Registration Code of Publication: 13-35-7-73 The article is published on the materials of speech at the XX All-Russian Conference "The structure and dynamics of molecular systems." Yalchik 2013. Publication is available for discussion in the framework of the on-line Internet conference "Butlerov readings". http://butlerov.com/readings/ Contributed: July 16, 2013.

Simulation of plant defensin interaction with phospholipid membrane

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Keywords: defensin, phospholipids, molecular docking.

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 solvatation and hydrophobic effects give a major contribution into interaction energy. Different orientation of proteins relative to membrane surface reveals the specificity of interactions.