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Molecular Docking Studies of Phytochemicals from *Persea americana* to Treat Alzheimer's Disease

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Abstract

Alzheimer's disease (AD) is a fatal brain disorder that progressively degenerates brain cells. It poses a significant burden on healthcare and social care systems. Currently, there are only five drugs available to treat AD, but their use is limited due to their adverse effects, toxicity, and limited targets in AD pathology. As a result, finding an effective compound to fight AD is critical. Antagonizing beta-site APP cleaving enzyme 1 (BACE-1) and Acetylcholinesterase Enzyme (AchE) has become a novel therapeutic approach. This study is aimed to uncover potential drug candidates from 8 phytochemicals from *Persea americana* (Avocado) to target BACE-1 and AchE through protein-ligand docking using Autodock vina 1.2.6. 3D structures of the targets were downloaded from RCSB, and the structures of the phytochemicals were retrieved from the NCBI PubChem database and then the docking procedure was executed. Receptor-ligand interactions were observed in BIOVIA-DS and pharmacological properties were analysed using SwissADME webtool. Naringin showed the lowest binding affinity (-9.7 kcal/mol) against BACE-1 and luteolin showed the lowest binding affinity (-10.1 kcal/mol) against AchE. With respect to H-bond, GLN73 and GLY34 were identified as common amino acids of BACE-1 while TYR71, VAL69 and PHE108 were identified to involve in hydrophobic bonds. Considering H-bond in AchE, TYR121 and GLU199 were identified in common while TRP84 was identified with respect to hydrophobic interactions. Luteolin obeys the Lipinski's rule whereas naringin does not obey pharmacokinetic properties. Based on the results, luteolin found to be a promising drug candidate to target both the receptors. In vivo and in vitro research can be developed based on this research findings.

Keywords: *AchE, Alzheimer, BACE-1, Autodock*