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**Crystal Structure of 2,3-Dihydroxybiphenyl 1,2-Dioxygenase from *Rhodococcus globerulus* P6 and Its Implications.** Mustafa Koksali<sup>1</sup>, Amparo Haro<sup>2</sup>, Lindsay D. Eltis<sup>2</sup>, Jeffrey T. Bolin<sup>1</sup>, <sup>1</sup>Purdue Univ., West Lafayette, IN 47907-2054, USA; <sup>2</sup>Univ. of British Columbia, Vancouver, BC, Canada.

*R. globerulus* P6, a polychlorinated biphenyl (PCB) degrading bacterium, carries three isoenzymes for 2,3-dihydroxybiphenyl 1,2-dioxygenase (DHBD) encoded by three *bphC* genes. In PCB biodegradation, DHBD catalyses the cleavage of the hydroxylated ring of 2,3-dihydroxybiphenyl (DHB). Having reversed order of specificity against mono-Cl DHBs, DHBD-I and DHBD-III presents an interesting case for structural effect on substrate specificity.

We determined the crystal structure of DHBD-I at 1.62 Å resolution, and of DHBD-I with 3'-Cl-DHB at 1.7 Å. Analysis of substrate specificity will be presented, based on these structures and recently found DHBD-III crystals at 2.4 Å resolution, and substrate complexes of DHBD-I and III. DHBD-I complex with 3'-Cl-DHB, prepared by introducing powdered substrate to crystal, contained three substrate molecules per enzyme molecule, one at the active site coordinated to Fe<sup>++</sup>, another at the mouth of the active site. This type of substrate positioning could suggest a mechanism for substrate inhibition, typical of extradiol dioxygenases.

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