

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

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Potential competing interests: No potential competing interests to declare.

The paper "Inhibition Success of a Virtually Created Molecule: Pseudoericiotin and Femtomolar Inhibition" (Qeios, CC-BY 4.0) is devoted to *in silico* research of new medicinal compounds. This research method allows predicting the structure and properties of new compounds and simplifying experimental research. It would seem, therefore, that the presented work, containing results regarding the carefully described docking of a new compound to the proteins with which this compound should interact, should deserve to be published. Unfortunately, I believe that the work cannot be published in its current form. Based on previously performed research on ericiotin, the authors proposed the structure of a new compound called pseudoericiotin and examined the docking of this compound to proteins. The text of the manuscript is difficult to read. Figures and figure captions 1 and 4 show ericiotin. The captions of the remaining figures contain the name pseudoericiotin, but only figures 7, 8, 10, 12, and 13 present the new compound, while the rest contain ericiotin. Therefore, not only the figure captions but also the entire text must be carefully verified. For the reader's convenience, I propose to add the pseudoericiotin structure to the ericiotin structure 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 whole range of interactions found based on distance. This criterion is insufficient due to the lack of angular dependencies. Sometimes the interaction found on the basis of the shortened interatomic distance does not actually occur due to nonlinearity.

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