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 authors must explain the following:

1. Criteria for choice of protein PDB structures.
2. How the mode of action of the observed experimental activity is related to the choice of docked protein structures.
3. Why docking validation is missing in the text?
4. Did you redock the co-crystallized ligand and calculate the RMSD? What proves that this docking procedure is reproducible?
5. Explain the choice of the docking site, knowing that several protein structures have different druggable sites.
6. Can you explain the procedure for protein preparation?
7. The ligand preparative procedure is unclear. You generated .mol files using ChemDraw but did not explain how 3D conformers were generated before docking.
8. How many conformers and tautomers were generated for each ligand?
9. What were the criteria for selecting the docked poses? Was it solely based on docking score or on ligand interactions?
10. Can you re-score your docked poses using another scoring method like MM-GBSA and attempt an interpretation of the structure-activity relationships?