ESRF	**Experiment title:** BAG for the structural biology groups of Madrid:	**Experiment number**: MX-256
Beamline: ID14-2	**Date of experiment**: from: 3/4/04 to: 5/4/04	**Date of report**: 23/06/2004
Shifts: 6	**Local contact(s)**: Dr. Sofia Mancedo	*Received at ESRF:*

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Measles virus hemagglutinin and CD46.

A second set of experiments were done at ID14-2 using crystals of the measles virus hemagglutinin complex to its CD46 receptor. Crystals of the complex were used in previous experiments during 2003 at the ID14-4 beam line, where native at 3.1 Å of resolution and two heavy atom derivatives (Se and Br) were collected. Identification of several heavy atom sites has given an initial phase information.

The aim of the experiment at ID14-2 was to collect additional heavy atom derivatives and to collect cystals grown in different salt conditions in order to improve native data. Native crystals were first tested and a maximum resolution of 3.5 Å was reached. Data was collected with a single crystal. Subsequently, crystals derivatized with three different Pt compounds were used for collection of three complete data sets for resolutions ranging from 50 to 3.5-4 Å (see table below):

protein-xtal	Resolution	Compl. (%)	Redun	I/σ	Rmerge (%)
Mx1	20-3.6	99,4	7,2	6.8(2.2)	7.5(26.7)
Pt3	20-4.2	99	4	4.5(1.9)	12(32.7)
Pt4	20-3.6	99,8	7,8	5.7(2.4)	8.1(40)
Pt5	20-3.9	99,2	14,2	3.4(1.9)	11.3(31.9)

Statistics from data processed with XDS and scaled with SCALA (CCP4). Resolution limits in Å. Statistics for the high resolution shell (0.1 Å) are in parentheses.

The heavy atom derivative data were used for location of heavy atom sites using anomalous and isomorphous difference patterson and fourier methodologies. However, no sites were found for any of the three Pt derivatives. Further experiments were carried in another trip at the ID29 and BM30A beamlines (see additional reports on the project).

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A. *Data sets of FPR (ferredoxin NADP+ reductase) and FPR: NADP+crystals.* Two data sets were recorded for native FPR crystals up to a resolution of 1.75 Å. Soaking experiments were preformed at different NADP+ concentrations, and soaking times. Finally, two data sets were recorded with 0.1 M and 0.25 M NADP+, respectively. Currently, structure determination is under way.

B. *Analysis of crystals of the complex between CPL-1 (lysozyme from phage CP-1) and the ligand NAM-L-Ala-D-iso-Gln (N-acetyl-muramyl-L-alanine-D-isoglutamine).* A complete data set up to a resolution of 2.4 Å was recorded. The final soaking experiment was done using a ligand concentration of 0.1 M. Currently, structure determination is under way.

C. *Data sets of crystals of the hemolytic lectin from L. sulphureus.* Two complete data sets were recorded, one for native crystals and another one for a Pt-derivative. This last derivative

was obtained by soaking native crystals with 0.1 M $K_2Pt(CN)_4$ during 24 hours. Structure determination is under way by the SIRAS method

D. *Data sets of native PLRP2 crystals.* Because of the low diffracting quality of the PLRP2 crystals, a great number of them were tested in situ. Fortunately, a complete data set was measured using one crystal that permitted to obtain data up to a resolution of 2.9 Å. This data has been successfully used for solving the structure of PLRP2 by the molecular replacement method.

Remarks: all the experiments together with the treatment of the data were done with no problems. The assistance of the local contact was perfect.