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.

This work, named „Inhibition Success of a Virtually Created Molecule: Pseudoeriocitrin and Femtomolar Inhibition, is about a virtual molecule, pseudoeriocitrin, which can inhibit various proteins at the femtomolar level. It is the first study to show the structure-activity relationship of pseudoeriocitrin via *in silico* dockings. Protein-ligand docking simulations performed by *in silico* molecular modeling are the first step towards drug development efforts. Eriocitrin is one of the eriodictyol-derived flavonoid glycosides. It has antioxidant, anti-inflammatory, and antiproliferative properties. Karaman et al. investigated the anthelminthic effect of eriocitrin in their previous study, which yielded *in silico* outcomes. Interestingly, it was found that there was an additional bond in the molecule when studying the possible interactions of eriocitrin with the proteins it inhibits and when studying the new molecule named pseudoeriocitrin. Pseudoeriocitrin has the same molecular weight, molecular formula, and atom types as eriocitrin. The only difference is an extra intramolecular bond between the C8 of chromene-4-one and the oxygen atom of O-β-rutinoside. The new and original thing in this article is that pseudoeriocitrin interactions with anthelmintic target proteins were researched *in silico.*

It seems fantastic that Karaman et al. wrote the preparation of the proteins and ligands process step by step; it is clear and can be followed.

Unfortunately, the docking method was totally new information for me, but it’s great because I can learn more about computational chemistry.

The figures and videos can help to understand what the authors described in this paper.

This study showed that the inhibition constant of pseudoeriocitrin against rat CPT 2 was 15.83 femtomolar. This result indicates that pseudoeriocitrin may be a very successful CPT 2 inhibitor, which is not accessible in the database; however, it can be useful for the design of *de novo* drugs. I am interested in practical protein chemistry, so it is fruitful to read this kind of technique to see how things are going *in silico*. It would be great if the results were the same in vivo and in vitro circumstances. In any case, it is great to be able to model the interactions between some antioxidant molecules and enzymes.