ESRF	**Experiment title:** Data collection on toxins	**Experiment number**: LS-1527
Beamline: BM14	**Date of experiment**: from: 21/11/1999 to: 22/11/1999	**Date of report**: 23/02/2000
Shifts: 3	**Local contact(s):** Vivian Stojanoff	*Received at ESRF:*

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Report:

1)   Epsilon-toxin (8 hours)

Epsilon-toxin is a causative agent in pulpy kidney disease, which effects economically important domestic livestock. We are working on solving the structure of the toxin by MIR and MAD methods. Previous experiments had provided both a high resolution native dataset ($P6_3$, a=b= 122.4, c= 125.5 Å, 4 in asu) and a likely mercury derivative. At BM 14.1 we carried out a four wavelength MAD data collection on a crystal soaked overnight in $Hg(CN)_2$. Following the scan the wavelengths chosen were: 0.826571 Å (remote), 1.0065 Å (peak), 1.008 Å (inflection 1), and 1.0079 Å (inflection 2). Two inflection wavelengths were required as the peak appeared to be split. Statistics for the data are given below; and initial maps and statistics from SOLVE, look promising. We are currently working in improving these maps and obtaining further derivatives.

	λ (Å)	R_{merge} (%)	Comp. (%)	R_{anom} (%)	AnoComp. (%)	$I/\sigma I$
Remote	0.826571	5.0	94.7	5.0	80.8	16.6
Inflection 1	1.0065	5.5	99.1	5.6	95.7	16.4
Inflection 2	1.008	5.4	99.3	5.4	95.8	16.5
Peak	1.0079	4.3	99.3	4.4	95.8	20.1

Table 1: Statistics for anomolous data

2) Staphylococcal exotoxin 1 (4 hours)

sET1 is a member of a novel family of superantigen-related proteins recently isolated from *Staphylococcal aureus*. A native dataset for this protein was collected to 2.9 Å. The previous highest resolution data available had been to 3.8 Å. The spacegroup is $P4_{1/3}2_12$, with cell dimensions a=b=81.7, c= 148.0 Å, suggesting 1-2 molecules in the asymmetric unit. The data between 50 and 2.9 Å have an R_{merge} of 8.5 %, an $I/\sigma I$=14.6. The data were 98,6% complete, with 4.5-fold redundancy. In the highest resolution shell the R_{merge} was 30.6%, and $I/\sigma I$=4.6, these data were 99.2% complete with a 4.6-fold redundancy. These data were used in extensive molecular replacement trials using primarily Toxic Shock Syndrome Toxin and streptococcal Exotoxin C as models. These trials have failed, and we are now initiating a search for heavy atom derivatives.

3) βB2 Crystallin (2.5 hours)

Higher resolution native data were required for this project. No crystals diffracted beyond the limit for previously collected data. No data were collected

4) HSP (4.5 hours)

MAD data were required for a new seleno-methionine derivative of these crystals. These crystals were extremely weakly diffracting (5 minute exposures resulting in weak diffraction to 3.5 Å). The time required for a three-wavelength MAD collection exceeded that available to us, and so a single wavelength data set (for spacegroup identification) was collected.

5) Alpha-toxin (2 hours)

Alpha-toxin is the key determinant in gas-gangrene, we solved the structure a little while ago. Data were collected for a crystal grown at a different pH, which should provide important information about the mechanism of the protein. Data were collected to 2.5 Å.