

## Simulation of plant defensin interaction with phospholipid membrane

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### Abstract

Molecular docking was used for studying plant defensin interaction with phospholipid membrane. Six defensins with different total charges and different charge distributions on the protein surface were used. Comparative analysis of interaction energy between proteins and membrane surfaces shows that defensins slightly interact with membrane surface. Electrostatic interactions and solvation and hydrophobic effects give a major contribution into interaction energy. Different orientation of proteins relative to membrane surface reveals the specificity of interactions.