ESRF	**Experiment title:** Structure determination of Epsilon toxin of *Clostridium perfringens*	**Experiment number:** LS1672
Beamline: BM14	**Date of experiment:** from: 12/04/2000 to: 13/04/2000	**Date of report:** 17/08/2000
Shifts: 1.5	**Local contact(s):** Gordon Leonard	*Received at ESRF:* 28 AOUT 2000

Names and affiliations of applicants (* indicates experimentalists):
Ajit K. Basak*, Claire E. Naylor*, David S. Moss & Ambrose Cole*

Depart of Crystallography,
Birkbeck College,
Malet Street,
London WC1E 7HX,
UK

Report:

We continued our heavy atom derivative search in order to solve the 3D-structure of this protein. During this period of experiment a MAD experiment was carried out on epsilon toxin which has shown a lack of isomorphism between crystals. This has made it hard to verify heavy atom binding to solve the phase problem using the MIR method. The experiment was done on crystals that had been soaked in $HgCl_2$ and then back soaked. A satisfactory plot of the mercury edge was obtained and wavelengths were chosen to maximise the anomolous effects of the L_{III} edge. The peak wavelength was taken at 1.0083Å, the point of inflexion at 0.9919Å and the remote dataset at 0.9184Å. All datasets were integrated using MOSFLM and scaled with the CCP4 program SCALA which indicated a poor anomolous signal. SOLVE was initially used to try to ascertain sites but the results were poor. Further work using the CCP4 package have also failed to resolve sites and so the phases remain unsolved.

	Peak	Inflexion	Remote
Diffraction Limit (Å)	3	3	3
Wavelength (Å)	1.0083	0.9919	0.9184
Rmerge (%)	6.4	6.3	7.5
Ranom (%)	6.1	5.6	6.9
I/sd	14.9	15.5	13
Comp (%)	98.7	98.6	98.6
Mult (%)	3.2	3.2	3.2

So we will continue with our heavy atom derivative search in order to solve the 3D-structure of this protein.