



Experiment title:  
**Epoxide hydrolases.** BAG: Uppsala (II)

**Experiment number:**  
LS-1804

**Beamline:**  
ID14-EH1

**Date of experiment:**  
from: 02 Dec 2000 to: 04 Dec 2000

**Date of report:**  
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**Shifts:**  
3

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*Received at ESRF:*

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**Report:**

Epoxide hydrolases are a group of functionally related enzymes that hydrolyse potentially harmful epoxides into their corresponding diols which are less toxic. We have been studying mainly two enzymes in this family: epoxide hydrolase from *Aspergillus niger* (AspEH) and Limonene-1,2-epoxide hydrolase from *Rhodococcus erythropolis* DCL14 (LEH).

The structure of AspEH had been previously solved by MAD method using data collected at beamline ID14-4. We have also collected a complete dataset of AspEH in complex with an inhibitor, Valpromide, to a resolution of 2.1 Å at the same beamline. The structure of the complex has been refined and it confirms the location of the active site and the roles of several important amino acids that we proposed in the previously published paper (Zou *et al.*, *Structure* **8**, 111-122).

During this visit we were able to collect a complete dataset on a Se-Met substituted LEH Crystal with a wavelength of 0.931 Å. Although this wavelength is far from the selenium absorption edge, the anomalous signal was strong enough for successful structure determination using the single-wavelength anomalous dispersion method. The structure has been refined to a resolution of 1.2 Å.