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ORIGINAL RESEARCH ARTICLE

Molecular docking and dynamics simulation studies on sakuranetin a phytomolecule targeting AChE receptor against Alzheimer's disease

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ABSTRACT

Alzheimer's disease (AD) is a common type of dementia, mainly characterized by neurodegeneration and memory loss with other cognitive impairments in the brain. AD is one of the fastest emerging irrecoverable diseases in the aging population. Moreover, the degeneration of central cholinergic neurons damages memory and leads to cholinergic dysfunction. Several natural phytomolecules and semisynthetic analogs have been used to treat AD for years. However, no preventive treatment is available to date because most of the available drugs/compounds have failed in clinical trials. AChE is one of the most promising therapeutic targets for symptomatic improvement in AD patients. The current study was done to screen several natural phytomolecules derived from the Verbenaceae family's Lippia graveolens (Mexican Oregano). Based on the in silico results, Sakuranetin was the best potential AChE antagonist (-8.24 kcal/mol), and the primary amino acid residues, i.e., Tyr124, Tyr341, Leu289, and Phe295, were involved in the active binding site of AChE. The compound has shown a good fit and can cross the blood–brain barrier (BBB) along with high levels of intestinal absorption. Furthermore, Sakuranetin and AChE complex was found to be stable as analyzed by 10 ns molecular dynamics simulations. Based on the free binding energy and stability, it may be concluded that Sakuranetin is a potential hit compound for treating Alzheimer's disease.