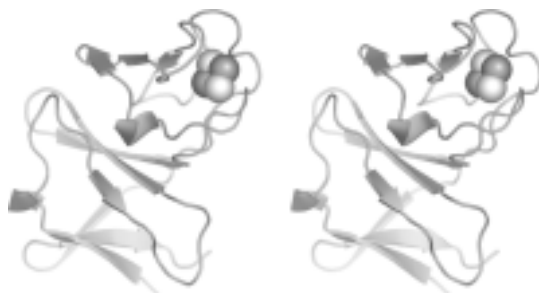


W0077

Structural Studies in Rieske Dioxygenase Electron Transport. E.N. Brown, D. Ferraro, C.-L. Yu, D.T. Gibson, S. Ramaswamy, Dept. of Biochemistry, Univ. of Iowa, Iowa City, IA 52242 USA.

Rieske dioxygenase systems are multi-protein systems of interest for their potential use in “green” chemistry, drug precursor synthesis, and environmental cleanup. Commercial use of dioxygenase systems requires an understanding of substrate specificity, product stereospecificity, and electron transport efficiency. New structures of the Rieske ferredoxin component of two dioxygenase systems are presented: *Pseudomonas putida* Naphthalene Dioxygenase Ferredoxin and *Sphingomonas yanoikuyae* B1 Biphenyl Dioxygenase Ferredoxin. Continuum electrostatics methods accurately predict ferredoxin reduction potential based solely on the structures of 13 Rieske ferredoxin proteins ($R^2 = 0.94$). Potential binding interactions between Rieske ferredoxin proteins and dioxygenase enzymes are determined with computational docking and refined using molecular dynamics simulations. Resulting Rieske [2Fe-2S] cluster distances of 11 – 14 Å are compatible with intra-protein electron transfer.



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