In Silico Molecular Docking Study of Flavonoids with Alzheimer's Target Receptor and Their Simultaneous Identification and Quantification by HPLC in Some Herbal Formulations

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Abstract

The inhibition of acetylcholinesterase (AChE) is considered as best strategy for the treatment of Alzheimer's disease (AD). In this study some possible interactions between the receptor acetylcholinesterase AChE and some neuroprotective agents are reported through molecular docking. Results of the docking study shows effective binding with the receptors. Simultaneous identification and quantification of flavonoids was carried out using simple, rapid, accurate and sensitive HPLC method in some herbal formulations. The proposed method was successfully applied in the simultaneous determination of five flavonoids in several herbal preparations selected from the local pharmacy and from online market. The flavonoids were analyzed using C_{18} column in a gradient elution with acetonitrile and buffer ammonium acetate with the flow rate of 1.0 ml min^{-1} with UV detection at 350 nm. The HPLC method was completely validated.

Keywords

Acetylcholinesterase, Alzheimer's disease, neuroprotective agents, herbal formulations, molecular docking