Review of: "Design and Molecular Screening of Various Compounds by Molecular Docking as BACE-1 Inhibitors"

Imam Siswanto[1]

1 Universitas Airlangga

Potential competing interests: No potential competing interests to declare.

This manuscript is of good quality; however, some points must be revised:

1. This manuscript misses Fig. 8. Please check.
2. Fig. 9 is never mentioned inside the text. It should be. Before Fig. 9, the author should use Fig. 8.
3. At Fig. 9, site 3, there are some substituents R1, R2, R3, R4, and R5; however, the table below Fig. 9 writes R6. Which substituent is R6?
4. In section 4.1, the Discovery Studio Visualizer software was mentioned twice. Is it necessary to write it twice?
5. In section 4.2.2, it was clearly stated that all ligands were prepared by using ChemDraw 2D software. After being prepared by using ChemDraw 2D, all of the ligands' structures must be geometrically optimized. This point was not explicitly written. For example, whether they are geometrically optimized using MM+, AM1, DFT, or HF methods of computation, using, for example, HyperChem or Gaussian. IF the author did the optimization, it should be written in the text.
6. In section 4.2.3, it was written that there are 2 models of BACE-1 (PDB ID: 2ZHT and 2WJO); which one was used ? It is better to use 2WJO because there is a native ligand complexed with the BACE-1. This can be utilized to validate the docking parameters (for example, to check the RMSD of this native ligand after redocking this ligand). Read, for example, : https://doi.org/10.22146/ijc.39943
7. In section 4.2.4, it was written "The grid box enclosing the receptor and ligand, having dimensions [center_X = 64.910; center_Y = 46.971; center_Z = -0.378].".
   No, it's not a dimension; it is a coordinate of the center of the grid box instead. The dimension itself was not informed. It should be, not just the coordinate but also the dimension.
8. The best conformation of ligands should be visually shown to ensure that all ligands are located inside the grid box after being docked. Read, for example, https://doi.org/10.22146/ijc.39943