

Review of: "Investigation and Synthesis of Benzothiazole-Derived Schiff Base Ligand Against Mycobacterium tuberculosis"

Sowmya Krishnan¹

¹ Life Sciences division, TCS Research, Tata Consultancy Services Limited, Mumbai, India

Potential competing interests: No potential competing interests to declare.

The article describes the synthesis and characterization of Schiff Base ligands to treat TB. There are several grammatical errors in the article, and the computational methods described are insufficient and technically incorrect.

1) Introduction - For this reason, he is not recognized in the department. - The authors should at least bother to check the contents of the manuscript before submission to a journal.

2) ADME prediction was done using SwissDock? SwissDock is a docking software, not an ADME prediction tool.

3) What is chemical chemistry? The authors really need to look into such typos and correct them.

4) By all parameters provided in Table 1, Isoniazid seems to be the drug of choice over MTA - lower molecular weight, higher TPSA, lower rotatable bonds, high hydrogen-bonding potential, and high intestinal absorption. Under what basis are the authors suggesting MTA to be a better drug apart from the docking score? A simple change in the docking program can easily give different binding free energy results for the two molecules.

5) What is Metab in Table 1? Metabolism is a complex task accomplished by multiple cytochrome P450 enzymes. The authors must have explained what the Metab score means. Is it a composite score of multiple CYP450 binding predictions? If so, what are the CYP isoforms considered?

6) Docking - We chose glutamine synthetase as the target of interest - Drug discovery does not work this way. A panel of targets must be experimentally selected and validated for drug-binding. Docking programs can provide highly plausible docking scores for any given protein-ligand combination. At least a minimal MD simulation should have been performed to prove that glutamine synthetase has a high affinity for the identified ligands. The approach followed by the authors is technically incorrect.

7) What are the docking parameters? How was the binding site identified? What is the grid box dimension? Several crucial details are missing in the manuscript.