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

Jyothi C Sistla[1]

1 State University of New York at Stony Brook

Potential competing interests: No potential competing interests to declare.

The study addresses a gap in Alzheimer's disease (AD) research by focusing on compound design and screening as BACE-1 inhibitors. Molecular docking techniques were used with modified compounds derived from natural products such as flavonoids and ferulic acid, demonstrating a novel drug discovery strategy for AD. The identification of active site key residues in BACE-1, as well as the rationale for selecting compounds based on docking scores, Lipinski's rule, and toxicity, suggests potential lead molecules.

Include detailed information about molecular docking methods, including the software and parameters used in the study. Discuss the limitations of in silico approaches and the importance of experimental validation in cellular or animal models. Discussions of lead compounds' mechanisms of action in inhibiting BACE-1 and how they affect amyloid-beta production are needed. Simple experimental validations, such as binding or enzymatic assays, would also improve the reliability of computational predictions.

Given the complexity of Alzheimer's disease and the challenges of drug development, include a sentence in the discussion about strategies for combination therapies or targeting multiple pathways related to AD pathology. The study's methodology and rationale are well-organized and scientifically informative. Addressing these issues would enhance understanding and applicability in the context of Alzheimer's disease drug discovery.