

**Enhancing *In Vitro* Propagation Efficiency and Exploring Wound Healing
Therapeutic Potential of *Rauvolfia tetraphylla* L.: A Multifaceted Approach**

Thesis submitted in partial fulfilment of the
Degree of Doctor of Philosophy in Botany

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Bioactive compounds identified through GCMS and LCMS analysis were subjected to molecular docking studies suggested that potential pharmacological implications of *R. tetraphylla* in drug design and development. *In silico* docking studies were accomplished using three different protein structures (PDB IDs: 6Y8M, 6B8Y, 1GEN) with various ligands selected for their potential in wound healing applications. The binding affinities of the ligands were evaluated, and their interactions with amino acid residues within the protein structures were analysed.

Protein structure with PDB ID 6Y8M, compounds such as Butyl cyclohexyl phthalate (-7.67 kcal/mol), and Isoreserpine (-8.25 kcal/mol) showed stronger binding affinities. Similarly, in the protein structure with PDB ID 6B8Y, Butyl cyclohexyl phthalate (-7.70) and Carapanaubine (-8.63 kcal/mol) exhibited strong binding affinities. In this background of the protein structure with PDB ID 1GEN, 1-Naphthalenepropanol (-7.69), Carapanaubine (-8.22 kcal/mol) displayed strong binding affinities, while others like Butyl cyclohexyl phthalate (-6.29 kcal/mol), Serpentine (-6.83 kcal/mol), Yohimbine (-6.23 kcal/mol), and Isoreserpine (-5.98 kcal/mol) also formed significant interactions.

The docking studies provide insight the potentials of ligand-protein interactions within the given protein structures, contributing to a respective understanding of their pharmacological significance and potential therapeutic applications in wound healing. It contributes the molecular mechanisms underlying alkaloid metabolism in *R. tetraphylla* and their implications for the development of novel therapeutic agents for wound healing property. Though, further research is required to investigate the clinical potential and safety profile of *R. tetraphylla* extracts to promote the formulation of wound healing drug.