



	Experiment title: Mechanism of L-2-haloacid dehalogenase from <i>Xanthobacter autotrophicus</i> GJ10	Experiment number: LS-824
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Names and affiliations of applicants (* indicates experimentalists):

I.S. Ridder *
 B.W. Dijkstra *
 F. Fusetti * (see also LS 954, BM14, 28-Mar-98 to 30-Mar-98)
 A. Oubrie * (see also LS 954, BM14, 28-Mar-98 to 30-Mar-98)

Laboratory of Biophysical Chemistry
 University of Groningen
 Nijenborgh 4
 NL 9747 AG Groningen (the Netherlands)

Report:

Three data-sets were collected on the dehalogenases from *Xanthobacter autotrophicus* GJ10;

DhlA, soak with 1-chloropentane, pH 5
 resolution 30-1.15 Å, R_{sym} 0.039 completeness 97.6%
 DhlA, soak with 1-chlorohexane, pH 5
 resolution 30-1.52 Å, R_{sym} 0.035 completeness 84.3%
 DhlB, soak with D,L-2-monochloropropionic acid, pH 8
 resolution 30- 1.52 Å, R_{sym} 0.064 completeness 92.7%

The data-sets of the DhlA experiments contain similar information and the model of the previously solved DhlA is currently being refined against the very high resolution data. It will allow a highly detailed study of the enzyme structure.

The DhlB data-set goes out to a higher resolution than collected before (1.95 Å) and completes the picture of the reaction cycle of L-2-haloacid dehalogenase together with data collected before on a covalent enzyme-ester intermediate.

Epoxide hydrolase, a bacterial enzyme which detoxifies toxic halohydrins

" native at pH 9.0 ; resolution 2.04 Å; R_{sym} .048; completeness 96.9 %
 Structure solved; it provided essential information on the relative positions of the active site residues at the pH of optimum activity.

Glucose dehydrogenase, a diagnostic enzyme used for quantitative glucose detection

- methylhydrazine soak ; resolution 1.5 Å; R_{sym} 0.034; completeness 97.8 %
 - lactose soak ; resolution 1.85 Å; R_{sym} 0.052; completeness 98.6 %
 Hydrazine binds in the active site of GDH in two distinct, functionally relevant modes; lactose was not bound in sufficiently high occupancy to draw conclusions.

GP39, an eukaryotic lectin involved in cell differentiation

" native : resolution 2.5 Å; R_{sym} 0.070; completeness 99%
 " pentasaccharide soak: resolution 2.7 Å; R_{sym} 0.069; completeness 99%
 " Gly-mutant : resolution 2.5 Å; R_{sym} - ; completeness 99%
 The structure has been solved, together with data collected at BM14. The pentasaccharide soak was not successful; the Gly-mutant awaits further processing.