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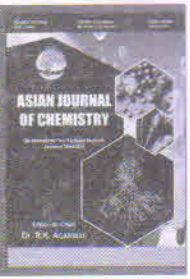

HR-LCMS based Metabolic Profiling, *in vitro* Analysis and Computational Insight of *Tabernaemontana divaricata* Hydroalcoholic Extract: A Multitargeted Approach to Combat Asthma

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Tabernaemontana divaricata (L.) is a prevalent horticultural species in Southeast Asia, also occurring in Australia, tropical Asia and Polynesia shows a diverse range of activities. To explore the molecular mechanisms and targets for prospective and effective therapeutic approaches, molecular docking enables the identification of the most promising targets in asthma. The present study investigates the multitargeted anti-asthmatic potential of phytocompounds isolated from *T. divaricata* by docking analysis. The hydroalcoholic extract of *T. divaricata* (TDHE) was obtained using the Soxhlet extraction and analysed for antiasthmatic activity. Chemical profiling of the extract was carried out using HR LC-MS/MS, which revealed the presence of 19 distinct phytocompounds. All the isolated 19 phytocompounds were docked against prime modulators in asthma such as histamine H1 (PDB: 3RZE), human interleukin-6 (PDB: 1ALU), IL4-IL4R-IL13Ra ternary complex (PDB: 3BPN), IL-25-IL-17RB-IL-17RA ternary complex (PDB: 7UWL), as well as IL-13 (PDB: 5KNH) receptors. The results demonstrated that TDHE possesses significant antiasthmatic potential, primarily through anti-inflammatory and antihistaminic mechanisms. Among the screened phytocompounds, kaempferol-3-O-rutinoside, 8-[4,5-dihydroxy-6-(hydroxymethyl)-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]-5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one and selaginpulvilin T exhibited strong binding affinities across all targeted receptors. In addition, ADMET profiling of the identified compounds supported their favourable pharmacokinetic and safety profiles. This study highlights the medicinal potential of *T. divaricata* phytocompounds as alternative or adjunctive therapeutic agents for asthma, offering a multitargeted strategy to modulate immune responses and alleviate disease symptoms. Future investigations should focus on clinical evaluation of the isolated phytocompounds to validate their efficacy and safety in asthma management.

Keywords: *Tabernaemonata divaricata*, Molecular docking, ADMET, Hydroalcoholic extract.