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# ANTITUBERCULAR POTENTIAL OF BIOACTIVE PHYTOCONSTITUENTS FROM *ANDROGRAPHIS PANICULATA*: TARGETING DprE1 OF *MYCOBACTERIUM TUBERCULOSIS*

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**Abstract**. Tuberculosis (TB) remains one of the leading infectious diseases worldwide, and the emergence of multidrug-resistant strains has intensified the need for novel therapeutic agents. Medicinal plants continue to provide structurally diverse bioactive molecules with significant drug discovery potential. *Andrographis paniculata* (Kalmegh) is widely recognized for its antimicrobial and immunomodulatory activities and may represent a promising source of antitubercular lead compounds.

**Keywords:** *Andrographis paniculata*; Tuberculosis; DprE1; Molecular Docking; Molecular Dynamics Simulation; Drug Discovery

**Introduction.** Tuberculosis, caused by *Mycobacterium tuberculosis*, continues to pose a major global health challenge. The increasing incidence of drug-resistant TB has reduced the effectiveness of existing treatment regimens and necessitates the identification of new therapeutic candidates. *Andrographis paniculata* is an important medicinal herb extensively used in traditional medicine for the treatment of infectious and inflammatory disorders. Although several pharmacological properties of the plant have been reported, its phytoconstituents remain inadequately explored against DprE1, a validated enzyme involved in mycobacterial cell-wall biosynthesis.

**Research Methodology.** Ten reported phytoconstituents of *A. paniculata* were selected from published phytochemical literature and screened against DprE1 of *M. tuberculosis* (PDB ID: 4P8N). Molecular docking studies were performed to evaluate binding affinity and interaction profiles within the active site. Top-ranked compounds were further assessed for physicochemical properties, drug-likeness, and pharmacokinetic behavior using in silico ADME tools. The most promising ligand–protein complexes were subsequently subjected to 100 ns molecular dynamics simulations to evaluate structural stability and persistence of binding interactions.

**Results and Discussion.** The investigated phytoconstituents demonstrated significant interactions with key residues present in the DprE1 binding pocket. Several compounds exhibited favorable docking scores and interaction patterns comparable to reported DprE1 inhibitors. Molecular dynamics simulations further confirmed the stability of the top-ranked ligand–protein complexes throughout the simulation period. ADME analysis indicated acceptable pharmacokinetic characteristics and compliance with commonly accepted drug-likeness parameters, supporting their suitability as potential lead molecules.

Conclusion. The present investigation highlights the potential of *Andrographis paniculata* as a valuable source of antitubercular phytochemicals. The identified compounds demonstrated promising interactions with DprE1 and favorable pharmacokinetic profiles, suggesting their potential utility in tuberculosis drug discovery. Further experimental validation is warranted to confirm their biological activity and therapeutic applicability.

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## CURRENT ISSUES OF USING MEDICINAL PLANTS IN PHARMACOLOGY

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**Abstract:** Medicinal plants have long served as an important source of therapeutic agents and continue to contribute significantly to modern drug discovery and pharmacological research. Plant-derived bioactive compounds, including alkaloids, flavonoids, terpenoids, and phenolic constituents, exhibit diverse pharmacological properties and have inspired the development of numerous conventional medicines. Despite their therapeutic potential, several challenges hinder the broader application and acceptance of medicinal plants in contemporary healthcare. A major concern is the lack of standardization and quality control, which leads to variability in the concentration and efficacy of bioactive compounds due to differences in geographical origin, cultivation conditions, harvesting practices, and processing methods. Furthermore, limited scientific validation, inadequate clinical evidence, insufficient toxicological evaluation, and the