عنوان مقاله:

Evaluation of berberine inhibitory effects on influenza neuraminidase enzyme: A molecular dynamics study

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خلاصه مقاله:

Introduction: Due to the high prevalence and drug resistance reported for the influenza virus in recent years, much research is being conducted on the discovery and introduction of more effective drugs against the virus. In this regard, the present bioinformatics study examined the inhibitory effects of berberine, a plant-based alkaloid, on influenza virus neuraminidase using docking and molecular dynamics studies. Methods: To conduct this study, the three-dimensional structure and PDB file of influenza virus neuraminidase were prepared from the protein and molecular information database, and the structure file of the berberine and oseltamivir (as positive control) molecules were prepared from the PubChem database. Using GROMACS software, simulation and molecular dynamics calculations were performed in the absence of an inhibitor. Molecular docking studies were performed using AutoDock software, and re-simulation of the protein-ligand complex was performed using GROMACS software. Results: Berberine was bound to the neuraminidase molecule with three hydrogen bonds and eleven hydrophobic bonds at the binding site. The amount of binding energy (BE) of berberine and oseltamivir was equal to -۷.۹۳ and -۶.۲۷ kcal/mol with the estimated inhibition constant (EIC) of ۱.۵ and ۲۵.۲ μM, respectively. Over simulation time, the radius of gyration (Rg) of the enzyme at berberine binding increased, but there was no significant difference in system energy changes (TE). Conclusion: Due to berberine binding, structural changes occur in the secondary and tertiary structures of influenza virus neuraminidase. The large number of created bonds, the low level of binding energy, and the low concentration of the EIC indicate the high tendency of berberine to bind to the binding site of neuraminidase.

کلمات کلیدی: