ESRF	**Experiment title:** Crystallographic studies of Staphylococcal exotoxin 1	**Experiment number:** LS-1672
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Shifts: 1	**Local contact(s):** Hassan Berhali	*Received at ESRF:* 28 AOUT 2000

Names and affiliations of applicants (* indicates experimentalists):
Dr Claire Naylor*, Dr Ajit Basak* and Prof. David Moss

Department of Crystallography
Birkbeck College
Malet St
LONDON, WC1E 7HX
UK

Report:

Staphylococcal exotoxin 1 (sET1) is a member of a newly discovered family of superantigen related proteins from *Staphylococcal aureus*. Superantigens in general interact with MHC class II molecules and T-cell receptors in a non-peptide dependent manner, thus eliciting a massive cytokine response from a wide rage of T-lymphocytes, resulting in a range of disease. Experiments with sET1 have failed to elicit this response from T-cells to date, and this protein may thus be able to shed light on the evolution of these toxins, and perhaps on the origin of their function, since utility of a large scale immune response for the bacteria's viability is still unclear.

SET1 is a 24 kDa, 230 residue protein which contains no cysteines and only a single methionine, it has, at best, 25% identity to any known structure. Structure solution is being attempted by standard multiple isomorphous replacement methods. Crystals grow readily using PEG-MME 2k as a precipitant, buffered at pH 6.5 with 0.1M MES in the presence of 0.2 M ammonium sulphate. The crystals are in spacegroup $P4_{1/3}$, with cell dimensions a=b=81.7 Å, c=148.0 Å, there are probably 2 molecules in the asymmetric unit. While at ID14-1, four complete datasets were collected: a native (to 2.7 Å), and three possible derivatives from crystals that had been soaked in platinum chloride, samarium nitrate and cobalt chloride. The crystals have a tendancy to form as near-perfect twins which are not detectable from crystal morphology, and this was the case for two of the derivatives. The last derivative did not reveal any strong peaks in a Patterson map. Since this trip, another

member of this family has become available for crystallisation, this protein contains 5 methionines, and it will now be used for initial structure determination.