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

Enade P. Istyastono[1]

1 Universitas Sanata Dharma

Potential competing interests: No potential competing interests to declare.

The research presented in the article is still very preliminary. The *in silico* methods should be validated rigorously. Please see Surely you are joking, Mr Docking! - Chemical Society Reviews (RSC Publishing) to examine some concerns in using docking to predict biological activities. Without “rigorously designed benchmarking studies and rigorous experimental validation,” the discussion and the conclusions in the article are merely speculation. The quality of the article could be improved, e.g., by using the retrospective structure-based virtual screening (SBVS) technique to examine the prediction quality of the docking method presented in the article. The retrospective dataset for BACE-1 is available at BACE1 | DUD-E: A Database of Useful (Docking) Decoys — Enhanced. Of course, some hits from the designed compounds should be verified experimentally.

Minor thing: Some molecules presented in figures are not at the correct distances and angles, which makes the molecules not in the right "shape."