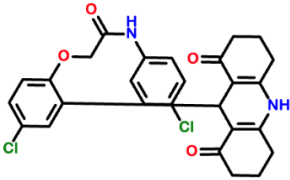
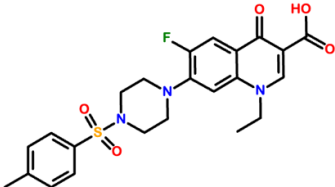
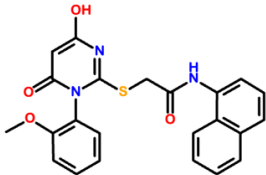
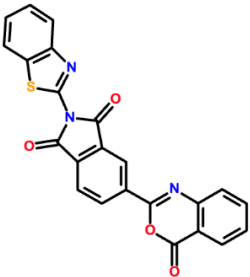
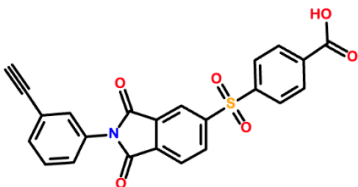
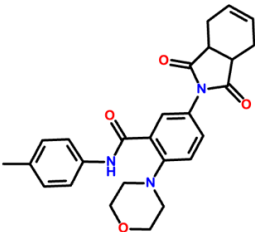


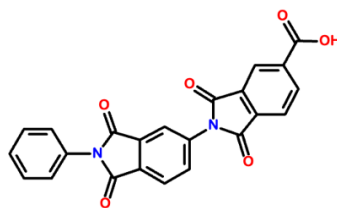
Table S1. Characterization of candidate compounds and maximum ligand RMSD values.

| Name | ID | IUPAC | maximum ligand RMSD [nm] |
|---------------|---------|--|-----------------------------------|
| Compound 1 | 7748081 | 2-[4-chloro-2-(1,8-dioxo-1,2,3,4,5,6,7,8,9,10-decahydro-9-acridinyl)phenoxy]-N-(4-chlorophenyl)acetamide | 0.418 |
| Compound 2 | 7036848 | 1-ethyl-6-fluoro-7-{4-[(4-methylphenyl)sulfonyl]-1-piperazinyl}-4-oxo-1,4-dihydro-3-quinolinecarboxylic acid | 0.509 |
| Compound 3 | 5353462 | 2-{[4-hydroxy-1-(2-methoxyphenyl)-6-oxo-1,6-dihydro-2-pyrimidinyl]thio}-N-1-naphthylacetamide | 0.602 |
| Compound 4 | 5766526 | 2-(1,3-benzothiazol-2-yl)-5-(4-oxo-4H-3,1-benzoxazin-2-yl)-1H-isoindole-1,3(2H)-dione | 0.609 |
| Compound 5 | 5224142 | 4-{[2-(3-ethynylphenyl)-1,3-dioxo-2,3-dihydro-1H-isoindol-5-yl]sulfonyl}benzoic acid | 0.643 |
| Compound 6 | 7159467 | 5-(1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2H-isoindol-2-yl)-N-(4-methylphenyl)-2-(4-morpholinyl)benzamide | 0.657 |
| Compound 7 | 5186895 | 1,1',3,3'-tetraoxo-2'-phenyl-1,2',3,3'-tetrahydro-1'H-2,5'-biisoindole-5-carboxylic acid | 0.671 |
| Compound 8 | 7732114 | 3-[4-(1H-1,2,3-benzotriazol-1-ylcarbonyl)-1-phenyl-1H-pyrazol-3-yl]-2H-chromen-2-one | 0.684 |
| Compound 9 | 7109157 | 3-{[3-(3,4-dihydro-2(1H)-isoquinolinylsulfonyl)benzoyl]amino}benzoic acid | 0.694 |

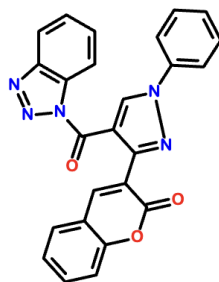
Table S2. Chemical structure of candidate compounds.

| Name | ID | Chemical structure |
|------------|---------|--|
| Compound 1 | 7748081 |  |
| Compound 2 | 7036848 |  |
| Compound 3 | 5353462 |  |
| Compound 4 | 5766526 |  |
| Compound 5 | 5224142 |  |
| Compound 6 | 7159467 |  |

Compound 7 5186895



Compound 8 7732114



Compound 9 7109157

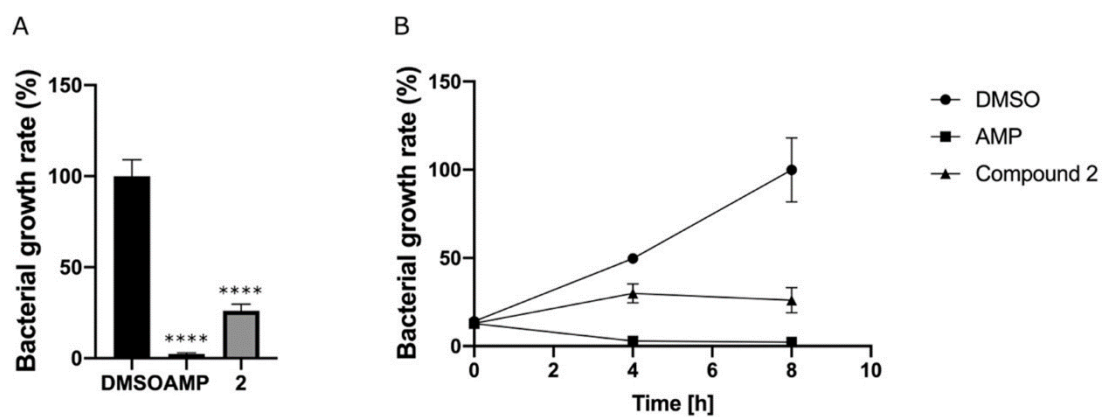
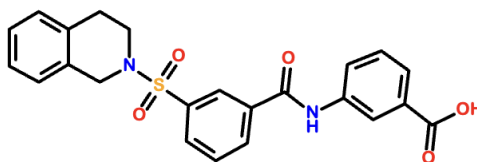


Figure S1. Pharmacological effects of Compound 2 on *E. coli*

(A) Growth inhibition rate against *E. coli*. (B) Change in bacterial growth over time. Negative control was 0.3% DMSO and positive control was 100 μ M ampicillin (AMP). Concentration of Compound 2 is 100 μ M. Dunnett's test: **** $p < 0.0001$.

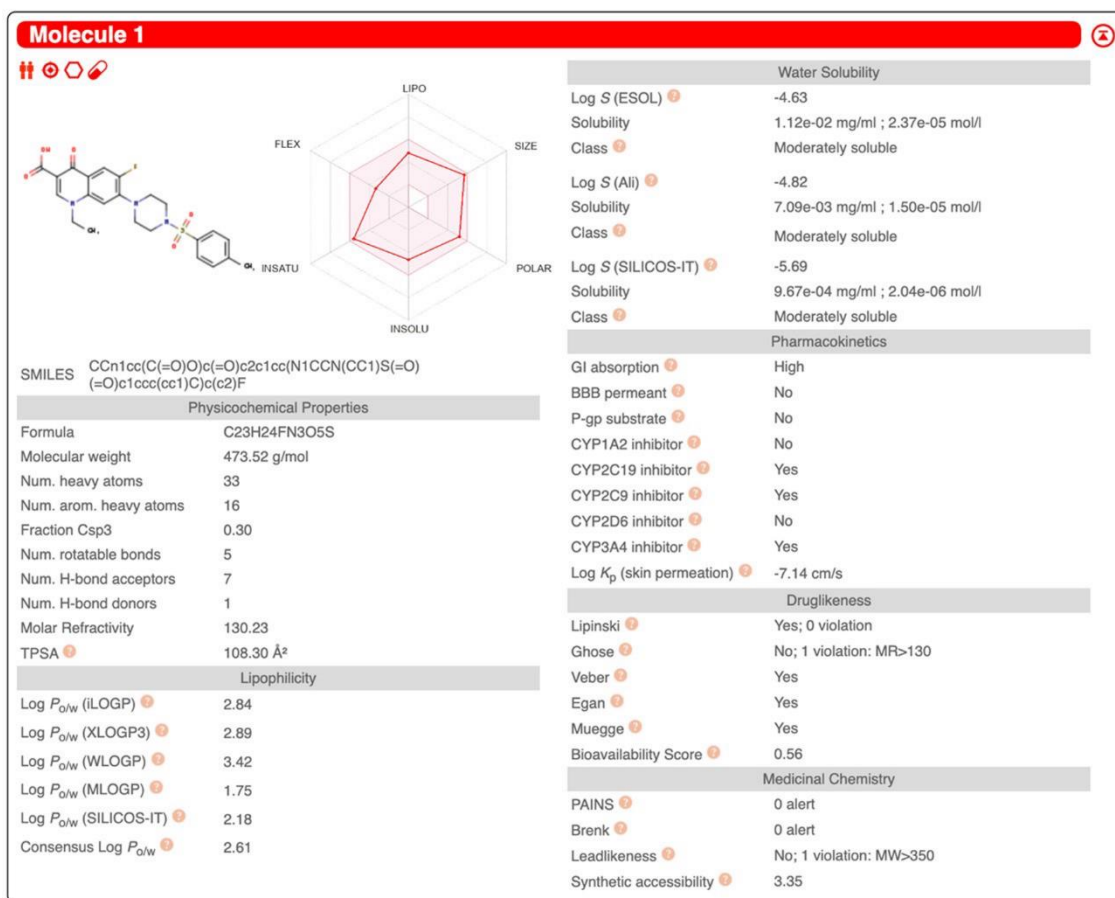


Figure S2. Chemical and pharmacological properties of Compound 2 predicted by SwissADME.

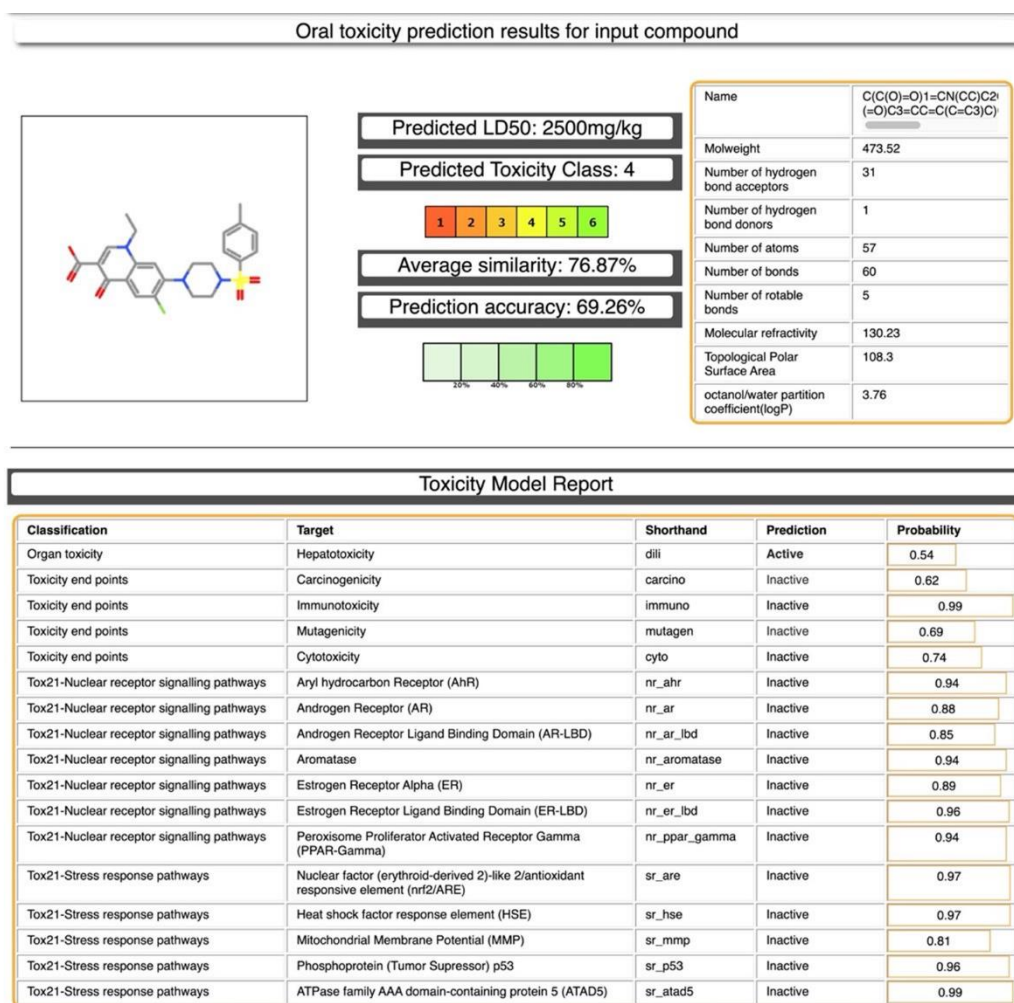


Figure S3. Toxicity prediction of Compound 2 by ProTox-II.

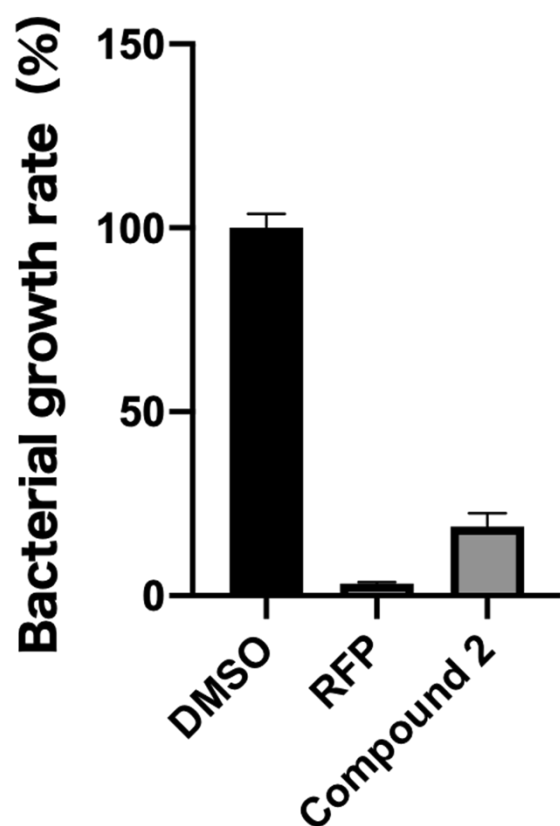


Figure S5. Growth inhibition rate against *Mycobacterium*

Negative control was 0.3% DMSO and positive control was 100 μ M rifampicin (RFP).

Concentration of Compound 2 is 100 μ M.