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.

Authors explain their work nicely in this manuscript

I recommend acceptance of the work in this format

Pseudoeriocitrin is a molecule that does not exist in reality but was created*in silico* by assuming the formation of oxygen radicals in eriocitrin and giving it a different geometry. It gave femtomolar results during *in silico* docking studies, being more successful than eriocitrin in inhibition. This study investigated what might be the reason for the ability of pseudoeriocitrin, an unusual molecule with superior inhibitory activity. In this study, 3D analysis of possible interactions was performed using the *in silico* protein-ligand docking method. Although it is difficult to say anything definitive, the absence of hydrogen donors renders the pseudoeriocitrin structure highly toxic. This new molecule, which can inhibit various proteins at the femtomolar level, was predicted to be responsible for the high binding ability due to its planar large structure and lots of oxygen radicals, which provide a number of hydrogen bonds with the atoms in the active site of the proteins. It is the first study to show the structure-activity relationship of pseudoeriocitrin via *in silico* dockings. In the results, it was shown that the large core structure, abundance of oxygen atoms, planar coordinates, and femtomolar level inhibition were related. The chemical properties leading to these new biological properties should be considered from different angles, and more research should be conducted on the synthesis of non-radical pseudoeriocitrin.