

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

Ricardo Luna¹

¹ Universidad Nacional Autónoma de México

Potential competing interests: Reviewing the manuscript, it is interesting, however: At least one of the compounds obtained and evaluated should be shown spectroscopic data, NMR, high resolution masses or elemental and infrared analysis. Since there are small and simple molecules to ignore their characterization. For certain conformations between the ligand and the protein, the lengths of the hydrogen bonds must be provided, and why this interaction has a consequence on the activity must be discussed. The π - π interaction, that is an interaction, not a bond. This important point must be modified, rewritten and explained correctly since there are enough aromatic rings for such stacking and therefore an effective interaction. What minimization energy and how did it couple to the protein receptor? Important information for this type of descriptions. Some images that are considered outstanding should be in 3D. With these observations, the work can be enhanced.

Reviewing the manuscript, it is interesting; however:

At least one of the compounds obtained and evaluated should show spectroscopic data, NMR, high-resolution masses, or elemental and infrared analysis, since they are small and simple molecules to ignore their characterization.

For certain conformations between the ligand and the protein, the lengths of the hydrogen bonds must be provided, and why this interaction has a consequence on the activity must be discussed.

The π - π interaction is an interaction, not a bond. This important point must be modified, rewritten, and explained correctly since there are enough aromatic rings for such stacking and therefore an effective interaction.

What minimization energy was used, and how was it coupled to the protein receptor? Important information for these types of descriptions.

Some images that are considered outstanding should be in 3D.

With these observations, the work can be enhanced.