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In silico pharmacokinetics and molecular docking of three leads isolated from Tarconanthus Camphoratus L

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Objective: To investigate the pharmacokinetic and toxicity profiles and spectrum of biological activities of three phytochemicals isolated from *Tarconanthus camphoratus* L.

Methods: Several integrated web based *in silico* pharmacokinetic tools were used to estimate the druggability of Hispidulin, Nepetin and Parthenolide. Afterward, the structural based virtual screening for the three compounds' potential targets was performed using PharmMapper online server. The molecular docking was conducted using Auto-Dock 4.0 software to study the binding interactions of these compounds with the targets predicted by PharmMapper server.

Results: The permeability properties for all compounds were found within the limit range stated for Lipinski ′s rule of five. Only Parthenolide proved to be able to penetrate through blood brain barrier. Isopentenyl-diphosphate delta-isomerase (IPPI), uridine-cytidine kinase-2 (UCK-2) and the mitogenactivated protein kinase kinase-1 (MEK-1) were proposed as potential targets for Hispidulin, Nepetin and Parthenolide, respectively. Nepetin and Parthenolide were predicted to have anticancer activities. The activity of Nepetin appeared to be mediated through UCK-2 inhibition. On the other hand, inhibition of MEK-1 and enhancement of TP53 expression were predicted as the anticancer mechanisms of Parthenolide. The three compounds showed interesting interactions and satisfactory binding energies when docked into their relevant targets.

Conclusion: The ADMET profiles and biological activity spectra of Hispidulin, Nepetin and Parthenolide have been addressed. These compounds are proposed to have activities against a variety of human aliments such as tumors, muscular dystrophy, and diabetic cataracts.

Keywords: *Tarconanthus camphoratus* L., Hispidulin, Nepetin, Parthenolide, *In silico* pharmacokinetic, Molecular docking, PharmMapper server, and Auto-Dock 4.0 software