

Supplementary materials

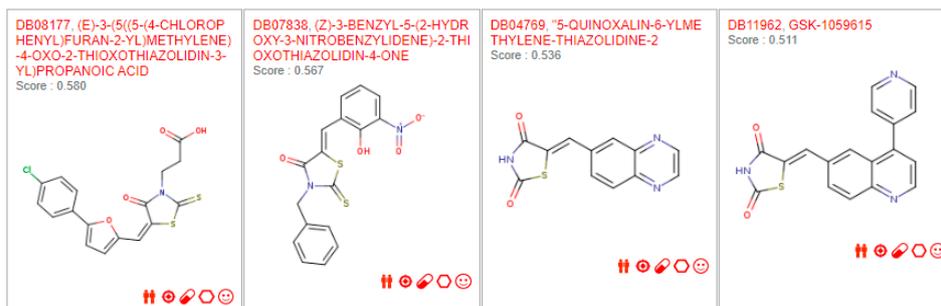


Figure S1. Similarity search on similar drug candidates or known bioactive molecules for the tested compound.

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Lysosomal protective protein	CTSA	P10619	CHEMBL6115	Protease	<div style="width: 100%; height: 10px; background-color: green;"></div>	315 / 0 ↓
Thromboxane-A synthase	TBXAS1	P24557	CHEMBL1835	Cytochrome P450	<div style="width: 100%; height: 10px; background-color: green;"></div>	230 / 0 ↓
Peroxisome proliferator-activated receptor gamma	PPARG	P37231	CHEMBL235	Nuclear receptor	<div style="width: 100%; height: 10px; background-color: green;"></div>	202 / 3 ↓

Figure S2. Target prediction for a tested compound using SwissTargetPrediction.