عنوان مقاله:

Anti-Dengue potential, Molecular Docking Study of Some Chemical constituents in the leaves of Isatis tinctoria

محل انتشار:

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خلاصه مقاله:

Dengue infection is a major public health challenge in several parts of the world, especially the sub-tropical and tropical regions. The development of agents that are able to inhibit the dengue virus (DNV) replication are therefore of utmost significance. I. tinctoria is one of the most investigated Chinese herbs, which has been recognised to be effective in the treatment of dengue fever. However, the mechanisms through which it exhibits such biological activity of great importance are still unclear. A total number of about 27 compounds isolated from I. tinctoria leaves which have been identified and reported in the literature to be effective against dengue fever were investigated for their inhibitory potencies against dengue virus as novel drugs for treating early attacks of dengue fever. The compounds were optimized by employing a method of Density functional theory (DFT) and a basis set of B3LYP (6-31G**). The results of Molecular docking investigation between the compounds and the dengue viral protein (PDB: 6MO1) revealed that three of the compounds (GB-20, GB-19, and GB-6) possessing best binding energy in of -27.051, -26.193 and -24.664 kcal/mol respective were observed to inhibit the target through hydrogen bonds and hydrophobic interactions with amino acids residue of the protease binding site. The results of these studies would offer relevant insight into structural requirements for the development of effective and a specific therapeutic treatment against dengue virus infection.

کلمات کلیدی:

Molecular docking, Binding energy, Hydrophobic interaction, Conventional hydrogen bond, Insatis tinctoria