

## The Interaction of Baicalein with Acetylcholinesterase is Comparable with the Known Acetylcholinesterase Inhibitor: A Molecular Docking Study

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**Abstract :** Background and Aim: Baicalein is a natural-origin flavonoid compound that has become the subject of recent research due to its therapeutic significance and pharmacological effects. Notably, reducing the risk of cancer, virus suppression and protective effects on several body systems, including the neurological system, is distinguished. It is known that the inhibition of acetylcholinesterase enzyme (AChE) is an effective mechanism in improving cognitive performance in patients with Alzheimer's disease (AD), the kind of dementia that is identified with loss of cholinergic pathways along with cognitive dysfunction. Accordingly, this study was planned to evaluate the interaction of baicalein with acetylcholinesterase (AChE) by molecular docking method in comparison with donepezil, the known AChE inhibitor that is used to improve the function of AD patients. Methods: The protein structure of AChE (PDB ID: 6CQT) was selected from Protein Data Bank; also, the molecular structures of baicalein (CID: 5281605) and donepezil (CID: 3152) were chosen from PubChem. Chimera 1.11.2 was used to prepare the enzyme structure and build all the pdb files. MGLTools 1.5.6, AutoDockTools-1.5.6 and AutoDock Vina (DOI: 10.1002/jcc.21334) were used for the docking process. The grid box included the binding site of chain A of AChE (PDB ID: 6CQT), which was defined as a rigid target with no flexible residue. Results: According to the results of blind docking by AutoDock Vina, the best-calculated affinity for baicalein and donepezil in interaction with AChE (chain A) were -9.8 and -8.4 (kcal/mol), respectively. Conclusion: The results of the blind molecular docking with the rigid target revealed that baicalein showed better affinity in interaction with AChE (chain A) in comparison with donepezil, the well-known drug used in the treatment of Alzheimer's disease patients. It appears that more investigation and experimental studies can be beneficial to reveal the effect of baicalein on inhibiting AChE enzyme and usage in Alzheimer's disease.

**Keywords :** acetylcholinesterase, baicalein, donepezil, molecular docking

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