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.

The article entitled: Expansion of the Experimental Antifungal Activities Through in silico Docking Study of Compounds from Albizia Lebbeck presents a very important objective, which consists of the search for new antifungal agents, but requires significant improvement to be published.

In the methods related to the in silico study, I missed mentioning the docking program used in the simulations. I did not identify it in the written methodology. You must include the access link to the Protein Data Bank (PDB) library and the access date. It must be informed how the molecular docking simulation was carried out, whether it was through a cavity or through a template; the identification of the active site of the proteins under study is not clearly described. How was the enzyme introduced into the simulation environment? Were cofactors removed or retained? Was the water contained in the enzyme retained? The settings of the software used must be informed, such as the number of rotations, etc. Other information that is not included refers to the fact of mining and preparing the compounds in the Maestro; what type of minimization was used, if it was molecular mechanics or some semi-empirical method. The reference of the PDB article must be cited with the corresponding IDs.

In relation to Table 01, what is the unit of free energy of connection adopted by the software used? This must be included in the table. In addition, all scores for the compounds of the series under study must be added, so where it is written: Docking score less than -2, the score value obtained must be provided in order to provide greater transparency of the results.

I don't understand why biological tests were not carried out on all compounds in the series under study. Compounds 1, 3, and 8 presented the best scores, together with compound 2, and these were not subjected to the biological test, and compound 7 was subjected to the biological test, but it did not present a more negative score when compared to compounds 1, 3, and 8. It is not possible to understand this. There must be a good justification for this.

In the results and discussion topic, as docking is a predictive theoretical approach, it must be made clear that the results referring to this simulation are predictions. The word active should be changed to greater affinity or greater potency, and the terms possibly, probability, should be used, since it is a theoretical simulation and not all results have been experimentally validated. The unit referring to binding free energy must appear in the text after the score value. It must be explained what each Pi-Pi interaction means (what is it? Which chemical groups are affected by this type of interaction?). Furthermore, it must be better explained and emphasized which groups are involved in the interactions and their polarity,

as well as whether there are crucial interactions for the enzyme under study. It should also be determined from the literature whether there is any evidence of the compounds under study for the activity addressed in the work.