Review of: "Design and Molecular Screening of Various Compounds by Molecular Docking as BACE-1 Inhibitors"

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Potential competing interests: No potential competing interests to declare.

The study investigates the critical realm of Alzheimer's disease treatment, specifically targeting the Beta Secretase Amyloid Cleaving Enzyme (BACE-1) as a key therapeutic path. The introduction clearly sets the stage by elucidating Alzheimer's disease as a difficult challenge in the medical landscape due to its neurodegenerative nature and lack of a conclusive cure. This contextualization is crucial for understanding the significance of BACE-1 inhibition and the potential of natural compounds in mitigating Alzheimer's progression. Molecular docking serves as a pivotal tool in elucidating potential interactions between target proteins and small molecules, which is effectively utilized in this study. By employing modified compounds derived from flavonoids, ferulic acid, and donepezil, the researchers explore paths for BACE-1 inhibition. Identifying key residues within the BACE-1 active site provides valuable insights into the mechanisms underlying effective inhibition. The emphasis on Asp228, Thr232, Tyr71, Thr72, and Gly11 elucidates the structural determinants of ligand binding, enhancing the study's credibility and relevance. The study's focus on derivatives of natural compounds such as Baicalein, Myricetin, and Quercetin underscores the potential of these agents in Alzheimer's therapy. By comparing docking scores, alignment with Lipinski's rule, and toxicity profiles, the researchers offer a comprehensive evaluation of their efficacy and safety.

While the study presents compelling findings, it is essential to acknowledge potential limitations such as the need for detailed BBB crossing ability of molecules. Additionally, elucidating the precise mechanisms underlying BACE-1 inhibition and exploring potential synergistic effects with existing therapies could enhance the study's translational impact.