

عنوان مقاله:

Bioinformatics study of the effect of thymol on inhibiting acetylcholinesterase enzyme compared to donepezil and galantamine

محل انتشار:

پانزدهمین همایش بیوشیمی فیزیک ایران (سال: 1397)

تعداد صفحات اصل مقاله: 1

نویسندگان:

Mojgan Naderi - *Department of Biology, Faculty of Basic Sciences, Nourdanesh Institute of Higher Education, Meymeh, Isfahan, Iran*

Azizeh Asadzadeh - *PhD in Biochemistry, Department of Biology, Faculty of Basic Sciences, Nourdanesh Institute of Higher Education, Meymeh, Isfahan, Iran*

Fatemeh Heidarian Naini

خلاصه مقاله:

Background and aims: Alzheimer s disease is the most common cause of dementia and its major pathological symptoms include synaptic loss and neurons, astrogliosis and accumulation of protein-containing sediment. Today, one method to control the progression of Alzheimer s disease is prescribing herbal medicine, which inhibits the cholinesterase enzyme (EC 3.1.1.7). Currently, four AChE inhibitors such as Tarystyn, donepezil, rivastigmine and galantamine are potentially approved by the FDA to treat Alzheimer s disease. Thymol is a phenolic chemical compound with antibacterial properties and it is an ingredient in the active ingredient of many plants. In the present study, the efficacy of thymol on the inhibition of acetylcholinesterase enzymes compared to donepezil and galantamine has been investigated. Methods: In order to investigate the connection method of this compound, two protein crystal structures of acetylcholinesterase (4EY7,4EY6) and AutoDock 4.2 software were used and in the final stage, the results were analyzed using three AutoDockTools, DS Visualizer and Ligplot programs. Results: Thymol was able to bind to aminoacids in the active site of the enzyme in a manner similar to donepezil and gelantamine. The binding energy for this compound was -5.89 Kcal / mol and -5.28 Kcal / mol, which is created hydrogen bond with amino acid PHE295 and PHE338. Conclusion: Considering the high efficacy of thymol in the bioinformatics study and the formation of similar hydrogen bonds with donepezil and gelatamine, for further studies, the effect of this compound .can be studied in vitro and in vivo

کلمات کلیدی:

The acetylcholinesterase enzyme, Molecular docking, Thymol and Alzheimer s

لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/875295>



