

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

Hussien Ahmed Khamees

Potential competing interests: No potential competing interests to declare.

I have thoroughly checked the manuscript entitled, "Expansion of the Experimental Antifungal Activities Through in Silico Docking Study of Compounds From Albizia Lebbeck. "

In my opinion, this article could be interesting for publication, but before that, the following points have to be revised.

In subsection 3. Results and Discussion:

- 1- Authors should mention the length of the hydrogen bonds, at least for the best ligand-protein conformations,
- 2-  $\pi$ - $\pi$  is not a bond; it is a stacking interaction, so authors should modify it accordingly.
- 3- It is better if the authors also analyze  $\pi$ - $\pi$  and  $X\cdots H-\pi$  interactions because the ligands have multiple rings .
- 4- As a computational paper, some information about the docking protocol should be included, like the minimization energy, receptor preparation, and glide grid box dimensions,
- 5- Authors should write the full term for each abbreviation, like extra precision (XP).
- 6- The authors used one of the best insilico software (Schrödinger), which provides excellent figures, but they presented only 2D visualization, so they should present 3D visualization of the best conformation.