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## Structural and functional characterization for interaction of silver nanoparticles with ergosterol in *Trichoderma harzianum*

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### Abstract

Silver ions, because of its recognised antimicrobial activity are reported in several regions for the very long time while ergosterol, apart from its role as a secondary metabolite, structural component of the fungal cell membranes, also turns out to be activating defence response in plants. Silver ions biosynthesized by terpene ergosterol producing *Trichoderma harzianum* could be used against other plant pathogenic fungi. In this work, possible interaction of the silver ions with ergosterol enzyme has been investigated using a computational approach. Protein model construction via prior knowledge of sequences and molecular ligand docking experiments as well as structural and sequence comparisons were executed to identify potential active-site in ergosterol enzyme. Moldock score of -48.5747 with the reranking score of -40.0228 has been reported by Molegro Virtual Docker(MVD) at ergosterol enzyme's active site positions for silver ion. Apart from the core of the active site, four other positions have been occupied by silver ion. The interacting site surrounded by Cys339, Arg343, Lue365, Leu336 and Trp371 formed hydrophobic bonds with silver. The anti-microbial activity against phytopathogens is believed to increase synergistically when combined with ergosterol enzyme. Thus the computational analysis of silver ion in conjugation with ergosterol enzyme provided additional strategies to

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