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

Ricardo Luna[1]

1 Universidad Nacional Autónoma de México

Potential competing interests: No potential competing interests to declare.

Based on previous research on eriocitrin, the authors proposed the structure of a new compound called pseudorierocitrin and examined its binding to proteins. The manuscript text is difficult to read. Figures 1 and 4 and their figure captions show eriocitrin. The titles of the remaining figures contain the name pseudoerocitrin, but only figures 7, 8, 10, 12, and 13 present the new compound, while the rest contain eriocitrin. Therefore, not only the figure captions but also the entire text should be carefully verified. For the reader's convenience, I suggest adding the structure of pseudoerocitrin to the structure of eriocitrin in Figure 1.

Another important point of the work is the analysis of weak interactions between the tested compound and the protein. The authors provide a wide range of interactions found based on distance. This criterion is insufficient due to the lack of angular dependencies. Sometimes, the interaction found based on shortened interatomic distance actually does not occur due to non-linearity.

The last point that raised doubts for me is the value of the dielectric constant of 10 in the docking process. Why was this value simply established? By the way, the term "dielectric constant" is incorrect and should be replaced by "relative permittivity."

I just recommend avoiding the same terms in the title and keywords. The article is very interesting, but I believe it requires more experimental work to be performed to be considered for publication. It has several grammatical errors that need to be corrected as well.

In the introduction, the rationale as to why novel anthelmintics need to be developed needs more justification.

Please describe the significance of docking studies.