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.

Antifungal potentials of compounds isolated from Albizia lebbeck: An in silico study

1. Significance and Novelty:

The paper provides a theoretical examination of natural compounds isolated from the fruit of Albizia lebbeck, evaluating their potential antimicrobial activities against Candida albicans. The study is significant in the field of natural product-based pharmaceutical research. The paper's strength lies in its comprehensive methodology, utilizing a combination of in-silico docking and molecular simulation studies to investigate the antifungal potential of the isolated compounds. The authors provide detailed descriptions of the docking process, receptor grid generation, protein preparation, and examination of ligand-protein binding, which adds credibility to their findings. The results of this study could be valuable in guiding future experimental research on Albizia lebbeck and its potential applications in developing new antifungal agents.

2. Weaknesses:

- One major issue with the paper is that the results section is overly descriptive and lacks critical analysis of the findings. For example, the docking scores need to be interpreted, not just stated, and related to those of other similar studies. What does -2 to -7 mean?

- The paper is missing adequate discussion or comparison with previous studies. Without this, it is difficult to gauge the novelty or relevance of the findings. The authors only mention studies that carry out docking of the compounds, but they did not discuss their main findings. For example, how do the docking scores compare to those of other studies that use similar proteins?

- Authors should remove repetitive statements. For example, “The virtual screening of the antimicrobial activity performed on the crystal structure of sterol 14-alpha demethylase (CYP51) from *Candida albicans* in complex with the tetrazole-based antifungal drug candidate VT1161 (VT1) (PDB Id: **5TZ1**) and the crystal structure of sterol 14-alpha demethylase (CYP51) from a pathogenic yeast *Candida albicans* in complex with the antifungal drug posaconazole (PDB Id:**5FSA**) with natural compounds isolated from the fruit of *Albizia lebbeck* have shown promising antimicrobial results. In addition, this is the first docking study using natural compounds as ligands with the **5TZ1** and **5FSA** proteins”, has been stated in

both the introduction and discussion sections.

-Lastly, the conclusion does not sufficiently summarize the key findings or discuss their implications, making it difficult for readers to understand the study's significance. Authors should enhance the conclusion by summarizing the key findings, discussing their implications, and suggesting directions for future research. This will help readers understand the value of the study and its contribution to the field.