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Report:

Structure of an aromatic ring-hydroxylating dioxygenase - naphthalene 1,2-dioxygenase

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STRUCTURE: in press.

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Background
Pseudomonas sp. NCIB 9816-4 utilizes a multicomponent enzyme system to oxidize naphthalene to (+)-cis-(lR,2S)-dihydroxy-1,2-dihydronaphthalene. The enzyme component catalyzing this reaction, naphthalene 1,2-dioxygenase (NDO) belongs to a family of aromatic ring-hydroxylating dioxygenases that oxidize aromatic hydrocarbons and related compounds to cis-arene diols. These enzymes utilize a mononuclear non-heme iron center to catalyze the addition of dioxygen to their respective substrates.

Results
The three-dimensional structure of naphthalene dioxygenase has been determined at 2.25 Å resolution. The molecule is an a3b3 hexamer. The a subunit has a b sheet domain that contains a Rieske [2Fe-2S] and a catalytic domain that has a novel fold dominated by an antiparallel 9-stranded pleated sheet against which helices pack. The active site contains a non-heme iron ion coordinated by His208, His213, Asp362 (bidentate) and a water molecule. Asn201 is at a longer distance, 3.75 A, at the missing axial position of an octahedron. In the Rieske [2Fe-2S] center, one iron is coordinated by Cys8 1 and Cys 101 and the other by His83 and His104.

Conclusions
The domain structure and iron coordination of the Rieske domain is very similar to that of the cytochrome bcl domain. The active site iron center of one of the a subunits is directly connected by hydrogen bonds through a single amino acid Asp205 to the Rieske [2Fe-2S] center in a neighboring a subunit. This is likely to be the main route for electron transfer.