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

Lohit Naik[1]

1 Christ University

Potential competing interests: No potential competing interests to declare.

The study titled "Inhibition Success of a Virtually Created Molecule: Pseudoeriocitrin and Femtomolar Inhibition" (Ref: C446VT) addresses a significant topic: the ability of molecular modeling to forecast potent bioactive compounds. Specifically, the study explores homology modeling techniques to refine an anti-anthelmintic agent. Incorporating minor revisions could further amplify the study's impact.

1. What are the key structural and chemical features of pseudoeriocitrin that contribute to its superior inhibitory activity compared to eriocitrin, as identified through in silico docking studies?
2. Can you expand on why various proteins were selected for the docking studies involving pseudoeriocitrin? Was the choice of proteins driven by specific biological targets, or was it intended to cover a range of protein families to assess the molecule's potential for broad activity?
3. The structure and disparities between both compounds under investigation lack clarity. In their modeling approach, the authors presented a depiction of the rutenoside-based sugar with an sp2 planar configuration alongside sp3 fragments. This representation persists throughout all figures and calculations, indicating an apparent error.
4. There is scope to enhance the quality of the paper.