## OP-22: Molecular docking simulation of *Aspergillus flavus* AlmA like protein binding with long chain alkanes (C16-C40)

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**Introduction:** AlmA is a bacterial enzyme known to initiate the degradation of long-chain alkanes. Although efficient degradation of alkanes has been observed in fungi, their mechanisms and the enzymes involved are poorly understood. The objective of this study was to identify the binding capability of AlmA like protein in *A.flavus* using *in-silico* methods.

**Methods:** A putative AlmA homolog protein sequence similar to the *Acinetobacter sp.* was identified from *Aspergillus flavus* and its 3D structure was modelled and validated using bioinformatics techniques. The 3D structures of Alkanes and the cofactors required for AlmA (FAD and NADP), were optimised using Orca Version 4.2.1 and molecules were docked stepwise using AutoDock Vina 1.2.0. The cofactors were initially docked on to the AlmA. The AlmA homolog bound to co-factors were then docked with alkanes (C16-C40). The RMSD value and binding affinity of molecules were evaluated. Hydrophobic interactions and docking site analysis of the *A. flavus* AlmA like protein and AlmA of *Acinetobacter sp.* were conducted using Chimera, Protein Ligand Interaction Profiler (PLIP), and ProteinsPlus and results were compared and analysed for ubiquity of similar interactions.

**Results:** FAD showed a higher affinity towards the AlmA like protein of *A. flavus,* than NADP suggesting it may bind to the active pocket initially. Hydrophobic interactions between the cofactor and active pocket amino acids showed comparable results with multiple programs (Chimera, PLIP and ProteinsPlus). Affinity and RMSD (0.0Å) values of tetracontane (C40 alkane) showed valid docking and docking site interactions showed ubiquity with Chimera and PLIP. The results imply that the identified AlmA homolog in *A.flavus* has great potential for bioremediation of crude-oil contamination which needs to be verified experimentally.

**Conclusions:** It was evident that the identified AlmA like protein of *A. flavus* uses long chain alkanes as substrates and therefore has a strong likelihood of structural and functional homology to the bacterial AlmA.

**Keywords:** docking, Aspergillus flavus, *alkane* degradation