

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.

major revision

In this study, the authors performed, a 3D analysis of possible interactions performed using the in silico protein-ligand docking method. This study investigated what might be the reason for this ability of pseudoeriocitrin, an unusual molecule with superior inhibitory activity. However, I think major revisions are needed to elucidate the mechanism underlying the high adsorption efficiency of the inhibitory activity of pseudoeriocitrin. Generally, the work is interesting but the **English** should be improved and more importantly, there are some problems you need to address: See below for my specific comments and suggestions.

Abstract:

1. I suggest that the authors revise their abstract and give more details about the systems plus some numeric examples of their results.

Introduction:

2. Please mention the novelty of this work compared to previously published work.

3. The performance of the employed docking technique must be evaluated before any calculations based on experimental data.

4. What are the implications of the study's results for the design of synthetic inhibitors for enzymes?

Material and method: (Preparation of proteins)

5. What is the reason for using the proteins used in this work?

Results and discussion:

6. Add more molecular docking details such as docking scores, and interaction distance, to the text.

7. In this work, hydrogen bond formation and hydrophilicity/hydrophobicity have been discussed only with the 3D and 2D

representation of pseudovariocitrine. It is suggested to add analyses such as hydrogen bond number and SASA for more details and discussion in this case.

8. Besides molecular docking simulation, it is better that some experiments be provided to confirm the obtained conclusion in this study,

Conclusion:

9. The conclusion section must be rewritten to be more informative and unveil the most beneficial outcomes.

References:

10. Make sure all references follow the same format.