A Repurposing Approach for Uncovering the Anti-Tubercular Activity of FDA-Approved Drugs with Potential Multi-Targeting Profiles

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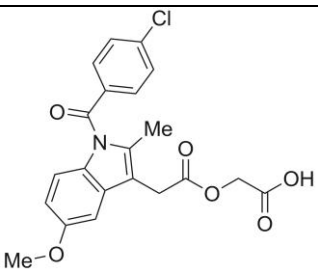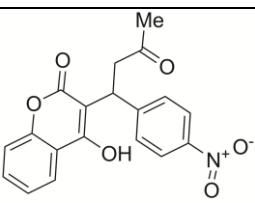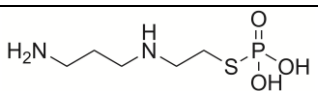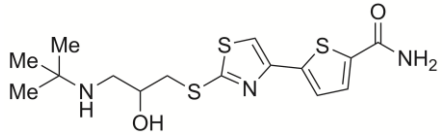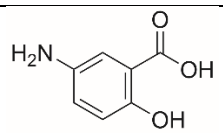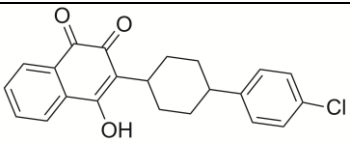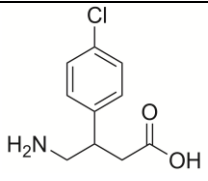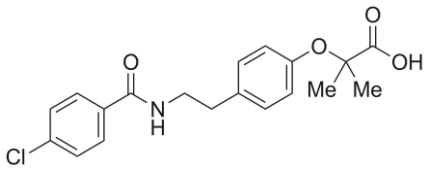
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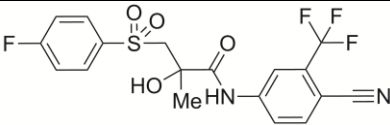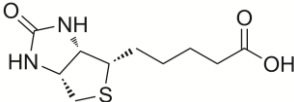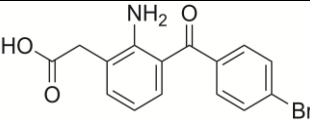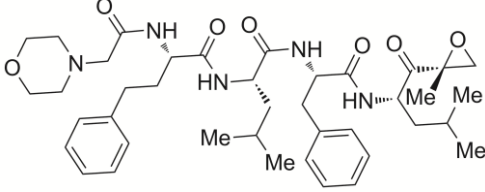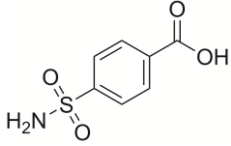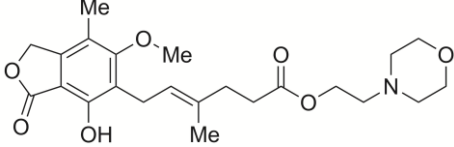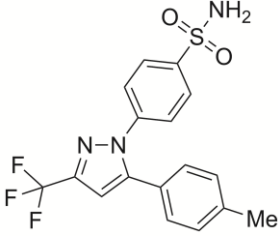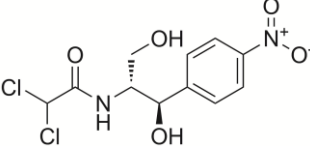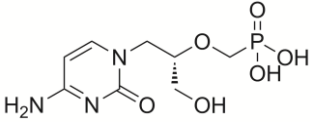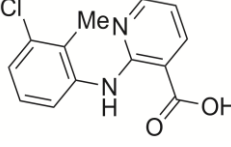
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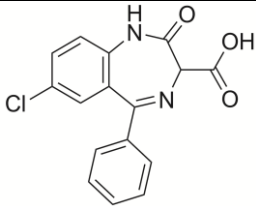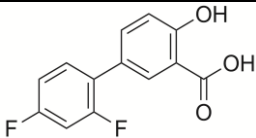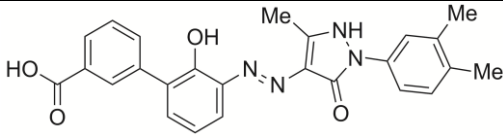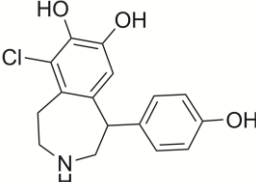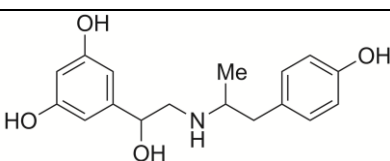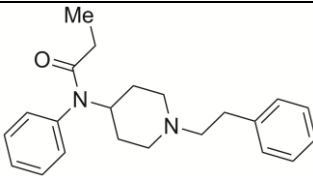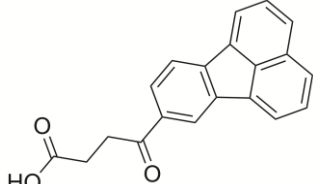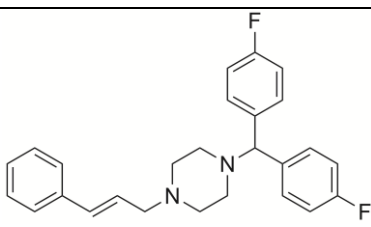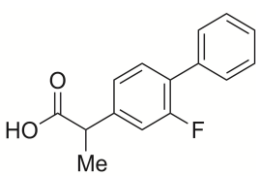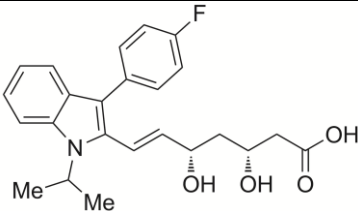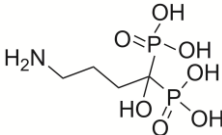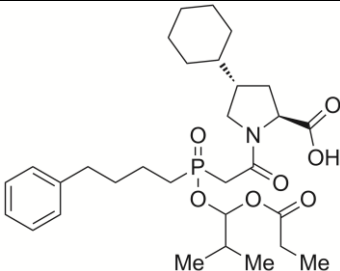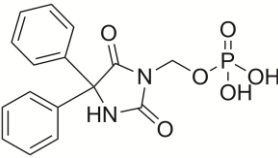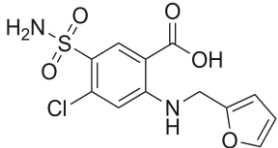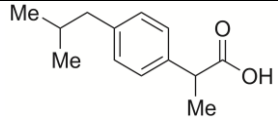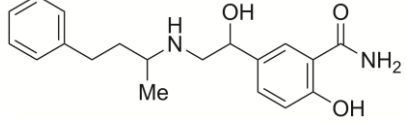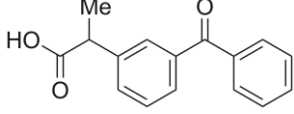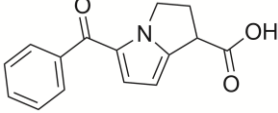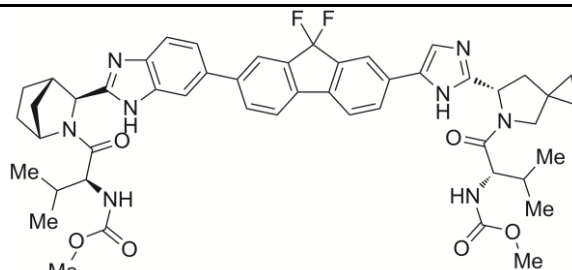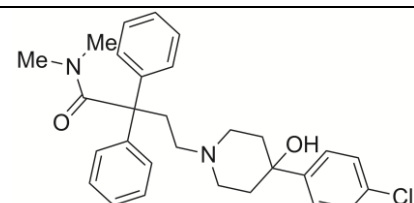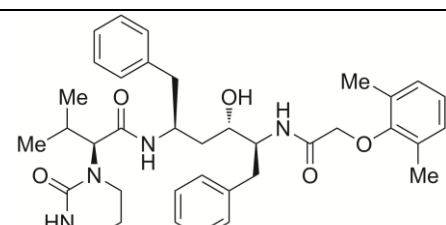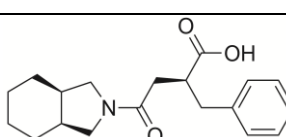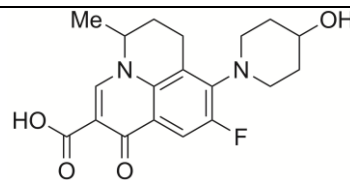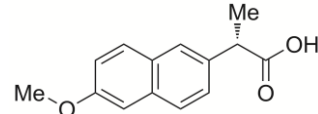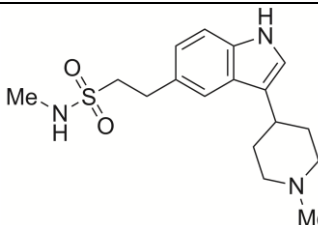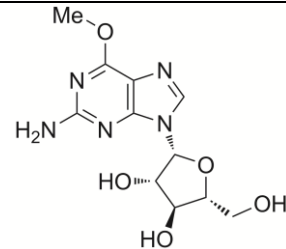
Table S1. Full list of FDA-compounds selected from virtual screening. The 29 compounds selected for the biological evaluation are underlined.
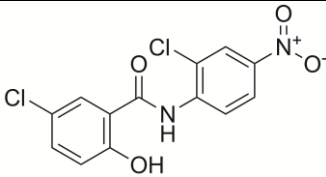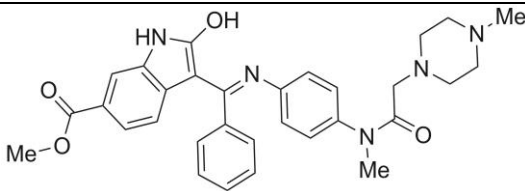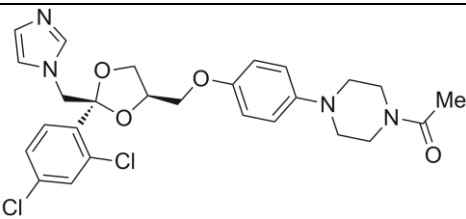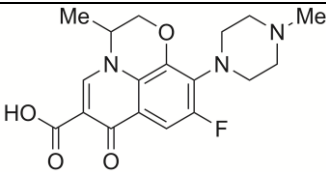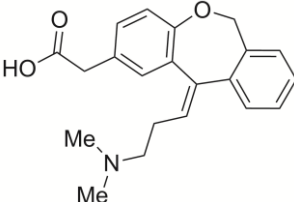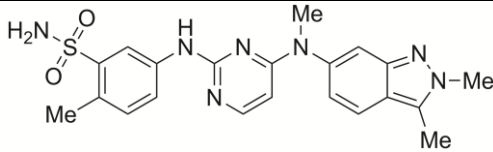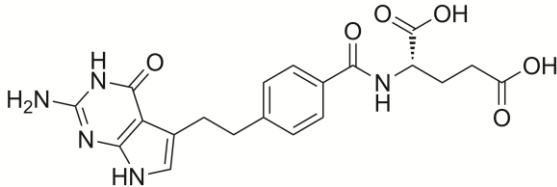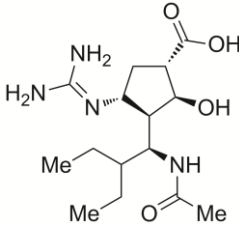
Compound	Structure	Test Performed Against *M. Tuberculosis*	Activity
Acemetacin		HTS against *M. tuberculosis* in 7H9 media HTS against H37Rv strain	inactive
Acenocoumarol		HTS against H37Rv strain	active
<u>Amifostine</u>		no	not previously determined
<u>Arotinolol</u>		no	not previously determined
Asacol		HTS against H37Rv strain	inactive
Atovaquone		HTS against H37Rv strain	active
Baclofen		HTS against H37Rv strain	inactive
Bezafibrat		HTS against *M. tuberculosis* in 7H9 media HTS against H37Rv strain	inactive
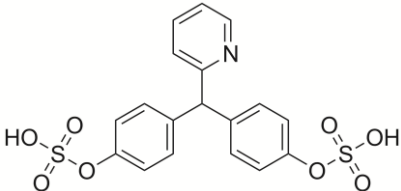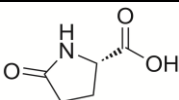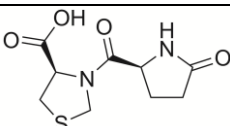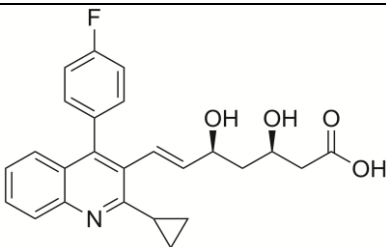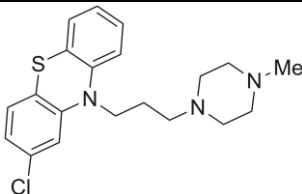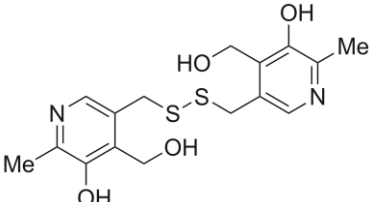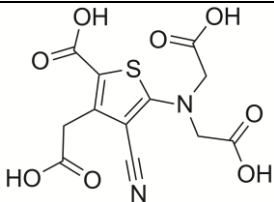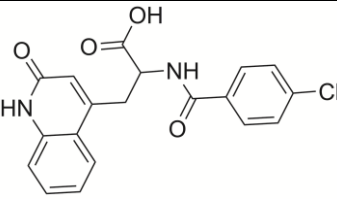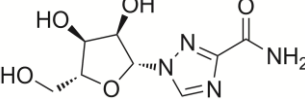
Name	Structure	HTS	Result
Bicalutamide		no	not previously determined
Biotin		no	not previously determined
Bromfenac*		no	not previously determined
Carfilzomib		no	not previously determined
Carzenide		HTS against *M. tuberculosis* in 7H9 media; HTS against H37Rv strain	inactive
Cellcept		no	not previously determined
Celecoxib		HTS against *M. tuberculosis* in 7H9 media	inactive
Chloramphenicol		HTS against H37Rv strain	active
Cidofovir		no	not previously determined
Clonixin		HTS against *M. tuberculosis* in 7H9 media	inactive
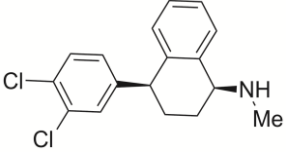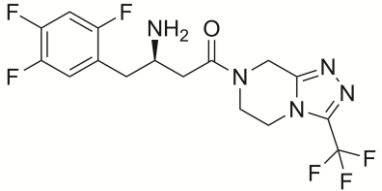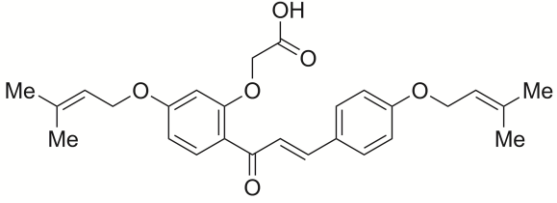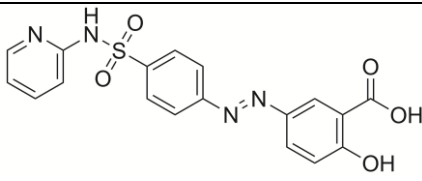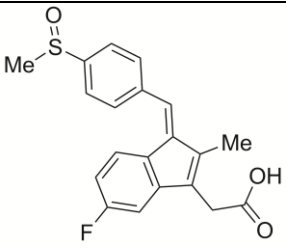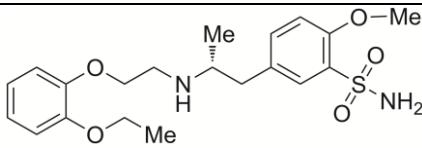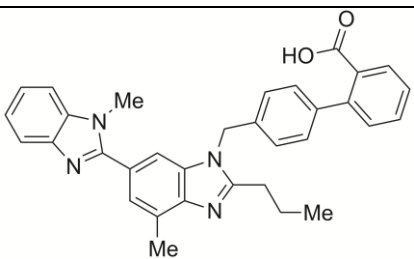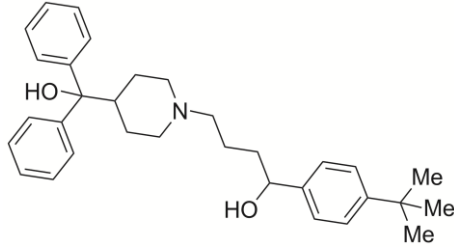
Clorazepate		no	not previously determined not purchased
<u>Diflunisal</u>		no	not previously determined
<u>Eltrombopag</u>		no	not previously determined
Fenoldopam		HTS against H37Rv strain	inactive
Fenoterol		HTS against *M. tuberculosis* in 7H9 media	inactive
Fentanyl		no	not previously determined not purchased
Florantyrone		no	not previously determined not purchased
Flunarizine		HTS against H37Rv strain	active
Flurbiprofen		HTS against *M. tuberculosis* in 7H9 media HTS against H37Rv strain	inactive
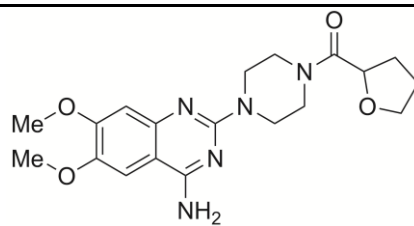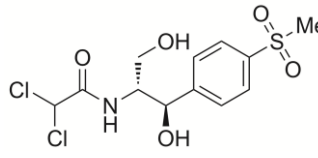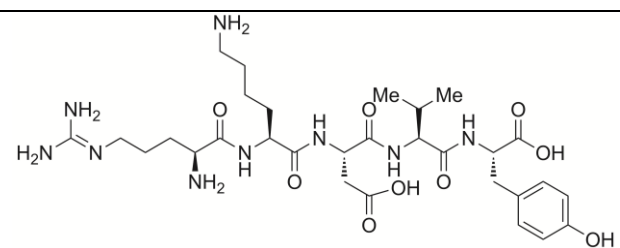
Fluvastatin		no	not previously determined
Fosamax		no	not previously determined
Fosinopril		no	not previously determined
Fosphenytoin		no	not previously determined not purchased
Furosemide		HTS against H37Rv strain	active
Ibuprofen		HTS against H37Rv strain	inactive
Labetalol		HTS against H37Rv strain	inactive
Ketoprofen		HTS against H37Rv strain	inactive
Ketorolac		HTS against H37Rv strain	inactive

Name	Structure	HTS	Result
<u>Ledipasvir</u>		no	not previously determined
Loperamide		HTS against H37Rv strain	active
Lopinavir		no	not previously determined not purchased
<u>Mitiglinide</u>		no	not previously determined
Nadifloxacin		HTS against *M. tuberculosis* in 7H9 media	inconclusive
Naproxen		HTS against H37Rv strain	inactive
<u>Naratriptan</u>		no	not previously determined
<u>Nelarabine</u>		no	not previously determined

Niclosamide		HTS against H37Rv strain	active
Nintedanib		no	not previously determined
Nizoral		HTS against H37Rv strain	active
Ofloxacina		HTS against H37Rv strain	active
Olopatadine		HTS against H37Rv strain	inactive
Pazopanib		no	not previously determined
Pemetrexed		no	not previously determined
Peramivir		no	not previously determined

Picosulfuric acid		no	not previously determined
Pidolate		HTS against *M. tuberculosis* in 7H9 media	inactive
Pidotimod		HTS against H37Rv strain	inactive
Pitavastatin		no	not previously determined
Prochlorperazine		HTS against H37Rv strain	active
Pyritinol		no	not previously determined
Ranelic acid		no	not previously determined
Rebamipide*		no	not previously determined
Rivabirin		HTS against H37Rv strain	inactive

Sertraline		HTS against H37Rv strain	active
Sitagliptin		no	not previously determined
Sofalcone		no	not previously determined
Sulfasalazine		HTS against H37Rv strain	inactive
Sulindac		HTS against H37Rv strain	inactive
Tamsulosin		no	not previously determined
Telmisartan		HTS against *M. tuberculosis* in 7H9 media HTS against H37Rv strain	inactive
Terfenadine		HTS against H37Rv strain	active

Terazosin		HTS against H37Rv strain	inactive
Thiamphenicol		HTS against H37Rv strain	active
Thymopentin		HTS against *M. tuberculosis* in 7H9 media	inactive

* These compounds showed high scores against Zmp1 only. Not purchased: compounds that were not available during the work or were available in a small amount for the tests. The data about the *in vitro* tests against *Mycobacterium* were found in PubChem (https://pubchem.ncbi.nlm.nih.gov/). The tests considered were against *M. tuberculosis* H37Rv strain (High Throughput Screen to Identify Inhibitors of *Mycobacterium tuberculosis* H37Rv AID: 1332 https://pubchem.ncbi.nlm.nih.gov/bioassay/1332; AID: 1626 https://pubchem.ncbi.nlm.nih.gov/bioassay/1626) and against *M. tuberculosis* in 7H9 media (High Throughput Screening Assay used to Identify Novel Compounds that Inhibit *Mycobacterium tuberculosis* in 7H9 Media AID: 449762 https://pubchem.ncbi.nlm.nih.gov/bioassay/449762).