

Review of: "Expansion of the antifungal activities through in silico docking study of compounds from *Albizia lebbbeck* fruits"

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Potential competing interests: No potential competing interests to declare.

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Authors: Bosco et al.

In this research article entitled "**Expansion of the antifungal activities through in silico docking study of compounds from *Albizia lebbbeck* fruits**", the authors evaluated the antimicrobial effects of some natural compounds, which had been previously identified in *Albizia lebbbeck* fruits. The authors used a combined in silico and in vitro approach.

Here are some points that should be taken into account before processing further.

Comments to the authors:

1. The list of authors is not the same. The author Serges Honoré Ediah Ngalaha does not exist in one of the versions. Please check.
2. In figure 1, the authors should respect the order of the studied chemical structures. For example, why did compound no. 14 exist in the middle and not at the end?
3. In the abstract, the authors did not mention the validation of their in silico findings by the experimental antimicrobial results, only by "supporting the experimental results."
4. The authors should report that the co-crystallized ligands have been removed after being used for the selection of the grid box. Some supporting references can be considered: <https://doi.org/10.3390/md22020085>, <https://doi.org/10.1080/15376516.2023.2301670>
5. What are the reasons behind the selection of only compounds no. 2 and 7 for the experimental assays, even though some other chemicals have better binding scores, particularly compound no. 7, which has only -3.5 and -5.2 Kcal/mol? So far, the sentence "the reason being the least quantities of most of the isolated compounds" sounds useless.
6. The experimental study concerned one fungal strain only (*Candida albicans*) and four bacterial strains, but the authors are reporting mainly the antifungal effect!!!
7. The antibacterial findings are overlooked.
8. It would be better to add some very recent supporting references to the sentence "Nowadays, almost all ... theoretical parts." with some references: <https://doi.org/10.1080/15376516.2023.2301670>, <https://doi.org/10.3390/ph16091305>

9. Insert the unit of the docking scores for the columns 2 and 3 of Table 1. I guess "Kcal/mol."
10. The conclusion of the study is already misleading as 7 compounds have affinities less than -2 kcal/mol and 10-11 compounds have affinities less than -6 kcal/mol, but the authors still mentioned the 14 natural compounds in the conclusion itself.
11. The English language is fine, but small editing is required; for example, the last sentence of the introduction should be checked.
12. The authors should think about mentioning the i) limitations of the study as it would add additional value to the discussion and ii) benefits of natural compounds and phytotherapy (<https://doi.org/10.1201/b22842-7>).