

Crystal Structure of the Haloalkane Dehalogenase DbjA

Yukari Sato^{a,b}, Ryo Natsume^b, Zbynek Prokop^c, Miki Senda^b, Jiri Damborsky^c, Yuji Nagata^a, Masataka Tsuda^a, Toshiya Senda^d,
^aGraduate School of Life Sciences, Tohoku University. ^bJBIRC, JBIC.
^cLoschmidt Laboratories, Masaryk University. ^dBIRC, AIST. E-mail: yukari@ige.tohoku.ac.jp

Haloalkane dehalogenases are key enzymes that catalyze hydrolytic conversion of halogenated aliphatic compounds to alcohol and hydrogen halide. The enzymes have good potential for bioremediation, biosensing and biocatalysis. Recently, the haloalkane dehalogenase DbjA from *Bradyrhizobium japonicum* USDA110 was revealed to have a sufficient enantioselectivity for industry scale synthesis of optically active alcohols. This is the first example of enantioselective catalysis among the haloalkane dehalogenases. To reveal the enantioselectivity mechanism of DbjA on the basis of the structure, we determined the crystal structure of DbjA at 1.47 Å resolution by the molecular replacement method. DbjA has an alpha/beta hydrolase fold. The architecture of specificity-determining cap domain is, however, different from three dehalogenases with known crystal structure. The results of structure-function analysis will be presented.

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