ray and neutron scattering, and that of its cross-section was 1.8 nm. The distance distribution function P(r) showed that the overall length of CR2 SCR 1-15 was 38 nm. Sedimentation equilibrium curve fits gave a mean molecular weight of 135,000 (±13,000) Da, in agreement with a fully glycosylated structure. Velocity experiments using the g*(s) derivative method gave a sedimentation coefficient of 4.2 (±0.1) S. In order to construct a model of CR2 SCR 1-15 for constrained fitting, homology models for the 15 SCR domains were combined with randomised linker peptides generated by molecular dynamics simulations. Using an automated procedure, the analysis of 15,000 possible CR2

SCR 1-15 models showed that only those models in which the 15 SCR domains were flexible but partially folded back accounted for the scattering and sedimentation data. The best-fit CR2 models provided a visual explanation for the versatile interaction of CR2 with four ligands C3d, CD23, gp350 and IFN-α. The flexible location of CR2 SCR 1-2 is likely to facilitate interactions of C3d–antigen complexes with the B cell receptor.