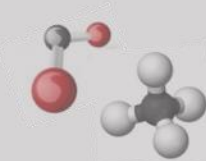
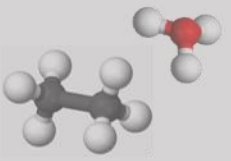


# Isolation of cytochrome monooxygenase (*cyp52*) gene from *Aspergillus* sp. MM1, *in-silico* protein modelling and molecular docking simulation of hexadecane binding



Madushika Perera<sup>1</sup>, C D Wijayarathna<sup>2</sup>, Sulochana Wijesundera<sup>1</sup>, Gamini Seneviratne<sup>3</sup> and Sharmila Jayasena<sup>1\*</sup>  
<sup>1</sup> Department of Biochemistry and Molecular Biology, University of Colombo <sup>2</sup> Department of Chemistry, University of Colombo <sup>3</sup> National Institute of Fundamental Studies, Kandy

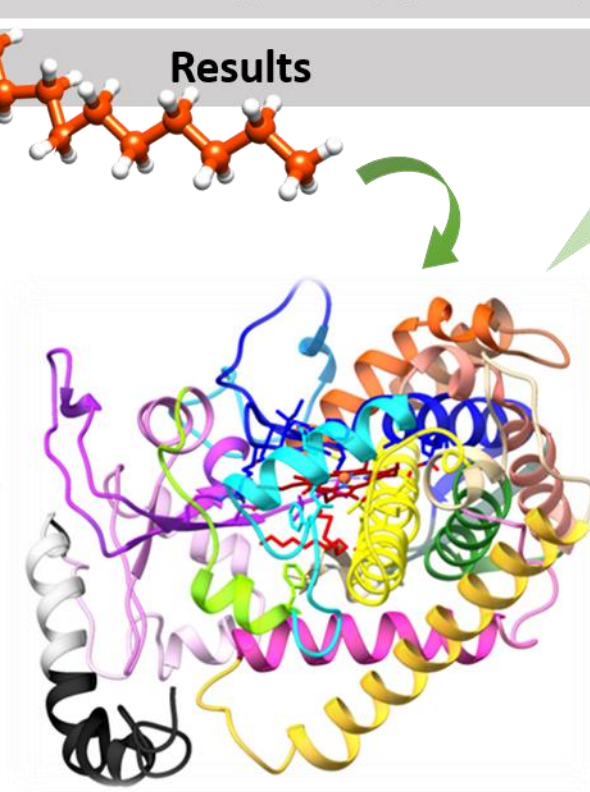
## Introduction



## Methodology

*Cyp52* gene from *Aspergillus* sp. MM1 was isolated comparing protein motifs to hexadecane-degrading Cyp52 from *Candida maltosa*. Quality models were prepared by I-TASSER. Haem and hexadecane structures were retrieved from Protein Data Bank and geometrically optimized with ORCA. Both protein and ligands were docked by AutoDock Vina. Visualized and analysed by UCSF chimera and BIOVIA discovery studio.

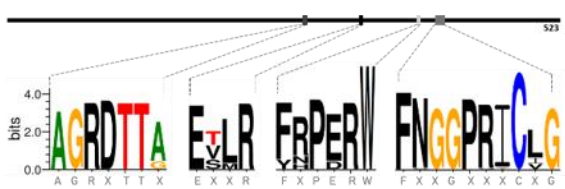
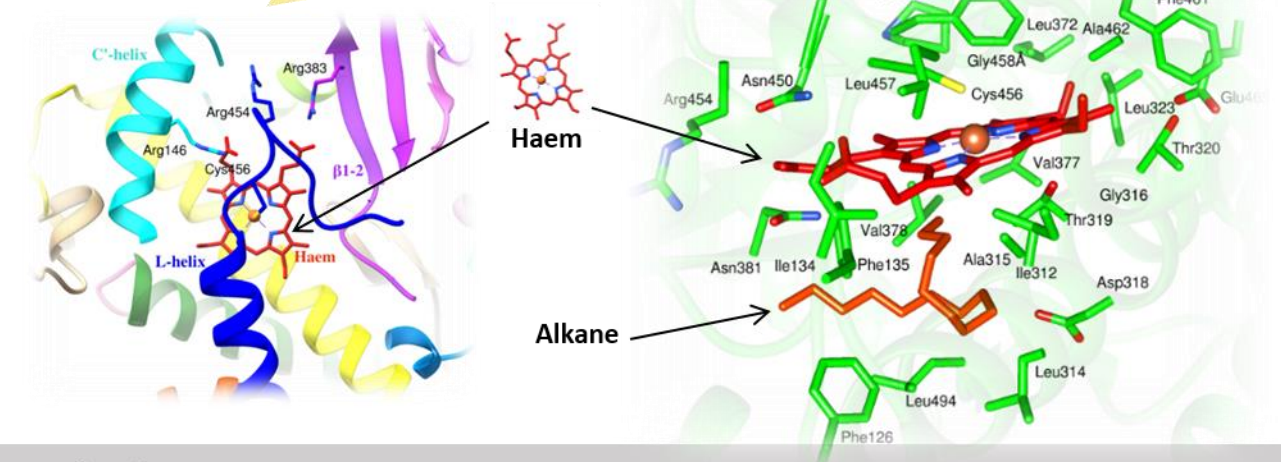
## Results



Hexadecane bound to *Aspergillus* Cyp52: haem complex by its terminal carbon atom

Positioning of haem at the distal face of *Aspergillus* Cyp52

29 active site residues were shared between *Candida* Cyp52 and *Aspergillus* Cyp52 with similar conformation of haem and hexadecane



The 4 Cyp52 motifs were present in *Aspergillus* Cyp52

## Conclusions

Isolated *Aspergillus* sp. MM1 *Cyp52* gene encodes a medium-chain alkane monooxygenase. This findings can support future biotechnological applications in bioremediation of petroleum hydrocarbon polluted environment