

Molecular Binding Study of the Main Constituents of Thymus Migricus with Trimmer Spike Protein of Corona Virus by Molecular Docking

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Abstract:

Thymus, which includes around 215 species, is an important genus of the Lamiaceae family. It comprises several species that are native to Iran and can serve as valuable medicinal plants because of their biological and pharmacological properties. Indeed, it is commonly used by the local inhabitants as an expectorant, antiseptic, antispasmodic, carminative, antirheumatic, and diuretic. Furthermore, this plants antibacterial, antifungal, and antiviral characteristics have made it a global source of potential antimicrobial agents. Analysis of the compounds of this plant by gas chromatography reveals the main compounds as the following: thymol (55.6 %), γ -terpinene (16.7 %), geraniol (4.6 %), p-cymene (4.0 %), limonene (2.6 %) E-Caryophyllene (1.9 %) and α -Pinene (1.8 %). The aim of this study was to investigate the molecular binding of the main components of Thyme migricus with the trimmer of spike protein of Corona virus by the molecular docking method. According to the method, first, the PDB file of ten main constituents of Thymus migricus was extracted from the Chempid database. Then, the PDB file of trimmer of spike protein was obtained from the rcsb site. In the next step, molecular binding analysis was performed for each compound using HDock online software. This study showed that although all of the analyzed compounds were able to bind to the coronavirus spike trimmer to some extent, Carvacrol exhibited the lowest docking energy and RMSD. To validate the genuine effectiveness of Thymus migricus compounds, more in vitro and in vivo researches are needed.

Keywords: Molecular Binding Study, Thymus Migricus, Trimmer, Spike Protein, Corona Virus, Molecular Docking

References:

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