Review of: "Inhibition Success of a Virtually Created Molecule: Pseudoeriocitrin and Femtomolar Inhibition"

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Potential competing interests: I have no competing interest

The manuscript is interesting, but there are a lot of issues to be accomplished in this manuscript for further consideration.

Point-1.

The authors must conduct the Gaussian-aided density functional theory (DFT) analysis in optimizing the energy-minimized structure of the unusual molecule/ligand. It is highly recommended for the authors; otherwise, the context is incomplete. In using DFT, the authors must cite - https://doi.org/10.1016/j.fuel.2024.130890.

Point-2.

In receptor preparation, the authors must optimize the protein/macromolecule structure, removing additional side chains, water molecules, unwanted ligands, and ions. Currently, the Gasteiger Method is followed globally in optimizing protein structure, where UCSF Chimera is used. I strongly recommend the authors optimize their receptor using the UCSF Chimera tool and cite the literature- http://doi.org/10.5455/javar.2021.h481.

Point-3.

Only SwissADME is not enough for profiling the ADMET properties. For a high-throughput analysis of the pharmacokinetic and pharmacodynamic properties through ADMET analysis, the authors are suggested to use the pkCSM web interface, following and citing this literature - https://doi.org/10.1007/s11030-022-10573-8.

Point-4.

Proteins from RCSB PDB have a lot of missing amino acid residues. Thus, before conducting a molecular docking, the authors should fill in the missing residues of the protein/macromolecule before optimization. Without this step, direct energy minimization downloading the PDB file from RCSB PDB is not accepted at all because the docking score would be faulty. The SEQATOMs server (https://www.bioinformatics.nl/tools/seqatoms/) is recommended for refilling the authentic missing residues in their right positions before UCSF Chimera optimization. For SEQATOMs, the authors must cite –

a. doi: 10.7555/JBR.35.20210111.
b. https://doi.org/10.1007/s40203-023-00144-6

Point-5.

The authors should explain the hydrogen bonds and hydrophobic interactions following the molecular docking, including their binding affinity (Kcal/mol) and RMSD upper and lower bound scores. Strongly recommend using the LigPlot+ tool to determine the hydrogen and hydrophobic bonds. Must cite for LigPlot plus –

a. DOI: 10.5455/javar.2022.i588
b. DOI: 10.5455/javar.2021.h544

Point- 6.

The authors should use PyRx instead of Autodock because of increased accuracy. In the case of using PyRx, the literature is strongly recommended -

https://doi.org/10.1007/s11030-023-10731-6

Point-7.

A molecular dynamic simulation dataset for at least 50 ns should be very significant in explaining all the analysis conducted here. Thus, the authors should reconsider an MD simulation following the molecular docking process. To conduct and explain the MD simulation process, the authors must study and cite the - doi: 10.5455/javar.2022.i565.

Point-8.

The presentation of the tables and figures is not satisfactory at all. The authors should follow the instructions given above. Besides, the manuscript writing is very average. The research novelty is missing. Each of the paragraphs needs smart rephrasing with strong English sentencing.

Point-9.

References older than 2017 must be replaced with recent-times literature as instructed above. Many of the citations are older than 10 and even 15 years, which is a very bad practice of citation. Must consider citing papers from 2017 - 2024 (seven years).

Point-10.

Please handle the common grammatical mistakes more carefully throughout the manuscript.

Thank you