In silico identification of a bacterial AlmA-like protein in *Aspergillus flavus* NRRL 3357

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Introduction

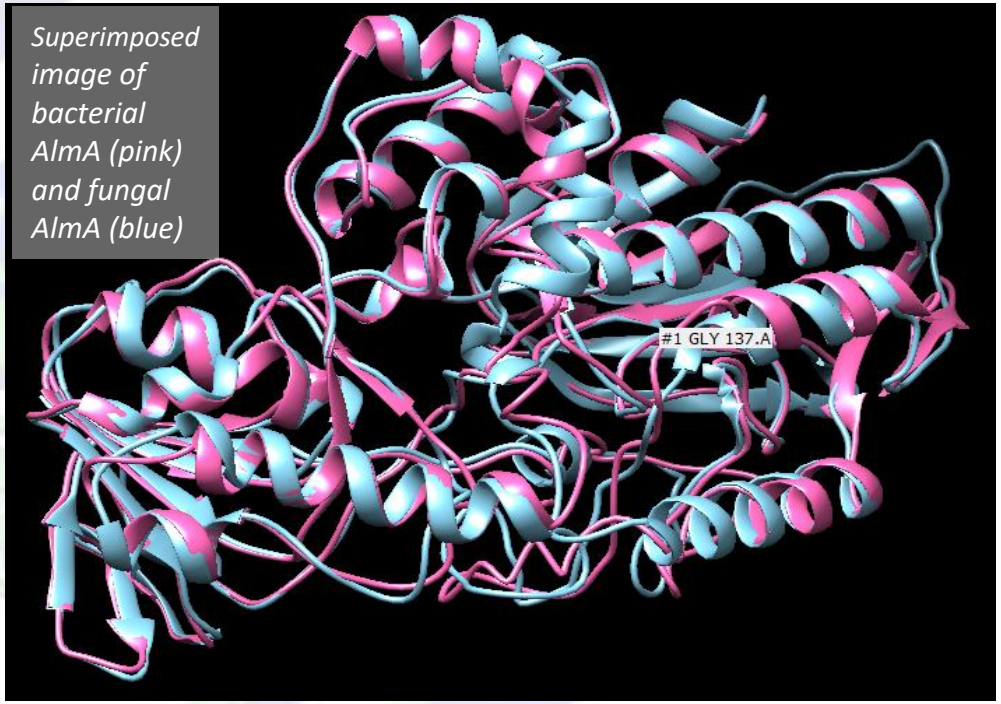
Accidental leak of crude oil during transport or storage poses a great environmental threat. Bioremediation is an effective method used to mitigate the effects of pollution on a large scale. AlmA enzymes found in bacteria are capable of degrading long-chain alkanes(C>32). Fungal AlmA enzymes that can use long chain alkanes as substrates have not been previously characterized . This study focuses on using an *in-silico* approach to identify a fungal AlmA homologue from *Aspergillus flavus* NRRL3357.

Methodology

- Verified bacterial AlmA sequence (UniProtKB).
- PSI-BLAST (20,000 sequences retrieved).
- Aspergillus flavus NRRL 3357 sequences selected.
- Similar domain search in Pfam database.
- 3D model preparation I-TASSER
- Superimposition of fungal and bacterial AlmA.
- Analysis using ERRAT, VERIFY3D and PROCHECK.

Results

Superimposition with model 1 gave the lowest RMSD value (0.547 Å). The validity of model 1, was further evaluated using ERRAT (87.7895), VERIFY3D (83.02 %) and PROCHECK (92.1%)



Superimposed image of bacterial AlmA (pink) and fungal AlmA (blue)

Validation scores demonstrate that model 1 is reliable. Together, these results indicate that the selected *A. flavus* sequence represents an AlmA-like monooxygenase, suggesting that AlmA-like enzymes present in *A. flavus* may play a role in degradation of long chain alkanes.

Conclusion

The results are conclusive evidence that the *Aspergillus flavus* NRRL 3357 has an enzyme similar to the bacterial enzyme AlmA.