

عنوان مقاله:

Investigation on Chemical Constituents of Foeniculum vulgare Essential Oil and the Molecular Docking Studies of its Components for Possible Matrix Metalloproteinase-13 Inhibition

محل انتشار:

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خلاصه مقاله:

Background: Foeniculum vulgare (Fennel) has a wide range of applications. Previous studies revealed the presence of different compounds in the essential oil (EO) of fennel fruit (FF). Matrix metalloproteinase-13 (MMP-13) participates in several human biological processes including the degradation of extracellular matrix proteins, activation or degradation of some significant regulatory proteins, and tumor cell invasion. Furthermore, the up-regulation of MMP-13 is associated with many disorders such as tooth caries and periodontitis, as well as the degradation of enamel and tissues around the implant and Alzheimer's disease. Therefore, the aims of the present study were to investigate the compounds of the EO of FF (EOFF) from the Hamadan district, along with performing molecular docking analysis to assess the binding affinity of four compounds originated from F. vulgare with the MMP-13. Finally, the study focused on evaluating the pharmacokinetic and toxicity characteristics of the compounds. Methods: Hydrodistillation method was used for obtaining the EO from FF. Then, gas chromatography-mass spectrometry was applied to identify the components of the EO. Molecular docking analysis was carried out using AutoDock software. Eventually, the pharmacokinetic and toxicity features of compounds were evaluated using bioinformatics web servers. Results: The results revealed the presence of fourteen compounds, among which e-anethole (86.86%), fenchone (74.3%), estragole (16.5%), and thymol (1.21%) were the main components. Based on the results, thymol, fenchone, e-anethole, and estragole could potentially bind to the MMP-13 active site, respectively. Conclusion: Regardless of several studies on the chemical constituents of EOFF, the subject has its own pharmacognostical importance. According to computational studies, EOFF has the potential for study on several human disorders such as cancer, tooth decay, and Alzheimer's disease.

کلمات کلیدی:

Foeniculum vulgare, Essential oil, Alzheimer's disease, Bioinformatics, Docking, Matrix metalloproteinase-13

