

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

Pınar Güller¹

¹ Atatürk University

Potential competing interests: No potential competing interests to declare.

Review Report,

In my view, the study entitled "Expansion of the Experimental Antifungal Activities Through in Silico Docking Study of Compounds From Albizia Lebbeck" is inadequate for publication in its current form in Qeios because of the followings:

1. The first sentence of the "Introduction" section should be deleted. It was also cited in the abstract. The abstract should be revised.
2. Why did the authors select Albizia lebbeck, and what are the uses of Albizia lebbeck? This should be mentioned in the "Introduction" section.
3. "A receptor grid was generated around the co-crystallized ligands for both proteins, and the ligands were docked using the glide XP module." How do the authors know that these ligands have affinity for the same site as the co-crystallized ligand? First of all, the binding sites on receptor proteins should be determined (allosteric site or active site), the grid box should be set to these sites, and the region to which ligands bind best should be selected; then an explanation should be made about the interaction types.
4. Grid box coordinates should also be given.
5. Validation of the method should also be done.
6. Statistical evaluations of the results should also be included.
7. Additionally, figures of antimicrobial studies should also be provided.
8. The results for *Candida albicans* were given, but where are the results on the four bacteria?