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. I find the following view problematic: "Nowadays, the modelization/production of new drugs is an easy task."
2. “The compound to establish a perfect connectivity”: revise this concept of perfection. Binding scores of -5 to -7 kcal/mol are nothing close to perfect. Also, authors assume a rigid receptor and a flexible ligand.
3. “This manuscript deals with the computational investigation of some naturally isolated compounds against*C. albicans*.” This statement is ambiguous. Kindly revise with specific pharmacological action. “Isolating a compound against *C. albicans* is meaningless.” Please be specific to enhance clarity.
4. Also, to do a “computational investigation of some naturally isolated compounds,” could predominantly suggest electronic structure calculation for structure elucidation. A proper rendition may be “A virtual screening experiment was conducted against protein targets or some selected proteins.”
5. What is the mechanism of action of “tetrazole-based antifungal drug candidate VT1161 (VT1)”? How closely related is this compound and its pharmacophore(s) to compounds 2 and 7? Was this ligand used as a positive control in the experimental assessment of the inhibitory potential of compounds 2 and 7? How did the MIC and binding affinity of compounds 2 and 7 vary with that of VT1?
6. "The technical characteristics of spectroscopic and spectrosmetric machines.” Kindly revise this!
7. "The experimental antifungal assays, as well as all the reported compounds in this study, were obtained from …". This suggests that authors were interested in providing docking scores to support the experimental results.
8. Molecular docking assessments carried out in this work lack validity. Authors should define a validation criterion for the molecular docking experiment and justify why the binding scores generated are correct.
9. The depth of this so-called “computational investigation” is shallow. Authors should consider expanding the scope of the computational study and possibly provide some data from experiments as well as some data from molecular dynamics simulations to support the potentially misleading conclusions drawn.
10. Authors should enhance writing, figure presentations, and the construction of the entire manuscript to avoid ambiguity.