

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

Edward Ntim Gasu<sup>1</sup>

<sup>1</sup> Abdus Salam international centre for theoretical physics

**Potential competing interests:** No potential competing interests to declare.

1. What does this excerpt of the introduction seek to convey? Kindly modify this!

"Because the unknown genome sequence and the lack of crystallized structure of the proteins belonged to *Syphacia obvelata*, the homology model of mitochondrial cytochrome c oxidase (COX) proteins can be useful *for in silico* docking experiments in order to investigate the antinematodal properties of some drug candidates against *S. obvelata* (Karaman, 2022)."

2. "*Haemonchus contortus*  $\beta$ -tubulin protein PDB ID: 1OJ0 (in complex with ABZ, theoretical structure)." How was this theoretical structure generated?

Entry **1OJ0** was removed from the distribution of released PDB entries in 2002 as part of the separation of theoretical model coordinate files from the main archive.

3. Kindly use AlphaFold to regenerate the structure of the  $\beta$ -tubulin protein PDB ID: 1OJ0 and compare the results to the obsolete version.

4. Also, for the "Homology Modelling" section of the paper, try to use AlphaFold for all the models generated in silico.

5. Kindly demonstrate the behavior of the interactions in the presence of water, and varying protein backbone orientations and conformations. Try to use molecular dynamics studies.