

**Experiment title:**

X-ray diffraction data collection on a group V major allergen Phl p5b.

Experiment number:

LS-892

Beamline:

BM14

Date of experiment:

from: 01-Feb-1997 7:00 to: 03-Feb- 1997 7:00

Date of report:

19-Feb- 1997

Shifts:

6

Local contact(s):

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*Received at ESRF:***- 3 MAR. 1998****Names and affiliations of applicants** (* indicates experimentalists):

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Report:

A MAD data set was collected for a mercury derivative of the allergen Phl p5b protein. Following the fluorescence scan, the wavelengths for data collection were set to 1.0065Å (white line - PK), 1.0078Å (point of inflection - PI) and 0.9357381 (remote - RM). We had to sacrifice around eight of our best crystals due to microscope alignment problem. However, data collection was started with one of the best among the remaining low quality crystals.

A total of 270 images, comprising 90 images for each wavelength, were collected. The spindle rotation for each image was 2°. As can be seen in the Table 1, the collected MAD data is nearly 99% complete with almost complete anomalous pairs. But, it is unfortunate that there is no significant anomalous signal which could contribute constructively for structure phasing. The reason for this is still unclear. It could be that the crystals would have suffered severe mechanical damage during the train transport. As suggested by the beam line scientist, Dr. Andrew Thompson, this time we plan attempt crystallisation/soaking experiments on the ESRF site, so as to reduce the mechanical damage to the crystals.

Table 1.

	PK ($\lambda=1.0065\text{\AA}$)	PI ($\lambda=1.0078\text{\AA}$)	RM ($\lambda=0.93573\text{\AA}$)
No. of independent reflections	2502	2500	2502
No. Centric reflections	498	499	504
No. of acentric reflections	2004	2001	1998
No. of reflections having anomalous measurements	1978	1976	1986
Completeness	99.0%	99.0%	99.0%
R_{cvm}	10.2%	10.2%	10.5%
R_{ano}	4.0%	4.0%	4.0%