Review of: "Flavocillin: a potent TrxR and OATP inhibitor"

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Potential competing interests: No potential competing interests to declare.

he manuscript contains valuable scientific information regarding a novel antibiotic-like, molecule and discovered enzyme inhibitor properties as determined by ligand affinity docking analysis to TrxR thus reducing the bacterial ability to neutralize lactamic antibiotics. The manuscript exhibit solid science in the area of bioinformatics that is meritorious of publication. However, some modifications are recommended.

M & M

There is insufficient information regarding the algorithms used for the docking analysis, I can see that some algorithms information is described at the results section but it should be here instead.

The source of the PDB files of TrxR and the ligands used for the docking analysis should be clearly indicated.

The amino acids described at M & M probably are from the TrxR active site but lack any further information that I consider necessary to describe in the results section.

A still image of the docking TrxR-Flavocilin should be included with a proper legend

A close-up still image of the TrxR active site interacting with Flavocillin should be included with a proper legend

Identification of the catalytic amino acids at the active site of TrxR are relevant for this analysis.