عنوان مقاله:

Molecular docking studies of Triphala with catalytic portion of HMG-CoA reductase enzyme

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خلاصه مقاله:

Introduction: Triphala, consisting of three fruits, Phyllanthus emblica L. (Phyllanthaceae), Terminalia bellirica (Gaertn.) Roxb. (Combretaceae), and T. chebula Retz, is a well-recognized Ayurvedic herbal formulation, used for various therapeutic purposes, including the treatment of dyslipidemia. Inhibitory activity against ۳-hydroxy-۳-methylglutaryl-coenzyme A (HMG-CoA) reductase, a rate-limiting enzyme in the endogenous cholesterol synthesis pathway, is an essential target for the management of hypercholesterolemia. This in silico study aimed to investigate the HMG-CoA reductase inhibitory activity of the phytochemical compounds derived from Triphala formulation by employing molecular docking analysis. Methods: Ten phytochemical constituents of Triphala formulation were selectively used for docking study by using the HMG-CoA reductase template (PDB: ۱HWK). Docking analysis was performed using AutoDock ۴.۲. The candidates were ranked by the binding energy parameters. Results: From the docking studies, the phytochemical compounds with HMG-CoA reductase inhibition could be classified into ۴ groups, including phytosterols, polyphenols, tannins, and flavonoids. Beta-sitosterol exhibited the highest binding affinity to HMG-CoA reductase with a binding energy of -۷.۷۵ kcal/mol. Conclusion: These ۱۰ phytochemical compounds in Triphala potentially exert their cholesterol-lowering effects via inhibition against HMG-CoA reductase. Nonetheless, .further in vitro and in vivo experiments should be conducted subsequently to confirm this finding

کلمات کلیدی:

In silico molecular docking analysis, Triphala-derived phytochemicals Dyslipidemia, HMG-CoA reductase inhibitor Beta-sitosterol