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POSTER ABSTRACT

COMPUTATIONAL EVALUATION OF PHYTOCHEMICALS FROM PLANTAGO OVATA L. AGAINST BREAST CANCER (Times New Roman, Font size 14)

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Breast cancer, a prevalent cause of female mortality globally, underscores the urgent need for effective treatment. Existing potent drugs for breast cancer often exhibit adverse effects and inefficacy. The emergence of resistance, driven by cancer-related mutations, further compromises treatment outcomes. This study focuses on exploring potential leads from *Plantago Ovata L.* against breast cancer through molecular docking analysis, specifically utilizing the Glide module within the Schrödinger suite, targeting EGFR (PDB ID: 2J6M). The objective is to identify bioactive compounds with significant efficacy and minimal adverse effects. A bioinformatic approach involving the screening of numerous phytochemical molecules was employed. Docking analysis helped filter these compounds, with the top three ligands for the protein receptor being selected. Subsequently, a screening process involving 44 phytochemicals from AS was conducted, and based on binding affinity scores, the top three molecules with the protein receptor were identified as the top 03 drug candidates. Among these, a single molecule was chosen for formulation. The comprehensive screening of diverse phytochemicals against breast cancer target proteins has yielded a promising therapeutic candidate. This discovery holds potential for the development of traditional medicine-based therapies and serves as a stepping stone for future lead optimization in breast cancer medication development. We anticipate that these findings will contribute significantly to advancing novel treatments and identifying potential candidates for further exploration in breast cancer research. (Times New Roman, Font size 12)

Keywords: Molecular docking, cancer, phytochemicals

Abstract should not exceed 250 words