Structure of Diol Dehydrase Containing Bitamin B_{12} Analogue

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Diol dehydrase is a membrane-binding enzyme that catalyzes the adenosylcobalamin dependant conversions of 1,2-diols to the corresponding deoxy aldehydes. Diol dehydrase apoenzyme is composed of three polypeptide chains with molecular weights of 60,000 (α), 24,000 (β) and 19000 (γ). The holoenzyme has two of each subunit and two adenosylcobalamins and its molecular weight is 230,000. Molecular cloning of genes encoding diol dehydrase and their sequences have been reported but a membrane binding site is remeins unknown.

Crystal structures of cobalamin-dependant enzymes, methylmalonyl-CoA mutase and methionine synthase, have been reported. Both enzymes have the structure that a cobalt-dimethylbenzoimidazole bond of a cobalamin is broken and a histidine coordinates to a cobalt ion, instead. On the contrary, diol dehydrase has been reported that it conserves the cobalt-dimethylbenzoimidazole bond. On the opposite site of a corrin ring, an adenosyl group coordinates to the cobalt ion via a Co-C bond. Activation of the Co-C bond is the initial step of the reaction.

Our interest is how diol dehydrase activate the Co-C bond and how the protein is bound to membrane. We crystallized diol dehydrase to solve its crystal structure.

Data sets for platinum and ethyl mercury chloride derivatives were collected at BL41XU equipped with the Rigaku R-AXIS IV detector system. A wavelength of an incident beam was 0.708 Å and a crystal-to-detector distance was 400 mm. The crystals were kept cooled at 278 K during the data collection by the Oxford Cryosystems. The crystals diffracted over 2.5 Å resolution for both derivatives. The data collection for platinum derivatives could not complete because all crystals were cracked. The mercury derivative crystal gave good diffraction at first, but most spots streaked at the 20th image due to diffraction damage. We had no time to try another crystal.

In spite of incomplete data set, an isomorphous difference Patterson map gave significant peaks in an u=1/2 Harker section. We hope we can complete the data collection at SPring-8 if the occasion arises.