



Experiment title:

Epoxide hydrolases. BAG: Uppsala (II)

Experiment

number:

LS-1520 c

Beamline: ID14-EH4	Date of experiment: from: 22 Sept 1999 to: 25 Sept 1999	Date of report: 29 Aug 2000 <i>Received at ESRF:</i>
Shifts: 3	Local contact(s): Sean McSweeney	

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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. During this visit we were able to collect a complete dataset of AspEH in complex with an inhibitor, Valpromide, to a resolution of 2.1Å. 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).

Around 25 crystals of putative SeMet derivatives of LEH were also tested during this visit. No Se signal, however, was detected with fluorescence scans. No phasing information was obtained from other 3 datasets that were collected on crystals soaked with different heavy-atom solutions. We were able to collect data on a native LEH crystal to 1.2Å resolution.