

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

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Potential competing interests: No potential competing interests to declare.

The paper highlights the promising inhibition ability of pseudoeriocitrin, a novel molecule derived from eriocitrin. Despite utilizing different proteins in docking procedures, and given the evaluation of only one new ligand, it is recommended to conduct more robust computational simulations, such as molecular dynamics, to yield more reliable results. Additionally, while it is mentioned that pseudoeriocitrin may not be druggable due to certain structural characteristics, it would be beneficial to discuss potential modifications to the molecule that could mitigate its toxicity while preserving its inhibitory efficacy.

Regarding the statement about 400 million people worldwide being infected with Enterobius vermicularis in 2015 (page 2), it is advisable to present more recent data on this infection.

In the third paragraph (page 2), please include bibliographic references to support the statements made.

Furthermore, consider including a picture of pseudoeriocitrin immediately following the eriocitrin picture (Figure 1).

During the protein preparation steps, it is recommended to assess the Ramachandran plot of the protein to ensure the structural integrity of the obtained model.

Lastly, please provide a table comparing the ligand-protein interactions for pseudoeriocitrin and eriocitrin to enhance clarity in the comparison. This table should include the residues each ligand interacts with (through hydrogen bonds or nonpolar interactions), docking energies, and any other pertinent information.

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