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72. Computational Analysis and Molecular Docking of Bioactive Compounds from *Strobilanthes glutinosus* Targeting the HER2 Receptor

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ABSTRACT

Strobilanthes glutinosus is a medicinal plant with limited scientific exploration despite its traditional therapeutic relevance. The present study aims to investigate the anticancer potential of bioactive compounds derived from *Strobilanthes glutinosus* through computational analysis and molecular docking against the Human Epidermal Growth Factor Receptor-2 (HER2), a well-established therapeutic target in breast cancer. Phytochemical constituents reported from *Strobilanthes glutinosus* were screened for drug-likeness using Lipinski's Rule of Five and ADMET prediction tools to evaluate their pharmacokinetic and toxicity profiles. The selected compounds were subjected to molecular docking studies against the HER2 receptor to assess binding affinity and interaction patterns. Docking results revealed that several bioactive compounds exhibited strong binding energies and stable interactions with key amino acid residues at the active site of the HER2 receptor, comparable to standard inhibitors. These findings suggest that *Strobilanthes glutinosus* harbors promising lead compounds with potential HER2 inhibitory activity. The study provides a computational foundation for further in vitro and in vivo validation of these phytochemicals as prospective anticancer agents targeting HER2-positive breast cancer.

Keywords: *Strobilanthes glutinosus, Lipinski's Rule, ADMET prediction, Molecular Docking*

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