

## 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.

Based on the extensive review of the document titled "Design and Molecular Screening of Various Compounds by Molecular Docking as BACE-1 Inhibitors," here are some of my observations and recommendations:

- Introduction provides a comprehensive background and includes relevant references to Alzheimer's disease, its
  pathology, and the role of BACE-1 as a therapeutic target.
- The references cited are highly relevant and current, focusing on Alzheimer's disease, BACE-1, and previous studies
  on molecular docking and inhibitors.
- The research design, focusing on molecular docking to screen various small molecules as BACE-1 inhibitors, is appropriate and well-justified for addressing the research question.
- The methods, including molecular docking procedures and construction of a chemical library, are adequately described, allowing for reproducibility.
- Results, including docking scores and interactions of screened compounds with BACE-1, are clear but figures
  are poorly presented with table details. Some of the figures look like they are cropped from some sources
  (maybe JPEG images) and out of the frame, look unevenly enlarged with some background texts and Fig. 8
  missing. ALL figures and texts need readjustments to look clear and precise. Revisions about the figures and
  tables look minor but are very important, informative and impactful part of the document.
- The conclusions are well-supported by the results, indicating that derivatives of Baicalein, Myricetin, Quercetin,
   Donepezil, and Ferulic Acid exhibit promising BACE-1 inhibitory activity.
- The quality of English is good, with a few minor errors that do not impede understanding but can be improved.
- Plagiarism has not been detected, and the document appears original based on its context and the detailed presentation of novel research findings.
- There are no obvious signs of inappropriate self-citations. The references are appropriate and contribute to the study's context.
- There are no apparent ethical concerns. The study seems to have been conducted with scientific integrity, and there is a clear declaration of no competing interests.
- The study presents original research on the molecular docking of various compounds as BACE-1 inhibitors, contributing novel insights into potential Alzheimer's disease treatments.
- The content is highly significant, providing valuable insights into potential new inhibitors for BACE-1, which is a crucial target in Alzheimer's disease research.



- The document is well-structured and presented logically and coherently.
- The study is scientifically sound, with a rigorous methodology, detailed analysis, and logical conclusions based on the
  results.
- The topic is of high interest to readers in neuroscience, pharmacology, and related fields focusing on Alzheimer's disease research.
- The document has high overall merit due to its contribution to understanding potential BACE-1 inhibitors, which is crucial for Alzheimer's disease treatment research.
- Based on the review, the document should be accepted for publication with minor revisions. The authors could benefit
  from a thorough proofreading to correct minor typographical errors and possibly expand on the discussion regarding
  the implications of their findings for future research and therapeutic development.
- In conclusion, the document presents valuable research on the molecular docking of compounds as BACE-1 inhibitors
  for Alzheimer's disease. With minor revisions, especially in proofreading and possibly expanding the discussion on
  implications, it should be a strong candidate for publication.

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