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.

This study presents a comprehensive investigation into the antifungal activities of various compounds isolated from Albizia Lebbeck, employing in silico docking methods. Using Maestro Schrödinger 4.2.1 software, the study focuses on the interaction of these compounds with sterol 14-alpha demethylase (CYP51) from Candida albicans. It integrates computational prediction with experimental validation for two of the compounds, providing insights into the potential antifungal properties of these natural substances.

Feedback and Suggestions:

Docking Validation: The study would benefit significantly from docking validation. While computational docking provides predictive insights, validating these predictions with experimental assays or additional computational methods can strengthen the reliability of the findings. This validation could involve cross-referencing with known inhibitors or conducting binding affinity tests.

Concerns with Docking Scores Below -2: The observation of some ligands having docking scores less than -2 warrants further investigation. This could indicate potential issues in the active site of the receptor or the methodology of the docking assay. It would be beneficial to revisit the docking parameters, including the consideration of receptor flexibility or the inclusion of water molecules in the docking site, to ensure accurate simulation of the binding environment.

Molecular Dynamics (MD) Simulation: Incorporating MD simulations would be a valuable addition to this study. MD simulations can provide dynamic insights into the stability of the ligand-receptor complex over time, offering a more comprehensive understanding of the binding interactions and the conformational changes of the protein-ligand complex.

Quantitative Structure-Activity Relationship (QSAR) Analysis: QSAR analysis can play a crucial role in understanding the relationship between the chemical structures of the compounds and their biological activities. Incorporating QSAR could aid in predicting the antifungal activities of these compounds more accurately and guide the design of new compounds with enhanced efficacy.

Density Functional Theory (DFT) Analysis: Including DFT analysis could provide deeper insights into the electronic properties of the ligands, such as the distribution of electron density, molecular orbitals, and their energy levels. This information can be vital for understanding the interaction mechanism at the molecular level and optimizing the compounds

for better activity.

Overall, the study presents a significant contribution to the field of natural antifungal agents. However, incorporating these additional computational analyses could significantly enhance the robustness and comprehensiveness of the findings.