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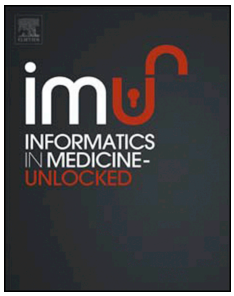

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Research Article

In silico drug design for *Staphylococcus aureus* and development of Host- pathogen interaction network

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Abstract

Staphylococcus aureus, a member of Staphylococcacea has been considered as an opportunistic pathogen in humans and livestock. Thus, the suggestion has been made to discover a potential drug to address Staphylococcus aureus infections. In the present study, drug designing of natural antistaphylococcal compounds, comprised of docking study of acetylated abietane quinone against ClfA (clumping factor A) using the AutoDock tool, was performed and the formed hydrogen bonds in the docked complex were analyzed using Pymol software. A drug library of 86 natural antistaphylococcal compounds was generated and screened with Lipinski and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) filters using Molinspiration and PreADMET tools. A host-pathogen interaction network of staphylococcus aureus and humans was developed using Cytoscape tool. After applying filters and performing an analysis, acetylated abietane quinone, which is a natural antistaphylococcal compound and a component of mint, was obtained. The binding energy of the docked complex of ligand acetylated abietane quinone against