

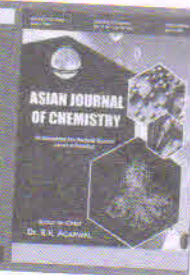


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Polyherbal Extracts as Antibacterial Agents: Phytochemical Profiling, MIC Assessment and *in silico* Targeting of Resistance Proteins

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This research explores the use of polyherbal extracts from *Eclipta prostrata*, *E. alba* and *Tridax procumbens* as a potent antibacterial solution, reflecting their significant role in contemporary medicine. Through gas chromatography-mass spectrometry (GC-MS) analysis, 45 distinct chemical compounds were identified in the ethanol extract, with the ethyl acetate extract revealing 35 different compounds. The chemical profiles of these compounds revealed substantial structural diversity and several demonstrated noteworthy antibacterial potential. The minimum inhibitory concentration (MIC) values against various bacterial strains indicated effective antibacterial activity, particularly against *E. coli* and *P. mirabilis*, with MICs as low as 6.25 µg/mL. The study emphasized three compounds, including 6-acetyl-5-(4-fluorophenyl) purine, for their potential in drug development, attributed to their chemical properties such as the ability to form hydrogen bonds and favourable solubility and lipophilicity. These findings underscore the therapeutic potential of polyherbal formulations, highlighting their value in addressing bacterial infections. The docking study demonstrates that 6-(3-fluorobenzylamino) purine exhibits a strong affinity towards ompC, murA and ESBL proteins through various interactions, indicating its potential as an inhibitory agent against drug-resistant proteins in the *Enterobacteriaceae* family. The positive docking scores across different proteins and interaction types underscore the compound's versatility and potential effectiveness in combating antibiotic resistance. Further research could validate these *in silico* findings and explore the clinical applicability of such compounds in treating drug-resistant infections.

Keywords: Polyherbal extract, Bioactive compounds, Lipophilicity, Molecular docking, Antibacterial activity.