

Peer Review

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

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The study presents an *in silico* investigation of the antifungal properties of compounds isolated from the fruit of **Albizia lebbeck** through molecular docking studies. This computational approach identifies specific interactions between the ligands and target proteins associated with **Candida albicans**, providing valuable data for antifungal drug development.

The manuscript is well-organized and addresses a relevant topic in computational chemistry and pharmacology. However, certain areas can be improved to enhance the impact and clarity of the article.

1- Add a table summarizing the docking scores for compounds (1-14) with the proteins 5TZ1 and 5FSA, along with the key interactions (H-bonds, π - π interactions, etc.).

2- Include bar charts or diagrams to visualize the differences in docking scores or the most frequent interactions.

3 - Expand the discussion on how *in silico* results predict the experimentally observed behavior.

4 - Include a comparative analysis showing how compounds with high docking scores might be prioritized for future experimental assays.

5 - Verify and clarify whether the compounds studied are indeed novel or if their known antifungal activities have been previously reported. For example, compounds like quercitrin and eugenol derivatives have already been established as antifungal agents, and this should be cross-checked with the new findings.

The manuscript is built on a solid foundation and addresses a relevant topic, but its impact and clarity can be significantly improved with visual enhancements, a deeper focus on experimental correlation, and more concise writing. Additionally, verifying the known antifungal activity of some compounds and derivatives considered in the study is essential. If these recommendations are implemented, the manuscript could make a valuable contribution to the field of antifungal drug discovery.

Declarations

Potential competing interests: No potential competing interests to declare.