Crystal Structures of Formaldehyde Dehydrogenase Complexed with Inhibitors

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Formaldehyde dehydrogenase from *Pseudomonas putida* (PFDH) is a member of the zinc-containing medium-chain alcohol dehydrogenase family. The pyridine nucleotide NAD(H) in PFDH, which is distinct from the coenzyme (as cosubstrate) in typical alcohol dehydrogenases (ADHs), is tightly but not covalently bound to the protein and acts as a cofactor. PFDH can catalyze aldehyde dismutations without an external addition of NAD(H). The crystal structure of PFDH was solved by the multiwavelength anomalous diffraction method using intrinsic zinc ions and was refined at a 1.65Å resolution [1].The 170-kDa homotetrameric PFDH molecule showed 222-point group symmetry. Although the secondary structure arrangement and binding mode of catalytic and structural zinc ions in PFDH were similar to those of typical ADH, a number of loop structures that differ between PFDH and ADHs in their lengths and conformations were observed.

Here we have determined the crystal structures of PFDH complexed with pyrazole inhibitors.

[1] Tanaka N., Kusakabe Y., Ito K., Yoshimoto T., Nakamura K.T., *J. Mol. Biol.*, 2002, **324**, 519.

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