

**W0130**

**Crystal Structure of a Quinohemoprotein Alcohol Dehydrogenase ADH-IIG from *Pseudomonas putida* HK5 and its Substrate Binding.** Zhi-wei Chen, F. Scott Mathews, Dept. of Biochemistry, Washington Univ., St. Louis Mo, 63110, Hirohide Toyama, Megumi Fukumoto, Megumi Yano, Osao Adachi, Kazunobu Matsushita, Dept. of Biological Chemistry, Yamaguchi Univ., Yamaguchi, Japan.

The structure of a soluble monomeric quinohemoprotein alcohol dehydrogenase from *Pseudomonas putida* HK5, ADH-IIG, had been determined at 2.2 Å resolution. The structure was solved by molecular replacement with MOLREP using ADH-IIB as the search molecule. The crystals are hexagonal, space group  $P6_1$  with cell parameters  $a=75.5$  Å,  $c=237.9$  Å with one molecule in the asymmetric unit. The structure was refined with CNS to  $R_{\text{work}}=0.173$  and  $R_{\text{free}}=0.226$ .

ADH-IIG consists of two domains, a PQQ-containing large N-terminal 8-stranded  $\beta$ -propeller domain and a small C-terminal four-helix, c-type cytochrome domain. The two domains are connected by a proline-rich linker segment of 19 residues. The heme is inclined by about  $70^\circ$  to the PQQ and their planes are about 13 Å apart at the closest point. The largest differences between the two ADHs occur in several loop regions and the linker segments as well the C-terminal region of cytochrome domain where there is one more helix in ADH-IIG. A substrate, 1,2-propanediol present during crystallization, appears to be bound in the active site cavity.