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: Parkia platycephala 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):

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Report:

The *Mimosoideae* subfamily of leguminous plants comprises 6 tribes (*Adenanthereae*, *Mimoseae*, *Mimozygantheae*, *Parkiae*, *Acacieae*, and *Ingeae*) which group 56 genera. At present the tribe *Parkiae* is the only taxon from which lectins has been biochemically characterised. These include the seed lectins from *Parkia speciosa* (Suvachittanont and Peutpaiboon, 1992), *Parkia javanica* (Utarabhand and Akkayanont, 1995), *Parkia platycephala* (Cavada *et al*., 1997; Ramos *et al*., 1999) and *Parkia discolor* (Cavada *et al*., 2000). To date, however, no structural data of any *Mimosoideae* lectin have been reported, and thus, the structural classification of these lectins remains obscure.

The seed lectin of Parkia platycephala represents the first lectin from a *Mimosoideae* plant whose primary structure has been elucidated. The protein is composed by three tandemly arranged β-prism domains. We have crystallized the Parkia platycephala lectin and obtained a complete dataset at 2.3 Å resolution. The asymetric unit of the $P2_12_12_1$ crystals contains two molecules of PPL. Molecular replacement methods, using available crystal structures of lectins made up by single β-prism domains, failed, and heavy-atom derivatives were not isomorphous with the native form. We obtained crystals in cocristallization with X-Mannose (a bromide derivative) that belongs to P21 space group with unit cells constants:

a=80.24

b=114.18

c=80.30

$\alpha = \gamma = 90$

$\beta = 119.88$

We performad a MAD experiment taking a complet dataset at three energies:

Peak:13.4864 KeV

Remote:13.450 KeV

Inflection: 13.4773 KeV

Using SOLVE we were able to find 9 bromides and to obtain phases. After density modification we obtained a map suitable to be traced. Now, we are building and refining the molecule.