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.

This work presents an interesting exploration into the design of potential BACE-1 inhibitors for Alzheimer's disease treatment. The in silico studies and detailed binding interactions discussed are promising, highlighting the potential of natural compounds like Quercetin, Myricetin, Baicalein, and Ferulic acid derivatives as anti-Alzheimer's agents. Overall, this study contributes to the ongoing efforts in developing novel treatments for Alzheimer's disease. However, the article can be improved if the authors address the following concerns: .

Abstract

- Mention the techniques/tools used for molecular docking.
- Mention the role of BACE-1 in Alzheimer's pathology.
- Specific compounds are mentioned but no docking scores, drug likeness, or toxicity profiles.
- Mention briefly how these results can be validated and the potential limitations of the study.

The Introduction and Literature Review. It does appear like a dissertation work, but the authors can reformat the article to the traditional form for journal publication.

Methods: The authors may wish to address the issue of promiscuity of ligands as this is very important in drug discovery. In silico tools can be used for this prediction, such as SWISSADME.

Results and Discussion: Limitations should be discussed, and these include methodological limitations, potential limitations in data interpretation, and the acknowledgement of the limited scope of the study and the need for broader investigations to validate findings across a wider range of compounds or biological assays.

Conclusion: It is too lengthy, and some of the facts presented may be moved into the Results and Discussion section. The conclusion briefly mentions the failure of certain BACE-1 inhibitors in clinical trials but does not discuss the avenues for future research.

Future research directions would include experimental validation (molecular dynamics simulation, in vitro and in vivo methods), more optimization of compounds, exploring mechanistic insights, clinical translation, and better comparison with existing inhibitors (pharmacodynamics and pharmacokinetics). `The authors must also consider the fact that binding does not necessarily suggest bioactivity.