

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

Muhamamd Naveed¹

1 University of Central Punjab

Potential competing interests: No potential competing interests to declare.

The authors have a good research topic, "Design and Molecular Screening of Various Compounds by Molecular Docking as BACE-1 Inhibitors," in which they designed a drug against Alzheimer's disease. However, the following points should be taken into consideration and addressed:

- 1. The title does not explain the main idea of the research manuscript. It should be changed to reflect the research, which involves designing a drug candidate for Alzheimer's.
- 2. In the abstract, "Beta Secretase Amyloid Cleaving Enzyme, or BACE-1, also known as β-secretase, is one of the major drug targets for the treatment of Alzheimer's disease. Molecular docking was performed with modified compounds derived from flavonoids (Quercetin, Myricetin & Baicalein), ferulic acid, and donepezil with the BACE-1 protein." What is the correlation of BACE-1 and flavonoids? This should be mentioned, and the abstract needs to be revised.
- 3. Is this a review or a research article? The authors need to clarify this confusion, as the research manuscript does not include subheadings in the introduction or any literature review like a thesis.
- 4. Again, the aims and objectives heading is not needed. The whole introduction needs to be revised and should follow typical manuscript guidelines.
- 5. In the materials and methods section, the numbering is totally wrong, and the headings are poorly made. There is no junction between any steps mentioned in the methodology.
- 6. In the results and discussion, heading 5.1 is totally missing.
- 7. The conclusion is too long, and it should discuss the future aspects, the main outcome, and the applications of your research.
- 8. There is no junction between any headings or results.
- 9. Please go through the following drug design articles in order to follow the pattern.
- Revolutionizing treatment for toxic shock syndrome with engineered super chromones to combat antibiotic-resistant
 Staphylococcus aureus
- Naveed, M.; Shabbir, M.A.; Ain, N.-u.; Javed, K.; Mahmood, S.; Aziz, T.; Khan, A.A.; Nabi, G.; Shahzad, M.; Alharbi,
 M.E.; et al. Chain-Engineering-Based De Novo Drug Design against MPXVgp169 Virulent Protein of Monkeypox Virus:
 A Molecular Modification Approach. *Bioengineering* 2023, 10, 11. https://doi.org/10.3390/bioengineering10010011
- Halogens engineering-based design of agonists for boosting expression of frataxin protein in Friedreich's ataxia

Overall review:



The authors should follow the typical guidelines and should go through several in silico-based drug designing articles to follow the pattern of a publication. The manuscript does not appear to be a thesis/manuscript or review article. A lot of work is required to convert this great research into a publishable article.