

**Experiment title:**

Solving the crystallographic phase problem of the thermophilic enzyme XT-6 by MAD experiments

**Experiment number:**  
LS 1199**Beamline:**

BM14

**Date of experiment:****from:** Apr. 5, 1998      **to:** Apr. 6, 1998**Date of report:**

Sep. 1, 1998

**Shifts:**

3

**Local contact(s):** Dr. Andrew Thompson (BM14)  
Dr. Vivian Stojanoff (BM14)*Received at ESRF:***Names and affiliations of applicants (\* indicates experimentalists):**

Prof. Gil Shoham and **Ms.** Anna Teplitski  
Institute of Chemistry  
The Hebrew University of Jerusalem  
Jerusalem 9 1904  
ISRAEL

**Report:**

Two BM14 beamtime “windows<sup>1</sup> were used for the XT-6 project in November 1997 and April 1998 together with our local collaborators at **ESRF** (**V.** Stojanoff and A. Thompson). In these **two** beamtime sessions we managed to perform the following experiments **on the** BM 13 beamline:

1. A complete native data set (2.4 Å res.) was collected at 95°K.
2. A full selenium MAD data set was collected on the Sel-Met derivative of XT-6 at 2.8 Å resolution (collected at 95°K).
3. Partial MAD data sets were measured for the Hg-, Sm- and U derivatives of XT-6.

A combination of these data sets resulted recently in a medium resolution map of *ST-6* which was used to build and **refine an almost complete** 3D mode of the native enzyme. A few **regions** of the protein are still disordered and could **not** be traced in the current electron density maps at this resolution.

**These data indicated that a higher resolution diffraction data (2 Å or better) is needed in order to complete the enzyme native structure and obtain the specific details needed for mechanism and thermostability interpretations.**