

# *In silico* identification and molecular docking analysis of long chain alkane monooxygenase (LadA) in filamentous fungus *Aspergillus flavus*

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## Introduction

*Aspergillus* sp. MM1 rapidly degrades long-chain *n*-alkanes (> C<sub>16</sub>) in crude oil. This led to the identification and characterization of an enzyme for the initial oxidation of long-chain *n*-alkanes using computational methods

## Methodology

*A. Flavus* NRRL3357 homolog of *Geobacillus* LadA was identified by BLAST (NCBI). A quality model was prepared by SWISS-MODEL server. FMN and alkanes were retrieved from Protein Data Bank and geometrically optimized by ORCA. Method was validated by redocking of *Geobacillus* LadA crystal structures by AutoDock Vina. Binding of long-chain alkanes to *Aspergillus* LadA was determined by validated method. Analysed by UCSF Chimera and BIOVIA discovery-studio

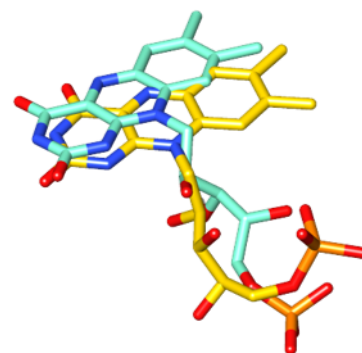
## Results

*Aspergillus* LadA successfully captured *n*-alkanes, C<sub>16</sub> to C<sub>30</sub> and C<sub>36</sub>

pi-alkyl interaction between FMN co-factor and the terminal carbon atom of C<sub>16</sub> - C<sub>24</sub> and C<sub>36</sub> indicate terminal oxidation of those long chain-alkanes when bound to the *Aspergillus* LadA: FMN complex (other alkanes may be oxidized through subterminal oxidation)



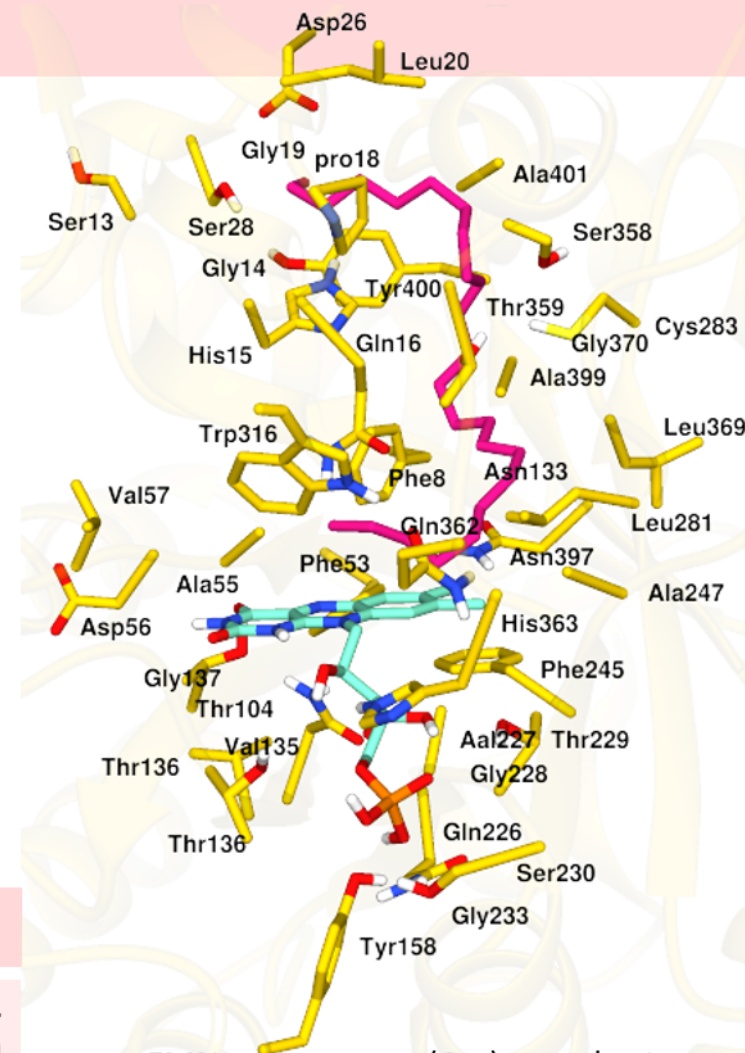
Homology model of *Aspergillus* LadA



Superpose of FMN of docked *Aspergillus* LadA: FMN (blue) and 3B9OchainA:FMN (gold) complexes



Long-chain alkane molecule



FMN: tetracosane (C<sub>24</sub>) complex in active site of *Aspergillus* LadA homolog

## Conclusions

This study reports the presence of a LadA in *Aspergillus flavus* for long-chain alkane oxidation. This finding supports future biotechnological applications in bioremediation of petroleum hydrocarbon pollution