

MOLECULES | LIFE | DIVERSITY

POSTER PRESENTATIONS DAY 1

FAOBMB2021.ORG















STRUCTURAL BIOLOGY



Madushika Perera¹, Sulochana Wijesundera¹, C D Wijayarathna², Gamini Seneviratne³, Sharmila Jayasena¹

¹Department of Biochemistry and Molecular Biology, Faculty of medicine, University of Colombo, Sri Lanka

²Department of Chemistry, Faculty of Science, University of Colombo, Sri Lanka

³National Institute of Fundamental Studies, Hantana Road, Kandy, Sri Lanka

FMN binding monooxygenase LadA, catalyses the oxidation of long-chain alkanes. LadAs have been characterized only in a few extremophilic bacterial species. Previously isolated *Aspergillus flavus* MM1, a rapid crude oil degrader, alluded to the presence of highly active long-chain alkane monooxygenases in them. Therefore, we searched LadA homologs in *A. flavus* using computational methods.

Six uncharacterized homologs of *Geobacillus* LadA, were identified from *A. flavus* NRRL 3357 by probing publicly available protein databases. Protein phylogeny inferred, five of *A. flavus* homologs to be LadAa class and one to be class LadAB.

Three-dimensional models of five *A. flavus* LadAa homologs (*Af1* to *Af5*) were predicted by SWISS-MODEL and their function was confirmed by docking simulations using AutoDcok Vina and UCSF Chimera.

FMN was captured only by Af1, Af3, Af4 and Af5 according to our blind docking experiments. FMN bound Af1, Af3, Af4, and Af5 were docked with *n*-alkanes (C_{16} - C_{30}). The four enzyme-cofactor complexes captured all alkanes inside the active pocket.

According to the BIOVIA discovery studio visualizer, the formation of pi-alkyl interaction between the isoalloxazine ring of FMN and the terminal carbon atom of captured alkanes (up to C_{30}) were observed in *Af3*, *Af4*, and *Af5*. *Af1* formed pi-alkyl interaction with alkanes only up to C_{24} . This indicates the possibility of oxidation of bound alkanes into their corresponding alcohol.

Our results confirm that identified *A. flavus* LadAa homologs bind long-chain alkanes within their active pocket. This suggests that they oxidise long-chain alkanes into their corresponding alcohol similarly to bacterial LadA.





MOLECULES | LIFE | DIVERSITY

Peak Bodies

FAOBMB

NZS

FAOBMB2021.ORG



Hosts

















