Detection of the Conformational Changes of FAD During the Catalysis

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BphA4 is the ferredoxin reductase component of biphenyl dioxygenase from *Pseudomonas* sp. strain KKS102. In order to provide a structural basis for disscussing the electron transport mechanism between ferredoxin and ferredoxin reductase, we determined the crystal structures of BphA4 and its NADH complex (blue semiquinone form) at 1.5Å and 1.6Å resolution respectively.

The crystal of the BphA4-NADH complex were prepared by the soaking method. The crystal color gradually changed from yellow to blue within 2 hours, and then the crystal was frash-frozen. Data collections were carried out at NW12 of PF (Tsukuba). The electron density of the blue semiquinone form shows that the nicotinamide ring of NADH is located beside the isoalloxazine ring of FAD. The difference Fourire map shows a bent of the isoalloxazine ring and a flip of the ribitol part of FAD in the blue-semiquinone form. These conformational changes seem to be caused by the conformational change of the N10 atom of FAD, which seems to have a non-planar conformation in the blue-semiquinone form.

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