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The Structure of Allene Oxide Synthase from *Plexaura homomalla*, a Catalase-like Fold. Michael Oldham¹, Alan Brash, Marcia Newcomer¹, ¹Dept. of Biological Sciences, Louisiana State Univ., Baton Rouge, LA 70803.

8R-Lipoxygenase and Allene Oxide Synthase (AOS) are parts of a naturally occurring fusion protein. AOS catalyses the production of an unstable epoxide (an allene oxide) from the fatty acid hydroperoxide generated by the lipoxygenase activity. We report here the structure of the AOS domain and its striking structural homology to catalase (rmsd 1.65Å [225 of 373 Cα]). While nominal sequence identity between the enzymes had been previously described, the extent of structural homology observed was not anticipated given that this enzyme activity had been exclusively associated with the P450 superfamily, and conservation of a catalase fold without catalase activity is unprecedented. While the heme environment is largely conserved the, AOS heme is planar and putative catalase charge relay residues are absent in AOS. These critical differences may explain the lack of catalase activity in AOS. The structure was solved by a combined FeMAD-MIR approach. Low resolution derivatives greatly improved phasing from the endogenous heme iron (1 Fe / 373 amino acids). The model was refined with 2 Å data to a R_{work} (R_{free}) of 20.0 (24.5)



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