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: Dioclea violacea seed lectin**	**Experiment number**: 16-01-653
Beamline: Bm16	**Date of experiment**: from: 23/9/04 to: 24/9/04	**Date of report**: 5/10/04
Shifts: 7	**Local contact(s)**: Dr. Ana Labrador	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Juan J. Calvete Instituto de Biomedicina de Valencia

*Francisca Gallego del Sol Instituto de Biomedicina de Valencia

Report:

Lectins isolated from seeds of *Diocleinae* (*Phaseolae, Leguminosae*) have highly related amino acid sequences but exhibit distinct pH-dependent dimer-tetramer equilibria, and show different biological activities. Since only the tetravalent form is able to cause cross-linking of receptors on the cell surface, the different ratio between divalent and tetravalent lectin species at a given pH may contribute to the variability of biological functions. We have reported the crystal structure of *D. guianensis* (Dguia) seed lectin at 2.0 Å resolution. Comparison of the structures of Dguia and D. grandiflora lectins (1DGL), a lectin which does not display dimer-tetramer equilibrium, indicated that substitution of His 131 for Asn drastically reduces interdimer contacts along with disordering of the loop comprising residues 117-123 which, in its ordered conformation, stabilises the pH-independent tetrameric association of the Dgran lectin. In order to test the hypothesis that replacement of His for Asn at position 131 may explain the existence of pH-dependent dimer-tetramer equilibrium, we searched for other lectins displaying pH-dependent tetrameric association. We have crystals from Dioclea violacea and Cratylia floribunda seed lectins. The aim of the experiment is to resolve this lectins, looking for a commom mechanism for the regulation of the dimer-tetramer association.

Crystals from Dioclea violacea seed lectin difracted to 2.5 Å and belongs to hexagonal P3 space group with unit cell constants:

a=b=73.06
c=161.99

We take two different data sets, one native and the other one in complex with a trimannoside. This structure may help us to elucidate de molecular mechanism of the dimer-tetramer equilibrium and sugar binding.

References

Wah DA, Romero A, Gallego del Sol F, Cavada BS, Ramos MV, Grangeiro TB, Sampaio AH, Calvete JJ. Crystal structure of native and Cd/Cd-substituted Dioclea guianensis seed lectin. A novel manganese-binding site and structural basis of dimer-tetramer association J Mol Biol. 2001 Jul 20;310(4):885-94. PMID: 11453695