Structure of Diol Dehydratase Reactivating Factor – A Novel Molecular Chaperone

<u>Naoki Shibata</u>^a, Koichi Mori^b, Naoki Hieda^b, Mamoru Yamanishi^b, Yoshiki Higuchi^a, Tetsuo Toraya^b, ^aGraduate School of Science, University of Hyogo, Japan. ^bDepartment of Bioscience and Biotechnology, Faculty of Engineering, Okayama University, Japan. E-mail: shibach@sci.u-hyogo.ac.jp

Diol dehydratase and glycerol dehydratase are adenosylcobalamin-dependent enzymes that catalyze the conversion of 1,2-propanediol, 1,2-ethanediol and glycerol to the corresponding aldehydes. Glycerol, a physiological substrate for the enzyme, inactivates the enzyme in an irreversible manner. Diol dehydratase reactivating factor is a molecular chaperone, reactivating the inactivated diol- and glycerol dehydratases in the presence of AdoCbl, ATP and Mg²⁺. Here we report the crystal structures of ADP-bound and nucleotide-free forms of diol dehydratase reactivating factor.

Initial electron density map of the selenomethionine-substituted ADP-bound form was obtained from the MAD diffraction data collected at the BL38B1 beam line, SPring-8, Japan. Diffraction data sets for native ADP-bound and nucleotide-free crystals were collected at the BL41XU beam line, SPring-8, Japan.

Structure of nucleotide-free diol dehydratase reactivating factor is similar to that of nucleotide-free glycerol dehydratase reactivating factor reported by Liao *et al.* [1]. The ADP-bound form of diol dehydratase reactivating factor shows rearrangement of domains with respect to its nucleotide-free form.

[1] Liao, et al., *Structure*, 2003, **11**, 109.

Keywords: diol dehydratase reactiving factor, molecular chaperone, crystal structure