**Inhibition of *Thermomyces lanuginosus* Chitinase by Allosamidin**

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**1. Introduction**

Chitinase

Structure information

Structure is unknown

Determination of the three-dimensional (3D) structure of a protein can provide important details about its biological functions and mechanism of action [1].

In this research report, we modeled 3D structure of chitinase from the aa sequence using homology modeling approaches. Further, we docked Allosamidin inhibitor into the active pocket of chitinase.

**2. Materials and methods**

*2.1. Homology modeling*

XXXXXXXX using modeler 9.xxxx []. First, NCBI BLAST, database, found 3 template. XXXXXXXX 1 paragraph.

*2.2. Molecular Docking*

Docking of Allosamidin has been performed into the active pocket of chitinase. Then xyz coordinates were XXXXXXX. The box size were XXXXYYYZZ. Exhaustiveness and num\_modes. Pdb to pdbqt, docking.

**3. Results and discussions**

*3.1. 3D model of Chitinase*

Figure 1. Chitinase PyMOL

Figure 2. PDBsum

Figure 3. Rama xxxx chitinase. It has 90% 1% llllllllllllllllllllllllllllllllllllllllllllllllllllllllllllllll.

3.2. Interactions of Allosamidin with Chitinase

Active site was Glu176

Interacting residues. XXXXXX.

Docking energy ??

We confirmed from the figure that it is docked in the active pocket.



Figure 4. (A) (B) (C) Pocket (D) 2D

**4. Conclusion**

**5. References**

1. Khan, F.I., et al., *Current updates on computer aided protein modeling and designing.* Int J Biol Macromol, 2016. **85**: p. 48-62.