

Phytochemical, antioxidant, and enzyme inhibition potential exploration of *Nyctanthes arbor-tristis* via *in vitro* and *in silico* methods

The article went through 2 rounds of review and all 2 reviewers agreed in advance to publish their review reports without 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: Anonymous

Recommendation: Revisions Required

In general, the work presented in here is of very high quality and very well explained. I liked that the authors mixed experimental with computational, it is very interesting. However, I believe that, at the moment, it still needs some small polishing.

- 1- During the manuscript, the authors cite kilo in capital, please check it, since it should be k.
- 2- There is some style changing in the free energy calculation description section
- 3- The experimental results are all presented as tables, and shown in a sequence for increasing activity. I miss some context about these data, otherwise the cut for the computational section is too sharp.
- 4- Docking scores normally consider a several amount of quantities, and the score is normally just a number. I maybe got lost in the text, I do not understand how did the authors managed to get a score as an energy value.
- 5- During the first paragraph in section 3.7.2.1, and other sections as well, an "apo structure" is cited. What would it be?
- 6- I would suggest to improve the connection between the computational data and the experimental one, it is still not so clear.

In general, the work is very well explained, all details are presented and the authors have done it in a very didactical way. Congratulations.

No Reviewer Files

Reviewer B: Anonymous

Recommendation: Revisions Required

I appreciate the authors for exploring the enzyme inhibition activity of *Nyctanthes arbor tristis* which is an important medicinal plant. I appreciate the extensive phytochemical analysis of the leaf extracts of the plant. I have a few suggestions to incorporate in the manuscript for its improvement:

- 1- In section 3.4. Antioxidant Antioxidant Activity, correct the typographical error. In place of HPPH, it should be DPPH.
- 2- In some references, the scientific name of the plant is not in italic; please make the correction.
- 3- In the text, at some places the author's name was mentioned, and again, in the bracket, the author's name with the year of publication is mentioned. My suggestion is that if a reference is mentioned in the bracket, then delete the name of the author before the bracket.

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- 4- My suggestion is to add the data of phytochemical/metabolic characterization of the extract, either GC MS, LC MS, or HRMS. It provides information about the presence of metabolites that you have selected for docking purposes.
- 5- Other than DPPH, some new methods can be used to measure the antioxidant activity of the extract.
- 6- My suggestion to the author is to read these manuscripts for better presentation and add the following references in the text: <http://dx.doi.org/10.1590/s2175-97902022e21180>; <http://dx.doi.org/10.1007/s40415-016-0283-x>.

No Reviewer Files

ANSWERS TO ROUND 1

Author's Files

ROUND 2

Reviewer A: Anonymous

Recommendation: Accept Submission

I would like to thank the authors for considering my comments.

No Reviewer Files

Reviewer B: Anonymous

Recommendation: Accept Submission

The review will not be published at the request of reviewer B.

No Reviewer Files

ARTICLE ACCEPTED