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In Silico Evaluation of Plant-Derived Phytochemicals and Phytopeptides as Potential Antimicrobial Agents

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Phytochemicals and phytopeptides derived from plants are known for their antimicrobial, anti-tumor, pesticide, and herbicidal activities. Among bioactive peptides, phytopeptides exhibit distinctive pharmacological and biological properties. Plant-derived antimicrobial peptides (AMPs) are of particular interest due to their structural diversity and potential for development into novel antimicrobial drugs. In this study, molecular docking was employed to investigate the interactions between antibacterial enzymes and phytochemicals extracted from *Vitex negundo* and *Prosopis juliflora*. Out of 102 docked complexes, 20 exhibited the highest binding energies and were further analyzed. The complexes revealed multiple interaction types, including Van der Waals forces, hydrogen bonds, Pi-Sigma, Pi-Alkyl, hydrophobic interactions, salt bridges, sulfur–X bonds, covalent bonds, and amide–Pi stacking, visualized in both 2D and 3D using Biovia Discovery Studio Visualizer. Higher binding energies were associated with stronger hydrophobic interactions between ligands and receptors. These findings suggest that phytopeptides and phytochemicals from Vitex negundo and Prosopis juliflora may serve as potent antimicrobial agents and warrant further in vitro evaluation for their potential in reducing food spoilage.

Keywords: Antimicrobial peptides, Food spoilage, Molecular docking, Phytopeptides, Phytochemicals

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