Review of: "Expansion of the antifungal activities through in silico docking study of compounds from Albizia lebbeck fruits"

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Potential competing interests: No potential competing interests to declare.

1. Did you perform redocking and check the efficiency of your docking software? Why did you select the software Maestro Schrödinger 4.2.1? How much was the RMSD? Highlight the pharmacophore features or pharmacophore functional groups of each molecule.
2. Is a clear 3D ligand-protein interaction pictorial depiction required? Define the selected molecular docking zone - 5 angstroms or 3 angstroms?
3. What's the worth of conducting artificial computational studies later than once you have already done and published the in-vitro real system studies in 2022?
4. Measure and mention the H-bond lengths, and discuss the active site amino acid residues of the fungal protein enzyme.
5. Where is the standard docking score of 5TZI and 5FSA with their PDB-bound drugs? How do you correlate these inhibitor results with standard drugs with respect to potency?
6. Correlate the compounds 2 & 7 in-vitro potency with docking results with respect to docking score values, both having similar in-vitro inhibitory concentrations of 32 µg/mL but showing different docking scores -7.7, -7.8, -3.5, -5.7, respectively. Why is it so?
7. What are the future perspectives of this core design of studies? Can anyone benefit from antifungal drugs in the future under these perspectives?
8. I can't see HEM interactions clearly. Kindly share the clear, separate graphics.