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

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Potential competing interests: None declared

Reviewer's Comment on Qeios ID: 9OCR7D:

The manuscript titled "Design and Molecular Screening of Various Compounds by Molecular Docking as BACE-1 Inhibitors" is engaging. It focuses on the devastating neurodegenerative disease known as Alzheimer's Disease (AD) and proposes a therapeutic solution in the healthcare sector. In this experiment, the authors employ the molecular docking technique to establish various modified compounds as anti-AD agents. The overall findings are promising and hold potential for effective treatment against AD. The authors' commitment to addressing this crucial disease is commendable. However, certain aspects of the manuscript require further clarification. Notable concerns are outlined below and must be resolved prior to acceptance.

1. The current manuscript title, "Design and Molecular Screening of Various Compounds by Molecular Docking as BACE-1 Inhibitors," lacks reference to Alzheimer's disease (AD). It is recommended to enhance clarity by incorporating "Alzheimer's Disease" into the title. The proposed new title would be: "In silico designing of various anti-Alzheimer's disease components by targeting β-secretase". This new title highlights the focus on repurposing modified drugs/components and targeting β-secretase as a potent treatment regimen against AD using computational methods.
2. Revise and improve the abstract to enhance its clarity and completeness. Integrate a brief description underscoring the significance of selecting BACE-1 as a focal point. A briefing about the materials/methods should be incorporated within the abstract. A few words that summarize the importance of this in silico study and future scope should be incorporated within the abstract section as concluding remarks. Conclude the abstract by emphasizing the pressing need for hands-on laboratory investigations to validate the outcomes presented in this manuscript.
3. The introduction section requires refinement as it currently lacks focus. It is suggested to consolidate the literature review and aims & objectives within the introduction, ensuring it provides a comprehensive overview of the materials and methods employed in this study. Furthermore, it is essential to incorporate a review of both dry and wet studies on anti-Alzheimer's disease (AD) components, including recent advancements. Emphasis should be placed on referencing recent studies that concentrate on the development of effective components for AD treatment, particularly those targeting BACE-1. This approach will enhance the significance and relevance of the current study by acknowledging existing findings and identifying gaps in the literature. Aligning the introduction with the revised abstract will ensure consistency between the two sections.
4. In the "Materials and Methods" section, it's recommended to include a flow chart for an overview of the computational

approach. This chart should detail the step-by-step process, including the software, server names, and addresses used for in-silico identification of potent anti-AD drugs. To facilitate replication, authors should provide specifications of the computational workstation they employed. For accurate molecular docking, proper preparation of the active site and grid box is necessary, along with validation of the docking method. After molecular docking, molecular dynamics must be included to support the findings. To bolster their results, the authors should incorporate studies on the molecular targets and biological activity analysis of the predicted anti-AD components. The authors can find relevant articles to enhance their "Materials and Methods" section and incorporate citations to support their revised manuscript.

a. https://doi.org/10.1186/s40064-016-2996-5 (May be used for active site analysis using CastP web server).
b. https://doi:10.1016/j.meegid.2021.104951 (May be used for molecular dynamics)
c. https://doi.org/10.1186/s42269-020-00479-6 (May be used for molecular target anticipation)
d. https://doi.org/10.1155/2023/5469258 (May be used for biological activity analysis)
e. https://doi.org/10.1007/s10989-023-10535-0 (May be used for molecular dynamics)

1. The conclusion section contains scientific inaccuracies and could benefit from additional clarity. Consider enhancing its comprehensibility. It might be beneficial to introduce a discussion section as well, addressing the potential for future improvements and strategies to enhance effectiveness in upcoming endeavors. The discussion section should contain a comparison of the findings of this research with relevant ones. It must contain the pros and cons of different types of anti-AD agents. This section could be further comprehended, and a paragraph can be added on demand and future scope within the section.
2. It is recommended to thoroughly review all references in the manuscript for typographical errors. Furthermore, ensure that the reference section adheres to the formatting guidelines specified by the journal.
3. The manuscript exhibits a lack of proficiency in English language usage encompassing grammar and writing skills. It is imperative to engage an expert language editing service or a native speaker adept in writing to thoroughly review the entire manuscript. A comprehensive revision is essential to enhance the manuscript's overall command of the English language.
4. The manuscript should incorporate an important section, namely ‘Author Contributions and Affiliation’. Top of Form
5. Please submit the revised manuscript after conducting a plagiarism check that yields a result between 10% and 15%.