

W0277

**Structural Analysis Reveals Determinants of Substrate Specificity of Biphenyl Dioxygenases.** Pravindra Kumar<sup>1</sup>, Christopher L. Colbert<sup>1</sup>, Nathalie Y.R. Agar<sup>2</sup>, Cheryl Whiting<sup>3</sup>, Emma R. Master<sup>3</sup>, Lindsay D. Eltis<sup>3</sup>, Justin Powloski<sup>2</sup>, Jeffrey T. Bolin<sup>1</sup>, <sup>1</sup>Dept. of Biological Sciences, Purdue Univ., W Lafayette, IN, USA; <sup>2</sup>Concordia Univ., Montreal, Canada; <sup>3</sup>Univ. British Columbia, Vancouver, Canada.

Biphenyl dioxygenase (BPDO) dihydroxylates polychlorinated biphenyls (PCBs) to initiate their biodegradation. The pathways and enzymes from different bacteria possess significantly different PCB-transforming abilities. For example, the capabilities of the BPDOs from *Burkholderia* sp. strain LB400 (BPDO-LB400) and *Comamonas testosteroni* B356 (BPDO-B356) differ and both enzymes have been targets of efforts to improve substrate range by directed evolution and other methods. We are in the process of defining the structural basis for substrate selectivity by determining the crystal structures of *Comamonas testosteroni* (BPDO-B356) (1.6 Å) and *Burkholderia str.* LB400 (BPDO-LB400) (2.2 Å) in their native forms and in anaerobic complexes with substrates. An analysis of the two BPDOs reveals variations in the interactions between substrate and enzyme and predicts variations for PCBs that may be reflected in substrate specificity.

Supported by NIH (R01-GM52381) and NSERC (224153-99), and various agencies that support BioCARs and SBC at the Advanced Photon Source.