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Molecular docking studies of a phytocompound kanzonol B as a potential acetylcholine esterase inhibitor for epilepsy

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Abstract. The third most prevalent neurological condition in the world is epilepsy. It has become a major concern for both medicine and public health in recent years. Currently, there are many approved therapies to address epilepsy diseases, but most of them are often associated with undesirable effects. Recent studies have pointed out the advantages of Acetylcholine Esterase Inhibitors (AChEIs) in the treatment of epilepsy with their ability to modulate cholinergic transmission and neuroprotective effects. However, AChEIs have adverse drug effects, necessitating the design of a novel drug. Flavonoids have emerged as promising alternatives in neuropharmacology due to their reported positive role in cognitive dysfunction, learning, and memory deficits. Thus, we aimed to identify the potential Acetylcholine Esterase (AChE) inhibitory activity of kanzonol B. The molecular docking simulation was used in the current in silico investigation to evaluate kanzonol B's capacity to bind with Torpedo californica AChE (TcAChE). Additionally, ADMET screening was performed on kanzonol B to forecast its pharmacokinetic characteristics. According to our findings, kanzonol B exhibited a considerable binding affinity (-10.58 kcal/mol) against the TcAChE enzyme. It also complied with the drug-likeness characteristics and Lipinski's RO5. The standard drug donepezil had a binding affinity of -11.73 kcal/mol. But both donepezil and kanzonol B interacted with ARG289, PHE331, PHE288, TRP84, PHE330, ILE287, SER286, TYR334, GLY441, HIS440, and PHE290. According to these computer studies, kanzonol B may have a therapeutic use for epilepsy as a strong AChE enzyme inhibitor. Therefore, to confirm the encouraging findings of the current in silico work, we advise more experimental research.

***Keywords*:** acetylcholine esterase; kanzonol B; molecular docking; pharmacokinetics; drug-likeness profiles; epilepsy.

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