ESRF	**Experiment title:** **Epoxide hydrolase from *Aspergillus niger*.** BAG: Uppsala (II)	**Experiment number**: LS-1376 b
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Report:

Epoxide hydrolases have important roles in the defense of cells against potentially harmful epoxides. Conversion of epoxides into less toxic and more easily excreted diols is a universially successful strategy. A number of microorganisms employ the same chemistry to process epoxides for use as carbon sources.

The x-ray structure of the epoxide hydrolase from *Aspergillus niger* was determined at 3.5 Å resolution using the multiwavelength anomalous dispersion (MAD) method, and then refined at 1.8 Å resolution. There is a dimer consisting of two 44 kDa subunits in the asymmetric unit. Each subunit consists of an α/β hydrolase fold, and a primarily helical lid over the active site. The dimer interface includes lid-lid interactions as well as contributions from an N-terminal meander. The active site contains a classical catalytic triad, and two tyrosines and a glutamic acid residue that are likely to assist in catalysis.

The *Aspergillus* enzyme provides the first structure of an epoxide hydrolase with strong relationships to the most important enzyme of human epoxide metabolism, the microsomal epoxide hydrolase. Differences in active-site residues, especially in components that assist in epoxide ring opening and hydrolysis of the enzyme-substrate intermediate, might explain why the fungal enzyme attains the greater speeds necessary for an effective metabolic enzyme. The N-terminal domain that is characteristic of microsomal epoxide hydrolases corresponds to a meander that is critical for dimer formation in the *Aspergillus* enzyme.

Reference: Zou, J., Hallberg, B.M., Bergfors, T., Oesch, F., Arand, M., Mowbray, S.L. and Jones, T.A. (2000). Structure of *Aspergillus niger* epoxide hydrolase at 1.8 Å resolution: implications for the structure and function of mammalian microsomal class of epoxide hydrolases. *Structure*, **8**, 111-122.