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.

Dear Peer Review Team, Qeios!

I am quite grateful for the chance to comment on this work. Our remarks, which centered entirely on the investigation's scientific findings, are mentioned in the text body.

Several excellent findings from this research include:

- The investigation of **Pseudoeriocitrin**, a chemical that was produced digitally, in this work is novel. It offers a fresh method for creating pharmaceuticals, especially when considering femtomolar inhibition.
- The paper provides a thorough docking analysis that looks at how different target proteins interact with **Pseudoeriocitrin**. This comprehensive investigation improves our knowledge of possible interactions between drugs and proteins.
- The discovery may have a substantial influence on the creation of novel medications, particularly in light of the molecule's femtomolar level of inhibition, which indicates strong effectiveness at low doses.
- The study shows how effective and accurate in silico approaches are for finding new drugs, which might speed up the process and lessen the need for *in-vivo* testing.

Even if the work's core notion is sound and helpful, I have a few remarks after reading this research:

- Above all, this work shows tremendous inventiveness in the area of molecular design. The authors offer fresh insights into drug design, particularly with regard to femtomole-level inhibitory effects, by examining the synthetically generated compound **Pseudohesperidin**. Furthermore, the work expands on our knowledge of possible drug-protein interactions by carefully examining the interactions that **Pseudohesperidin** has with various target proteins using docking analysis. These discoveries may have a beneficial effect on global health challenges and have significant implications for the development of new medications.
- Nonetheless, this study has a few significant flaws. The most evident issue is that**Pseudohesperidin**'s effectiveness and safety have not been scientifically proven. Additionally, there may be toxicity concerns as a result of the **Pseudohesperidin** structure's absence of hydrogen donors. Understanding the molecular mechanisms underlying the observed interactions is essential for comprehending the molecule's metabolic pathways and its side effects, but it was not thoroughly investigated in the study. The study also needs to be upgraded in the areas of data reliability and comparative comparison with already-approved medications.

In summary, although this work offers groundbreaking perspectives on virtual drug design and molecular docking, it also emphasizes the need for more study, particularly in experimental validation and toxicity evaluation, to fully realize **Pseudohesperidin**'s potential as a therapeutic agent.

Best regards,

Nguyen Minh Quang