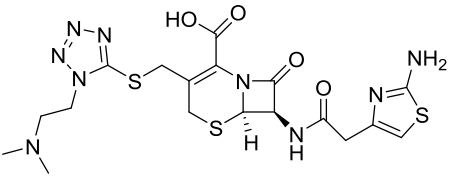
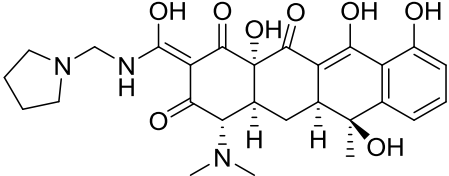
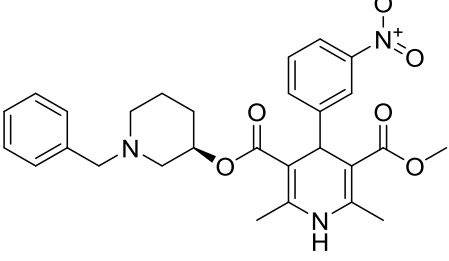
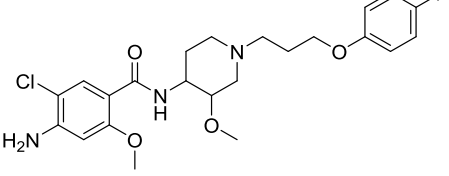
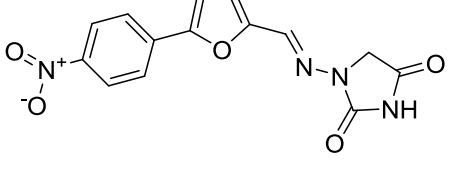
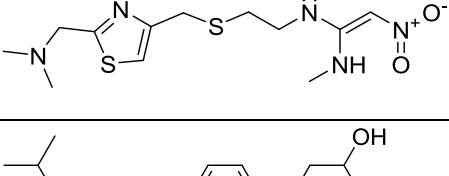
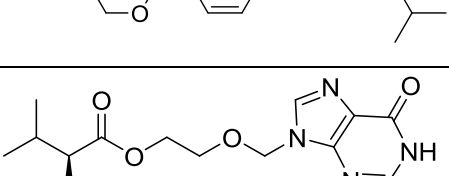
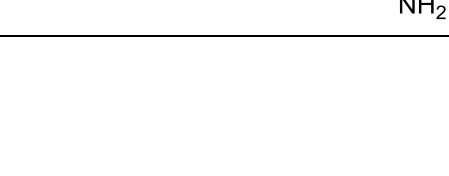
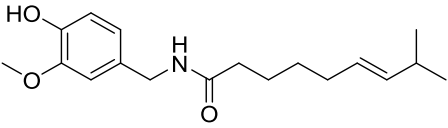
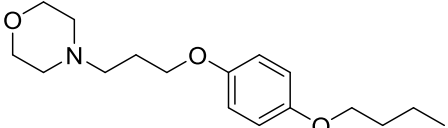
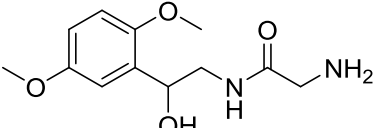
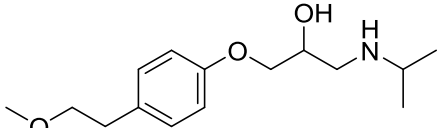
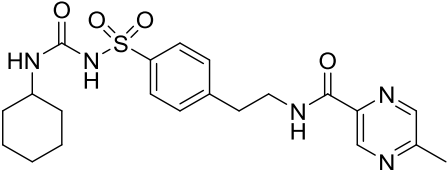
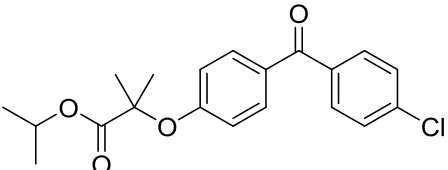
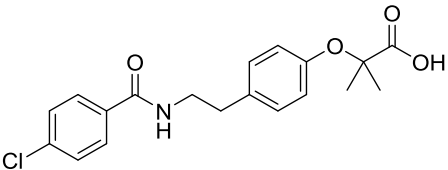


Supplemental Table S1: Top-Scoring FDA-Approved Drugs

Drugs	Names	Structures	Uses	AMBER Scores (kcal/mol)	In-Silico Rankings
1	Cefotiam		Cephalosporin antibiotic	-41.201	1
2	Roli-tetracycline		Tetracycline antibiotic	-9.602	24
3	Benidipine		Ca ⁺ channel blocker for hypertension	-21.671	16
4	Cisapride		Gastroprokinetic agent	-23.399	15
5	Dantrolene		Muscle relaxant	-39.587	3
6	Nizatidine		H ₂ receptor agonist for acid reflux	-40.980	2
7	Bisoprolol		Beta blocker	-37.168	4
8	Valacyclovir		Antiviral for herpes treatment	-23.795	13

9	Pantoprazole		Proton pump inhibitor for acid reflux	-19.377	19
10	Acitretin		Retinoid for psoriasis treatment	-17.884	20
11	Oxybutynin		Anticholinergic for frequent urination	-11.123	22
12	Pentamidine		Antimicrobial	-10.383	23
13	Furaltadone		Antibiotic	-32.090	6
14	Butacaine		Local anesthetic	-32.215	5
15	Bifonazole		Imidazole antifungal	-30.647	7
16	13-cis-retinoic acid		Accutane, acne treatment	-30.110	8
17	Gabexate		Serine protease inhibitor for treatment of pancreatitis	-29.313	9
18	Sulcotidil		Vasodilator	-26.382	11

19	Capsaicin		Active component of chili peppers	-25.876	12
20	Pramoxine		Topical anesthetic	-23.735	14
21	Midodrine		Vasopressor/ Antihypertension	-19.520	18
22	Metoprolol		Beta blocker	-15.643	21
23	Glipizide		Anti-diabetic	-6.506	25
24	Fenofibrate		Cholesterol lowering drug	-26.537	10
25	Bezafibrate		Cholesterol lowering drug	-21.133	17