Review of: "Expansion of the Experimental Antifungal Activities Through in Silico Docking Study of Compounds From Albizia Lebbeck"

Ali Bahadur

Potential competing interests: No potential competing interests to declare.

Title: Expansion of the Experimental Antifungal Activities Through in Silico Docking Study of Compounds From Albizia Lebbeck

General Comments:

This manuscript describes an in silico molecular docking study investigating the antifungal potential of compounds isolated from Albizia lebbeck against Candida albicans. The study aims to support and expand previous experimental antimicrobial testing of the compounds. Overall, the work is well presented, and the computational approach is relevant to the research objectives. A few minor revisions are suggested to improve clarity and address limitations.

Specific Comments:

Introduction: - Clearly introduce the protein targets (5TZ1 and 5FSA) used in the docking earlier in the introduction for context. Recent literature should be cited in the Introduction section, and improve the introduction by consulting these papers.: 10.1016/j.molstruc.2021.131136, 10.3390/molecules27217368 , **10.1002/bio.4044**, 10.1016/j.molstruc.2020.129422, 10.1016/j.arabjc.2023.104847, 10.1016/j.molstruc.2021.131145

Methods: - Provide more details on the docking protocol parameters like docking algorithms, scoring functions used.

Results & Discussion:

- The discussion of structure-activity trends could be expanded, e.g., relating activity to physicochemical properties.

- Limitations of the docking methodology should be acknowledged.

Tables/Figures: - Table 1 could include compound names for clarity, and the Figure quality could be improved for clarity.

Conclusions: - Overstatements about validating experimental results should be toned down given the limitations of docking methods.

Minor Revisions: - Ensure consistency in compound numbering. And - Standardize the formatting of references.

Recommendation: The study demonstrates a novel application of molecular docking to investigate natural products. With minor revisions to address limitations and improve clarity, the manuscript is suitable for publication after peer-review. The

work contributes computational insights that can aid future experimental assays.