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

Oddepally Rajender

Potential competing interests: No potential competing interests to declare.

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

It is suggested to show the full forms of hERD-7-*O*-Gluc and hERD-4'-*O*-Gluc.

Rewrite the sentence: “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.”

It is stated as “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,” but if Pseudoeriocitrin and eriocitrin have the same molecular weight, molecular formula, and atom types, then the extra intramolecular bond between the C8 of chromene-4-one and the oxygen atom of O-β-rutinoside should also be present in eriocitrin. If the same extra intramolecular bond exists in eriocitrin, provide the reference; if not, then give a proper justification about the difference.

Rewrite the sentence: “Before one molecule showed anomalous binding in the docking studies, we retrieved the PDB file of this molecule from the FooDB database.”

As the proteins were modeled using HOMOLOGY, provide the structure validation of the modeled protein. Structure validation of the modeled protein is very important before further studies, so provide structure validation of the modeled protein, and that should be incorporated in the manuscript.

As stated in the manuscript, “On the other hand, this molecule (pseudoeriocitrin) searched in the ZincDatabase is not present in the database. The interactions associated with pseudoeriocitrin are intended to be used in the discovery of a new anthelmintic based on its very favorable binding free energies.” In such cases, further validation of the protein-ligand interactions has to be done by molecular dynamic studies.