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

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Potential competing interests: No potential competing interests to declare.

The manuscript entitled "*Expansion of the Experimental Antifungal Activities Through in Silico Docking Study of Compounds From Albizia Lebbeck*" has been submitted by Bosco *et al*., and contains the computational evaluation of some naturally extracted compounds. After careful evaluation, the author(s) are instructed to qualitatively improve the manuscript before submission of the revision. As a medicinal chemist, this study is okay for me, but I have some concerns related to molecular docking studies of this study. Molecular docking studies were performed so basically in this project. Some of the points that need to be considered for improvement in the manuscript are listed below:

1. Authors are suggested to evaluate the *in-vitro* anti-fungal activity of all the compounds, which will make the manuscript more interesting.
2. Clarify the order of figures/tables in the manuscript - why does table 1 come before figure 1? Though in the text, initially authors explain about figure 1 and then about table 1.
3. How did you determine the active site of the enzyme?
4. Could you please provide the superposition of the complex of the receptor and positive control compounds with the modeling complex of receptors and the extracted compounds?
5. Docking validation should be made by calculating RMSD values for molecular docking.
6. Explain the choice of the drugs taken as references for antifungal candidates.
7. English language, grammar, format, and typo mistakes are present and need to be fixed.