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

Hiba Hassan Sulieman Omer

Potential competing interests: No potential competing interests to declare.

Title: "Success of a Virtual Molecule: Pseudoeriocitrin's Inhibition at an Extremely Low Level"

General Comments:
The manuscript explores the inhibitory properties of a virtual molecule called pseudoeriocitrin. The study investigates why pseudoeriocitrin exhibits higher inhibitory activity compared to eriocitrin. In silico protein-ligand docking studies were conducted to analyze possible interactions. The authors propose that the large core structure, abundance of oxygen atoms, planar coordinates, and extremely low level of inhibition are related. The study provides insights into the structure-activity relationship of pseudoeriocitrin and emphasizes the need for further research on its synthesis and biological properties. Overall, the study contributes to drug development and should be published after addressing minor concerns.

Specific Comments:

Introduction:
The introduction briefly discusses the significance of helminth infections and the need for alternative treatments with fewer side effects. Additional background information on the limitations of current synthetic drugs and the potential of natural compounds or virtual molecules would be helpful.
Please clearly state the research objectives and the research gap that this study aims to address.

Methods:
The methods section provides sufficient information on ligand and protein retrieval and preparation for docking studies. Adding specific software and parameters used for the docking simulations would enhance reproducibility. Please provide version numbers and references for the Biovia Discovery Studio 2020 Client and AutoDock Tool (ADT) software.
Mention any validation or verification steps taken to ensure accuracy and reliability of the docking results.
Clearly state the specific proteins and enzymes used in the study, providing references or accession numbers for their crystallized structures.

Results:
The results section presents findings from the docking studies and pseudoeriocitrin's inhibitory properties. Well-organized data, such as binding affinities and interaction analyses, support the findings. Including representative figures or diagrams illustrating docking poses or interactions between pseudoeriocitrin and target proteins would be beneficial.
Provide a clear and concise summary of the key findings and their implications.

Discussion:

The discussion section elaborates on the implications of the results and provides insights into the structure-activity relationship of pseudoeriocitrin. Discuss potential applications or implications of pseudoeriocitrin as an anthelmintic or in other therapeutic areas.

Acknowledge the limitations of the in silico docking approach and discuss the need for future experimental validation.