

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

Nguyen Minh Quang<sup>1</sup>

<sup>1</sup> Industrial University of Ho Chi Minh City

Potential competing interests: No potential competing interests to declare.

Dear Editor and Peer Review Team, Qeios!

I sincerely appreciate the opportunity to offer a critique of this work. The text body contains a mention of our comments, which were all focused on the scientific facts from the investigation.

After reading this research, I think it should be published because it addresses antimicrobial outcomes using new and improved methodologies. However, I have a few observations regarding this study, even if the main idea of the work is valid and beneficial:

- The authors should include spectroscopic analysis for chemicals such as elemental analysis, IR, H-NMR, and <sup>13</sup>C-NMR.
- The lengths of the hydrogen bonds and the reasons why this interaction affects the activity must be explained for certain conformations between the ligand and the protein.
- How was the minimizing energy related to the protein receptor, and what was the nature of its use? Crucial details are needed for these kinds of descriptions.
- Given the limits of docking approaches, overstatements on the validation of experimental data should be moderated.
- There should be some 3D photographs among the best ones.

In summary, the research is excellent, and I approve it without changes because the simulation was performed using the final compound's active sites and stereoscopic structures, and the inhibition results were good—especially when compared to those of some antifungal medications.

Best regards,

Nguyen Minh Quang