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Peer Review Reports

Computational assessment of hypoglycemic potency and ADMET evaluation of *Alpinia galanga* bioactive compounds against the alpha-glucosidase enzyme

The article went through 4 rounds of review and all 3 reviewers agreed in advance to publish their review reports disclosing all identities.

The authors agreed to disclose the reviewers' reports and their responses to the reviewers' comments.

Disclaimer: The peer review report content is the entire copy of the reviewers' and authors' comments. Typing and punctuation errors are not edited.

ROUND 1

Reviewer A: Arif Nur Muhammad Ansori
Recommendation: Revisions Required

First of all, this manuscript is good and well-written. However, I may require some comments on the following issues. Basically, this manuscript is acceptable.
However, in order to improve the readability of the paper by an English editing service as various sentences are mistyped.
Title: The title is easy to follow and no mistakes.
Abstract: This section was well-written and easy to understand. In addition, the study's objective and the state of the art of the study is clear. Furthermore, the keywords should represent the study.
Discussion: The discussion of the study is lack of information about the important topics. To develop a systematic discussion, the authors should mention the limitation(s) of the study.
Conclusion: In this part of the paper, the authors have established the conclusion of this study.
References: Many references are out of guidelines. Please kindly check the references again, do not include the old references, and check the abbreviation of the journals/proceedings. Please mention many high-quality related publications, such as:
> https://journal2.unusa.ac.id/index.php/IJMLST/article/view/1854
> https://www.scienceopen.com/hosted-document?doi=10.15212/bioi-2024-0032
> https://www.sysrevpharm.org/abstract/a-review-of-an-important-medicinal-plant-alpinia-galanga-l-willd-66295.html
> https://medicopublication.com/index.php/ijfmt/article/view/14730
> https://www.ajchem-a.com/article_201715.html

Reviewer B: Faruk Hasan
Recommendation: Revisions Required

Please go through the manuscript, read carefully and follow the instructions
Reviewer's Files

ANSWERS TO ROUND 1

Author's Files

ROUND 2

Reviewer A: Arif Nur Muhammad Ansori
Recommendation: Accept Submission

The reviewer did not leave any comments at this stage.

Reviewer B: Faruk Hasan
Recommendation: Accept Submission

The reviewer did not leave any comments at this stage.

Reviewer C: Deiver Alessandro Teixeira
Recommendation: Revisions Required

This article seeks to relate the compound Miglitol, which is currently used in the treatment of diabetes, with compounds alpha-glucosidase-α-bergamotene, alpha-glucosidase-β-farnesene, alpha-glucosidase-β-bisabolene, alpha-glucosidase-gal acetate, alpha-glucosidase-β-pinene, and their respective complexes with the alpha-glucosidase protein.
The researchers present Binding Affinity and Chemical Interaction as arguments. In this sense, the researchers work on the hypothesis that the "new" structures have a lower interaction energy when compared to the alpha-glucosidase-miglitol complex, which is -21.8 kJ/mol. In view of this, I have some questions:
1. When the computer simulations were performed, were all the atoms in the system free? Could they adjust freely?
2. Could the difference of no more than 3kcal/mol between the complex with Miglitol and the other complexes be associated with a conformational adjustment of the protein? Or is this difference related only to the interaction in the active site? How could this be proven?
3. From what I can see in Table 1, the interactions of these "new compounds" with the protein are of a physical nature, is that correct? Therefore, is it possible to say that these interactions can influence the inactivation of a protein?
4. Was the solvent effect considered in the simulations?

The answers to these questions are crucial for the work, because if they are not sufficiently acceptable, the work would be a good hypothesis to continue the studies.

ANSWERS TO ROUND 2

Author's Files

ROUND 3

Reviewer C: Deiver Alessandro Teixeira
Recommendation: Revisions Required

I congratulate the authors for the research carried out; however, since the calculations were performed without considering the solvent effect and the differences in interaction energies between the complexes are very low, I assess the manuscript as still needing further study.
The purpose of the study is very important and has great impact, but I see that the conclusions still need to be better supported by the calculations.
Solvent effects can significantly alter the results and, as stated, were not considered in the calculations.

ANSWERS TO ROUND 3

Author's Files

Peer Review Reports

ROUND 4

Reviewer C: Deiver Alessandro Teixeira
Recommendation: Accept Submission

Congratulations to the authors for the study carried out.

ACCEPT SUBMISSION

29 May 2025