

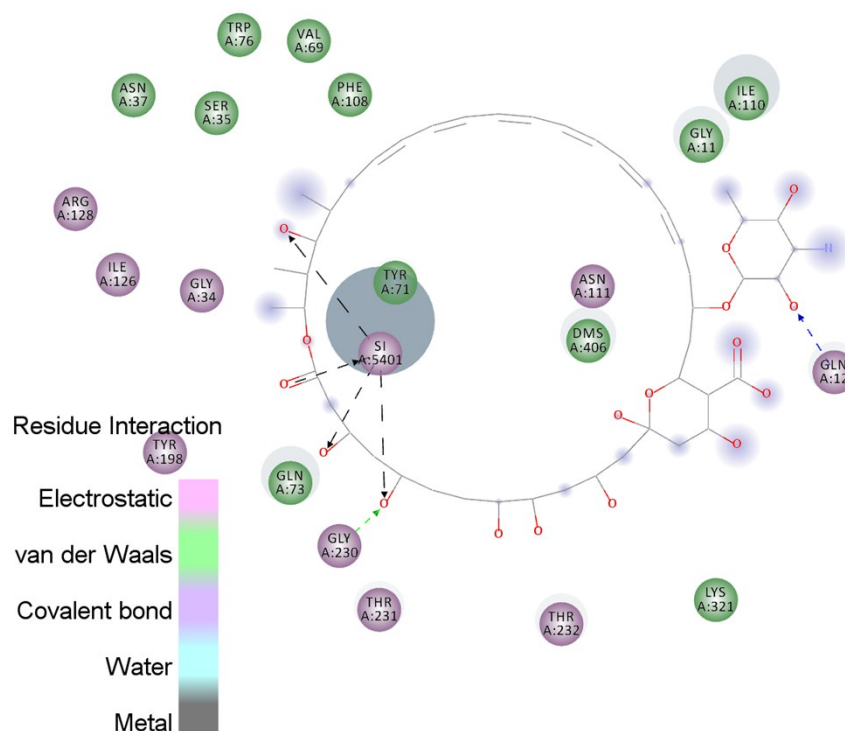


Fig. S1 Ligplot of Amphotericin B to BACE-1

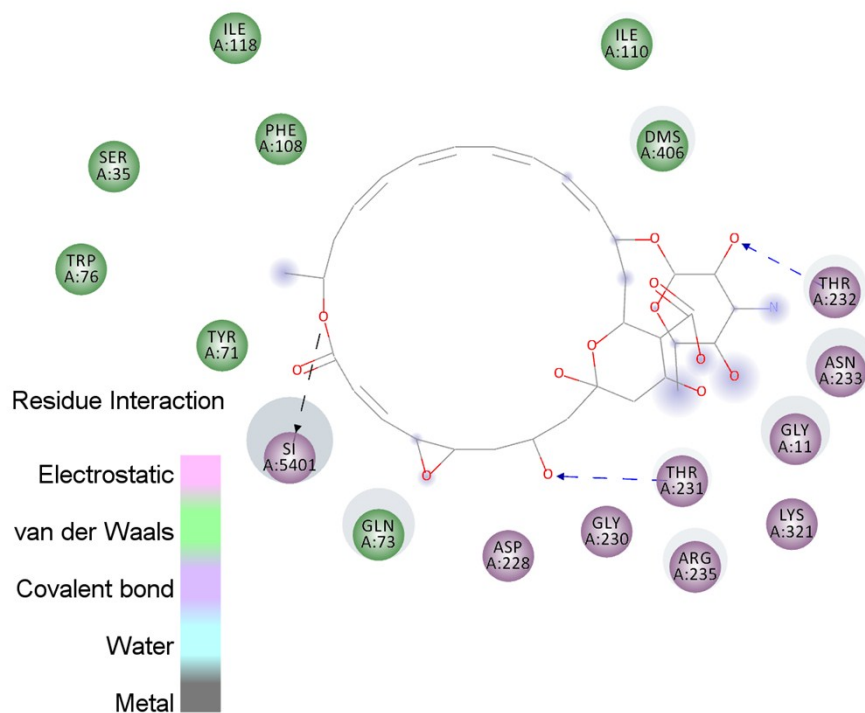


Fig. S2 Ligplot of Natamycin to BACE-1

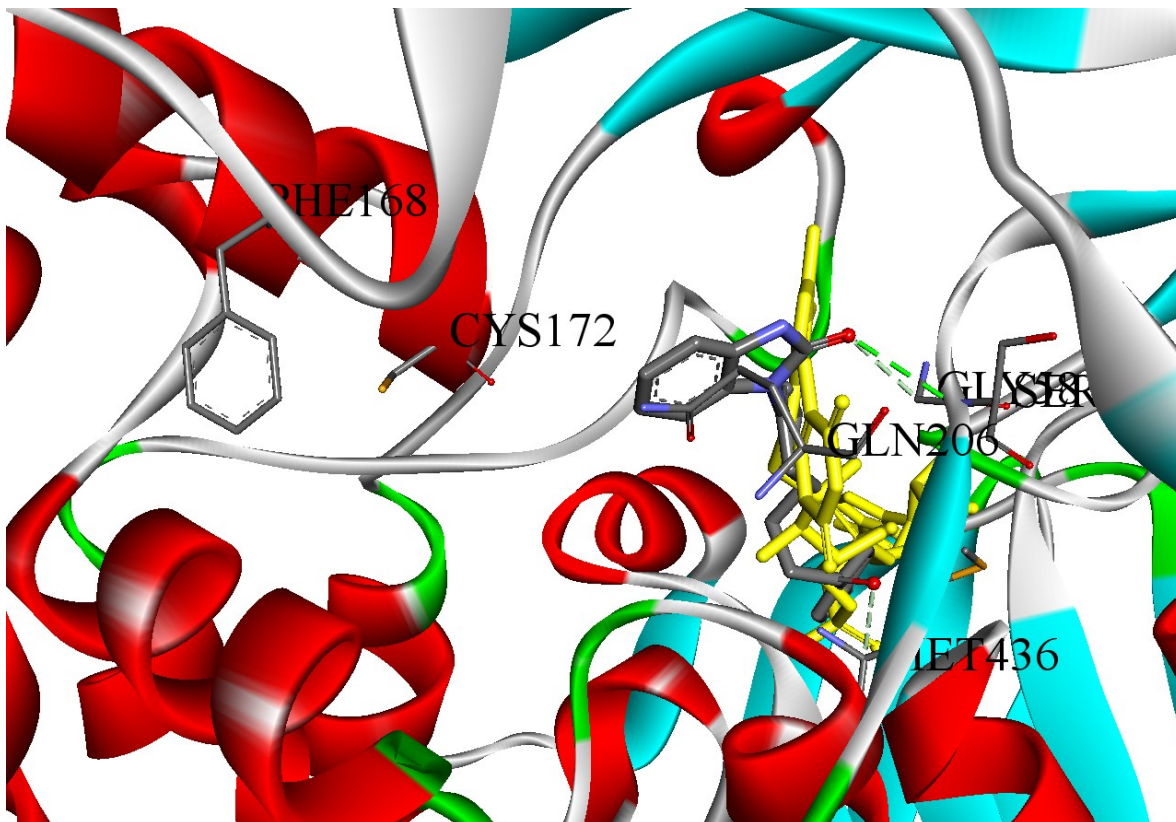


Fig. S3 The comparison of binding conformations between co-crystallized ligand of monoamine oxidase B (PDB code: 4A7A) and droperidol

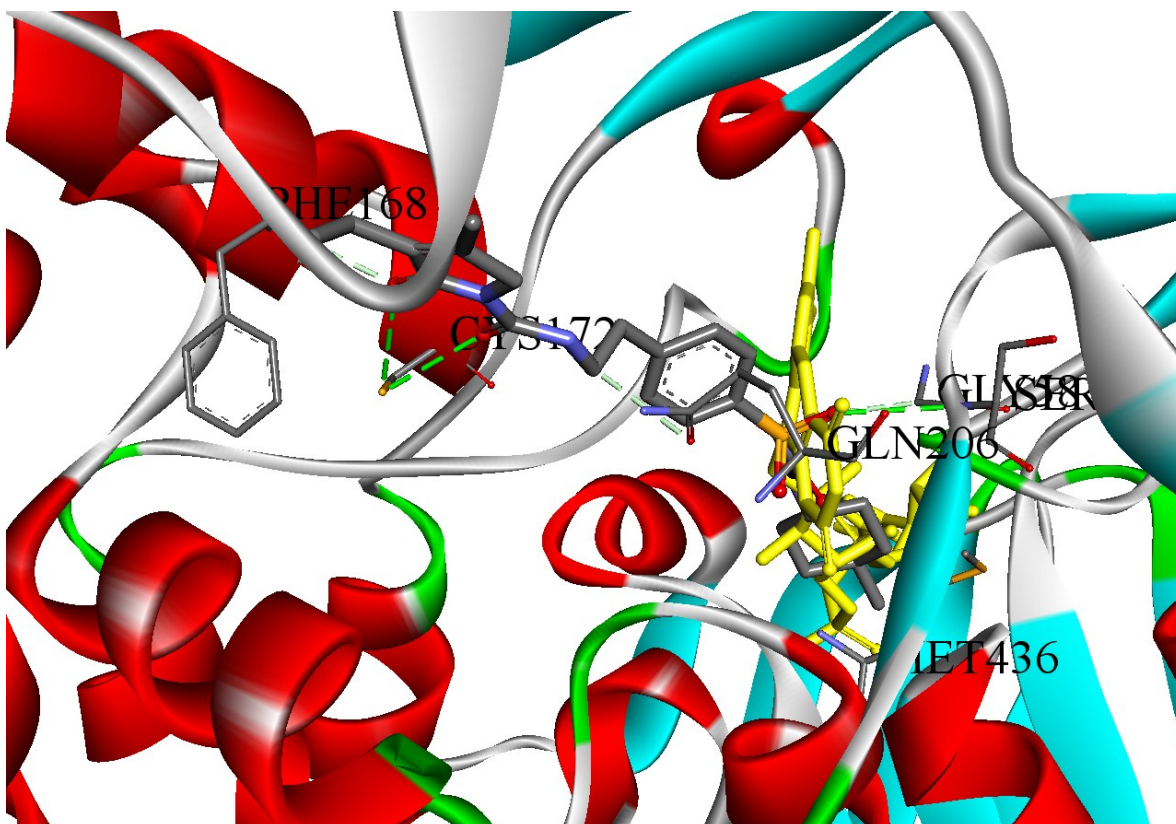


Fig. S4 The comparison of binding conformations between co-crystallized ligand of monoamine oxidase B (PDB code: 4A7A) and glimepiride

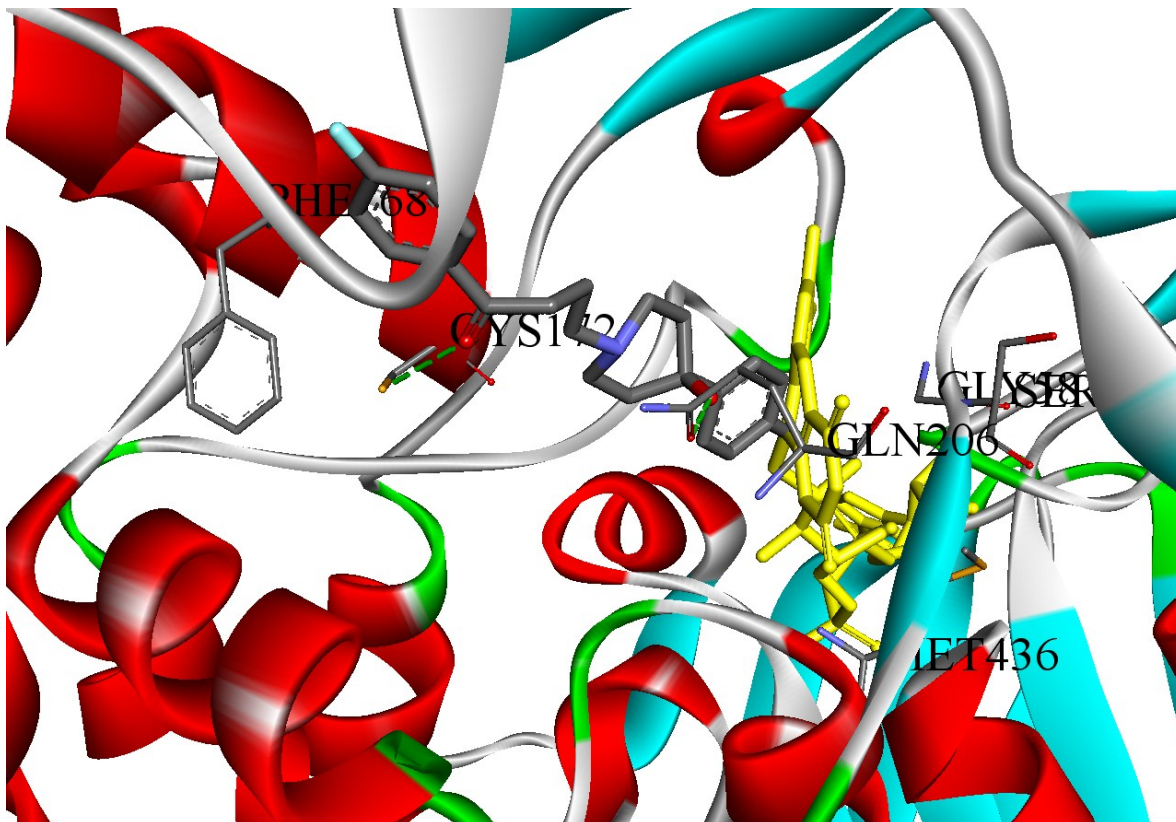


Fig. S5 The comparison of binding conformations between co-crystallized ligand of monoamine oxidase B (PDB code: 4A7A) and haloperidol

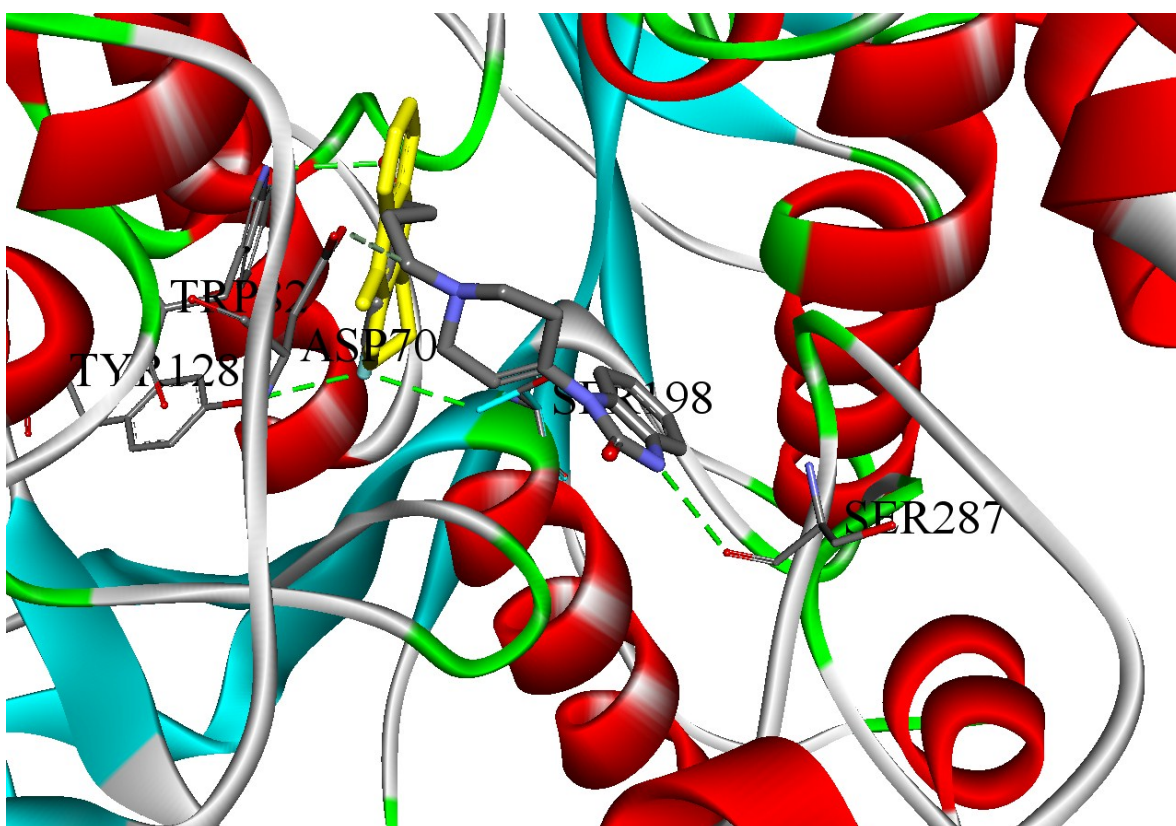


Fig. S6 The comparison of binding conformations between co-crystallized ligand of butyrylcholinesterase (PDB code: 4BDS) and droperidol

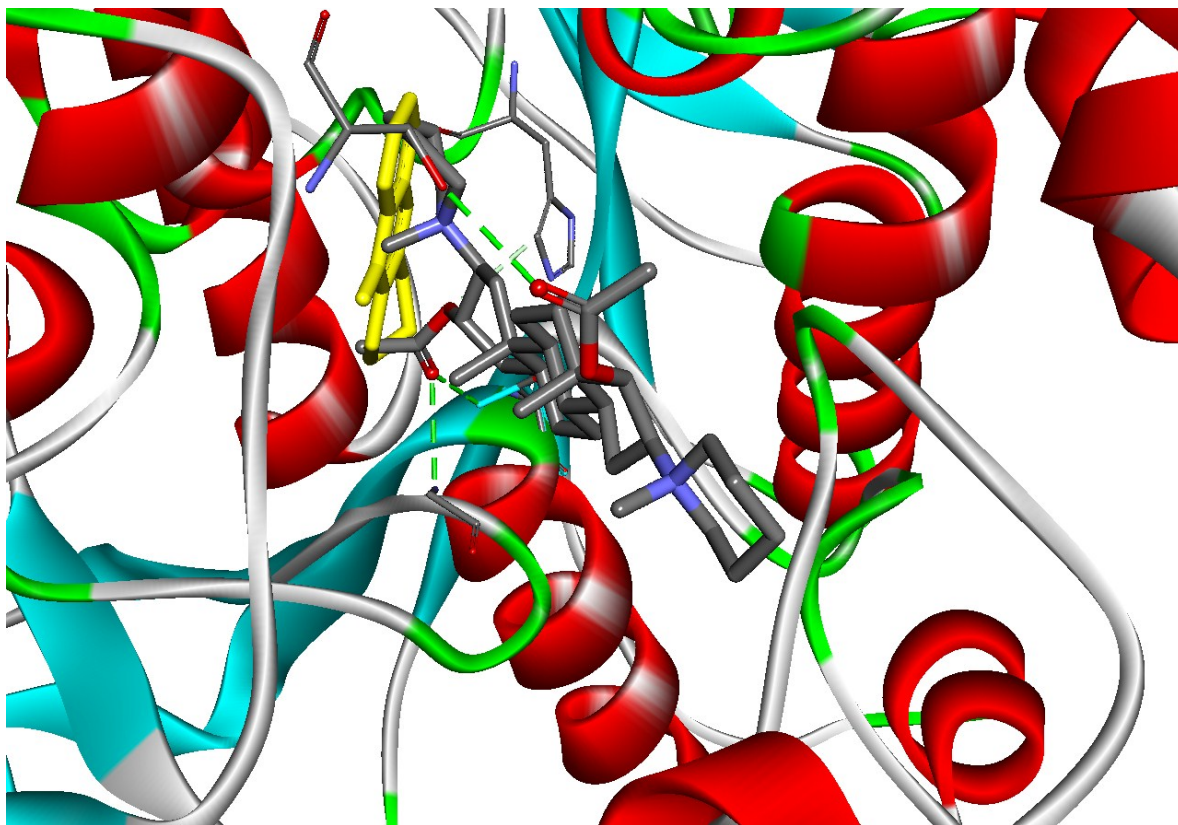


Fig. S7 The comparison of binding conformations between co-crystallized ligand of butyrylcholinesterase (PDB code: 4BDS) and pancuronium

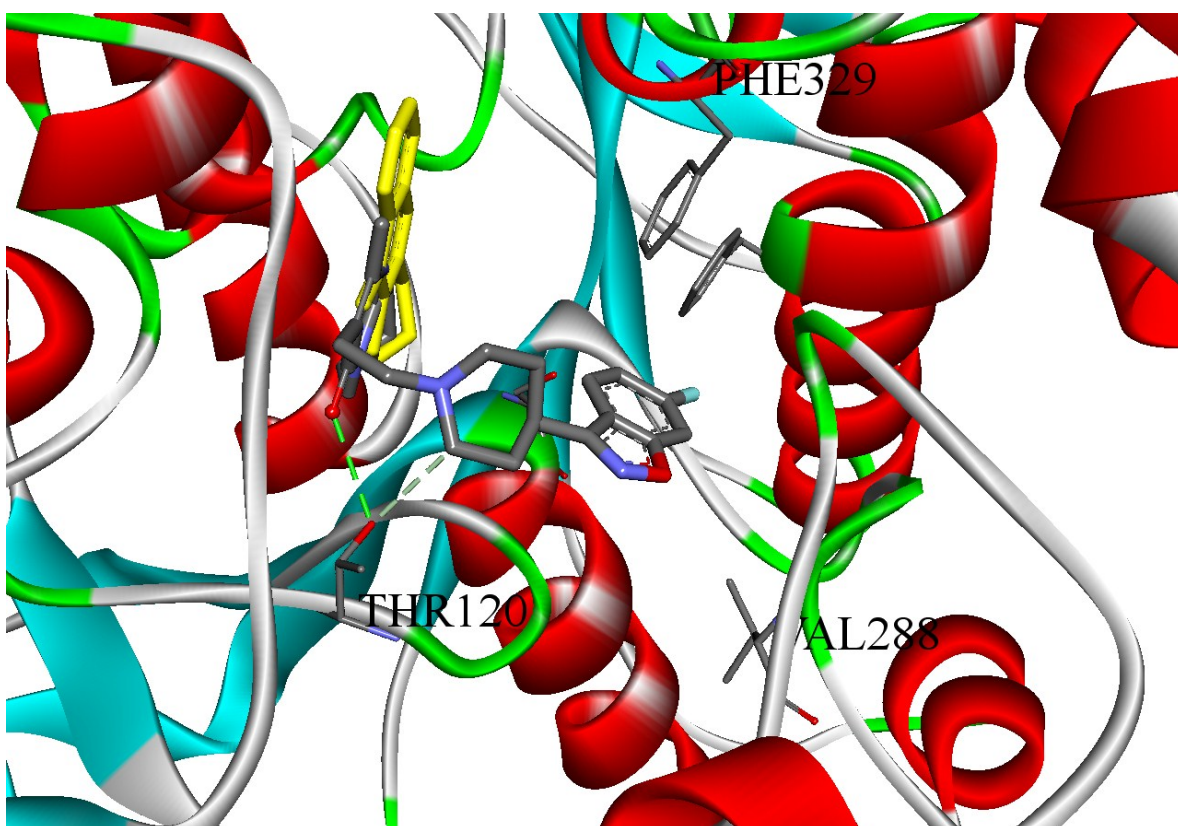
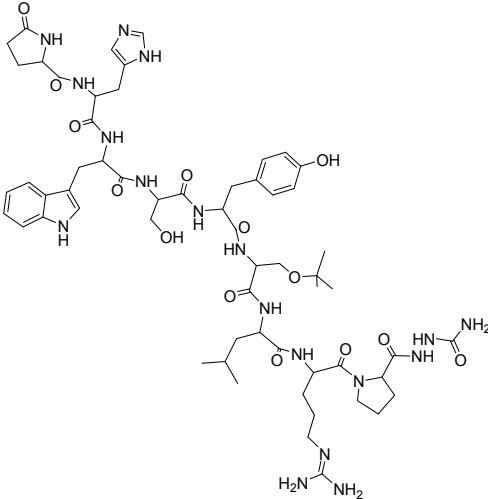
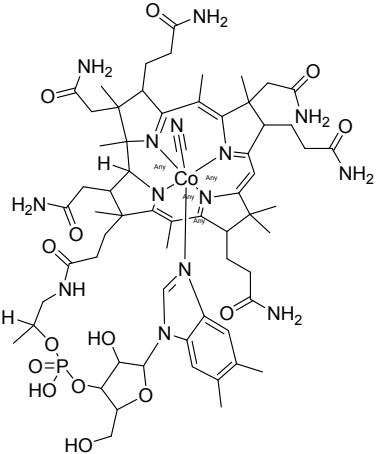
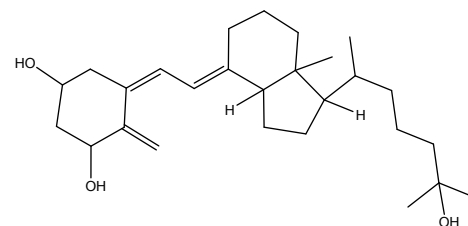


Fig. S8 The comparison of binding conformations between co-crystallized ligand of butyrylcholinesterase (PDB code: 4BDS) and risperidone

Table S1 The docking results of 211 FDA-approved drugs to the seven targets

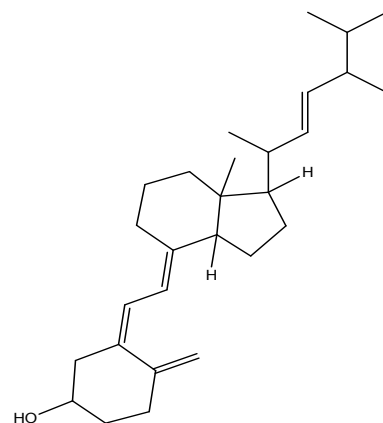
Drugs	Structures	Docking results (kcal/mol)						
		NMDA	CDK5	BChE	AChE	GSK-3 β	BACE1	MAO-B
Goserelin		-8.8	-7.9	-10.6	-8.5	-9.1	-9.8	-9
Cyanocobalamin		-9.3	-9.4	-7.8	-8.4	-10.9	-8.1	-8.9

Calcitriol



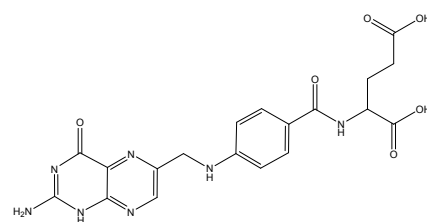
-8.7 -8.6 -9.4 -8.7 -8.6 -9.7 -10.6

Ergocalciferol



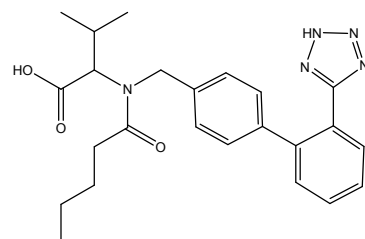
-8.8 -8.4 -10.2 -8.3 -9 -9.9 -11.6

Folic Acid



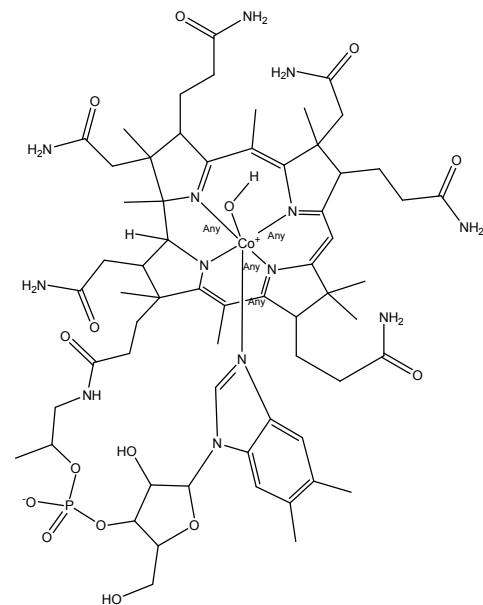
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Valsartan



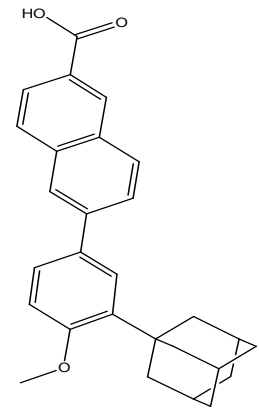
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Hydroxocobalamin



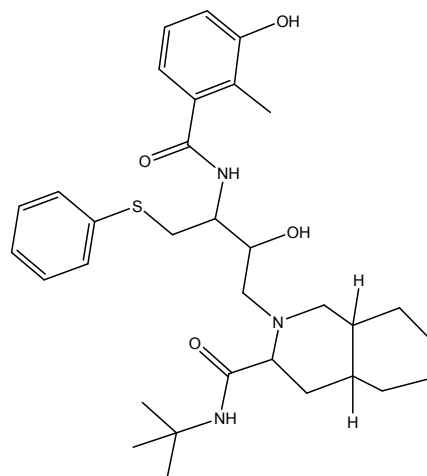
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Adapalene



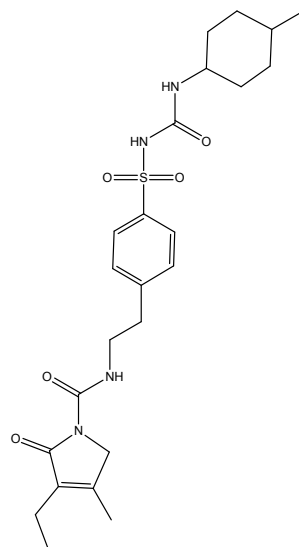
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Nelfinavir



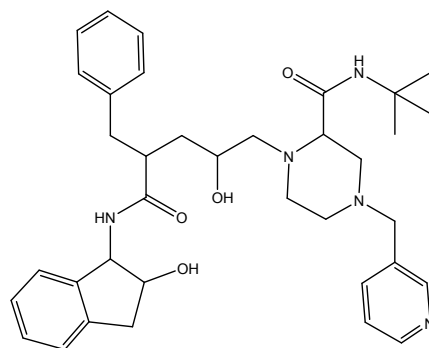
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Glimepiride



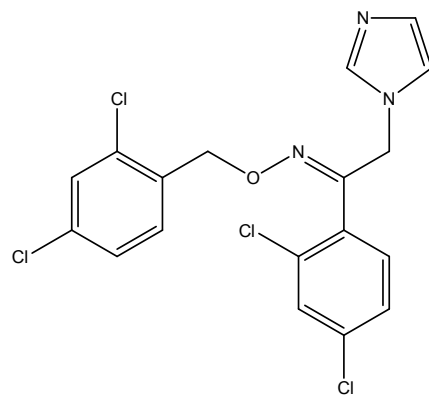
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Indinavir



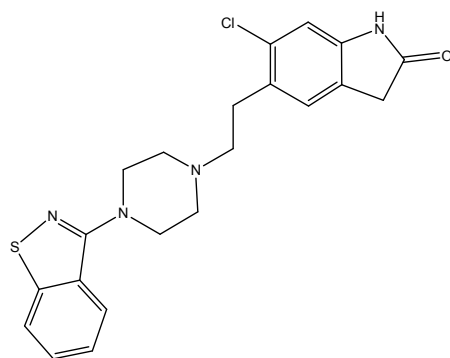
-9.9 -8.9 -10.8 -9.6 -9.3 -10.1 -8

Oxiconazole



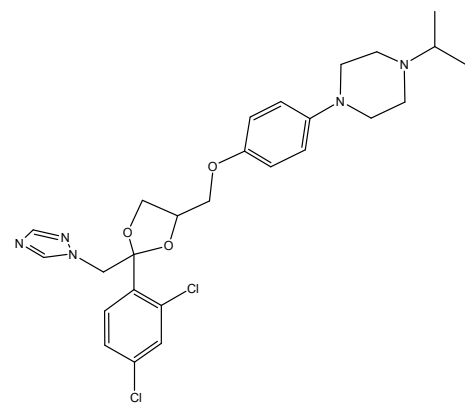
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Ziprasidone



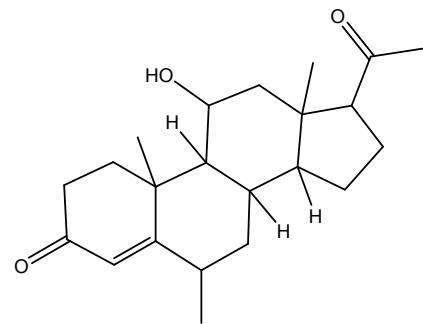
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Terconazole



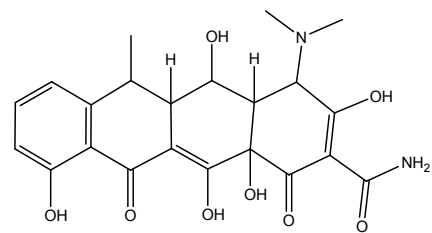
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Medrysone



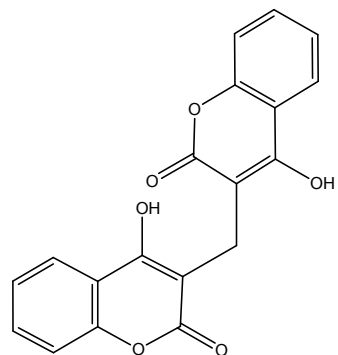
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Doxycycline



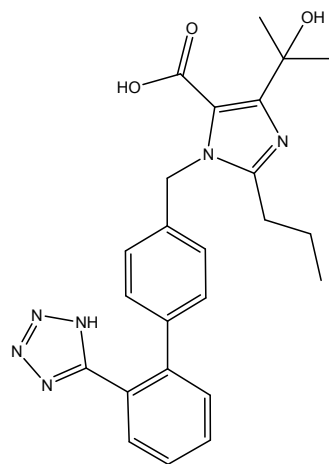
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Dicoumarol



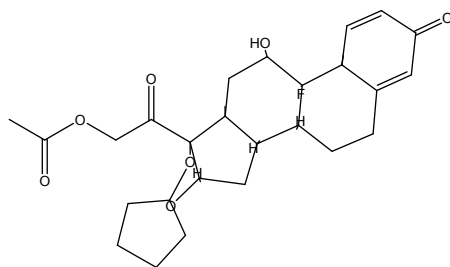
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Olmesartan



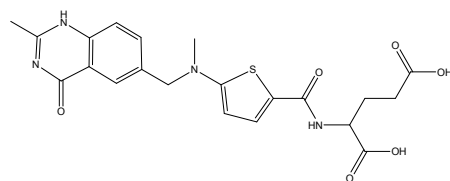
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Amcinonide



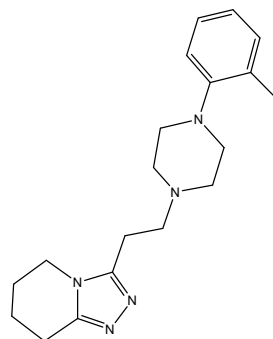
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Raltitrexed



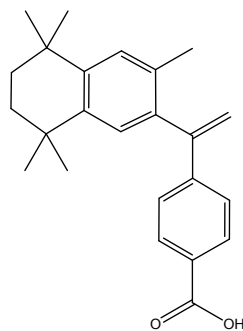
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Dapiprazole



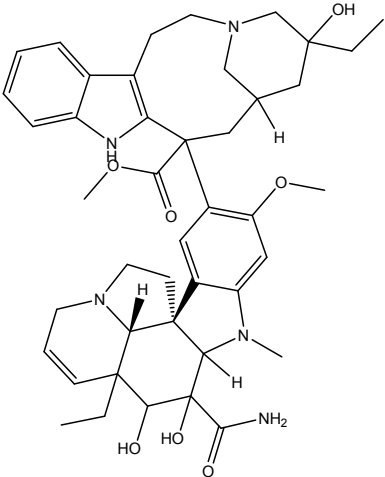
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Bexarotene



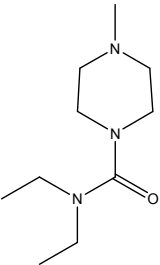
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Vindesine



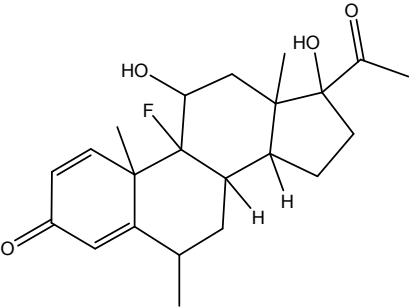
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Dihydroergotamine



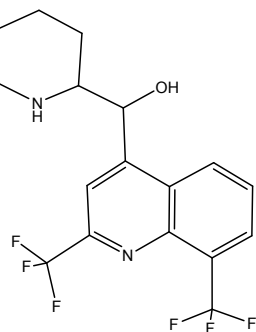
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Fluorometholone



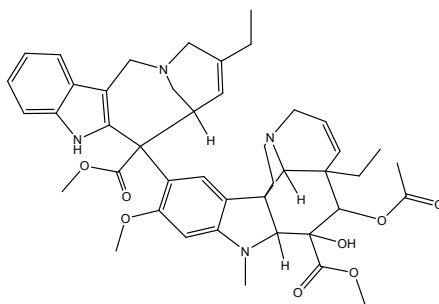
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Mefloquine



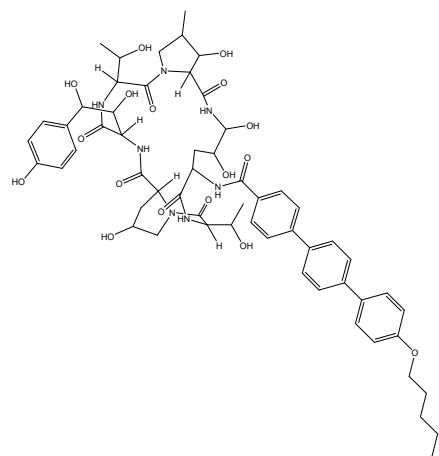
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Vinorelbine



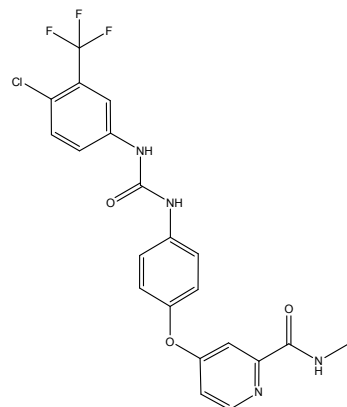
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Anidulafungin



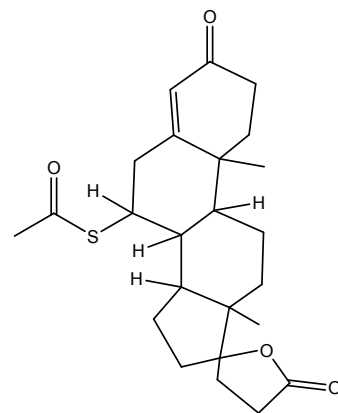
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Sorafenib



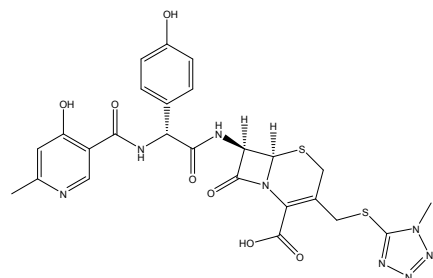
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Spirolactone



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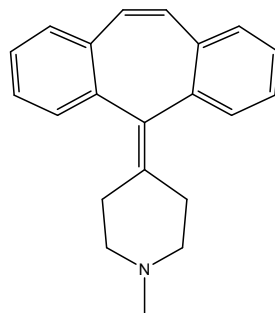
Cefpiramide



Chiral

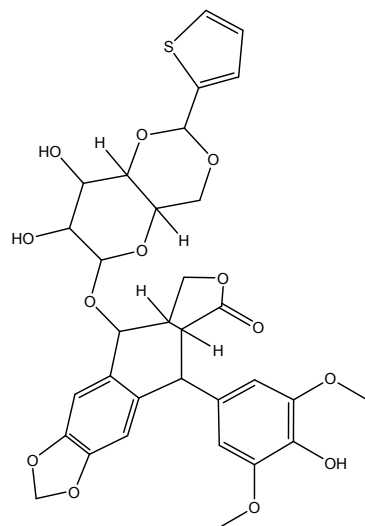
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Cyproheptadine



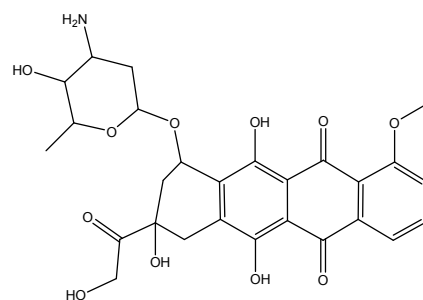
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Teniposide

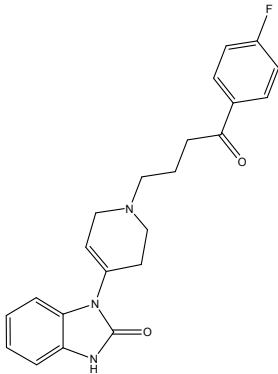
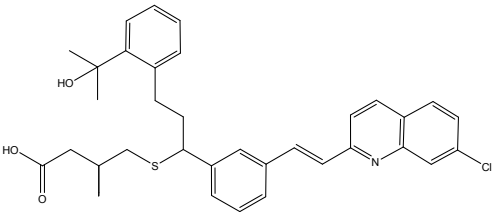
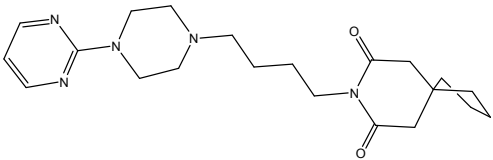
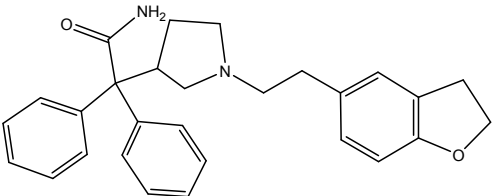


-9.5 -8.3 -11.7 -9 -9 -11.1 -8.9

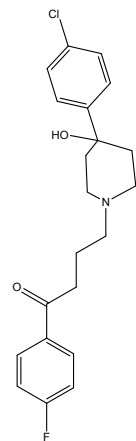
Epirubicin



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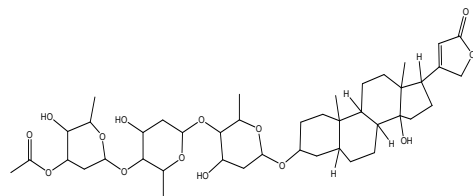
Droperidol		-8.4	-8.4	-10.4	-9.3	-8.5	-8.8	-10.7
Montelukast		-9.5	-8	-10.6	-10.5	-8.8	-9.2	-9.4
Buspirone		-7.9	-8.1	-9	-7.7	-7.6	-7.4	-10.5
Darifenacin		-7.1	-6.6	-10.5	-9.9	-8.7	-9.5	-9

Haloperidol



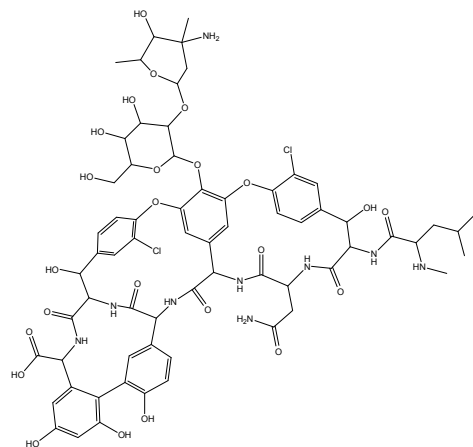
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Acetyldigitoxin



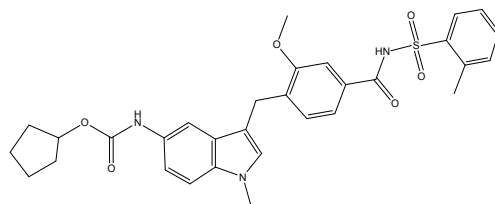
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Vancomycin



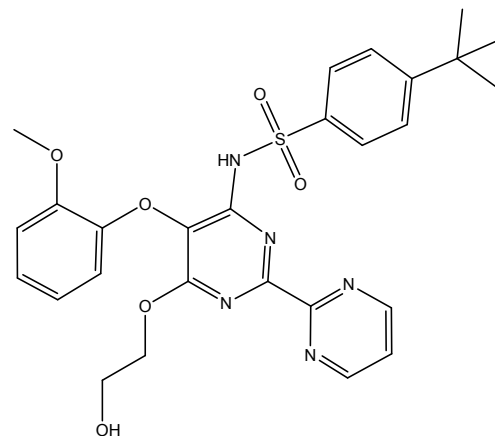
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Zafirlukast



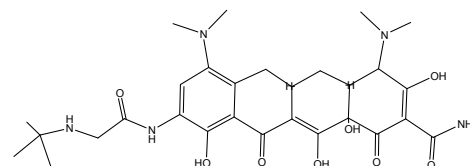
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Bosentan



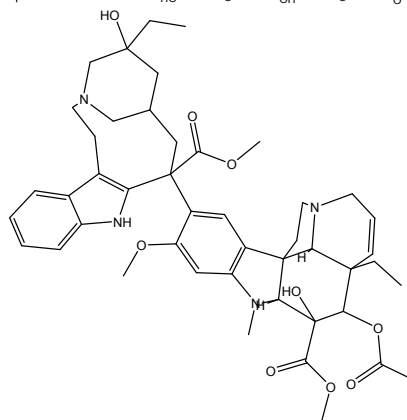
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Tigecycline



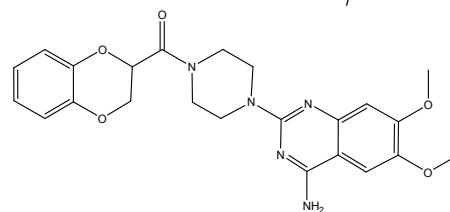
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Vinblastine



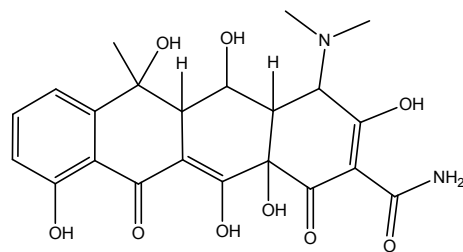
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Doxazosin



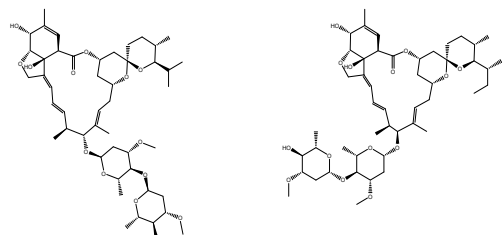
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Oxytetracycline



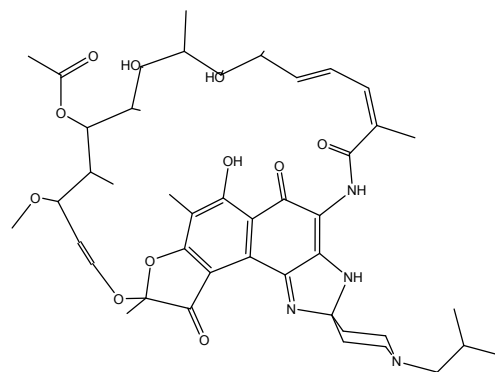
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Ivermectin



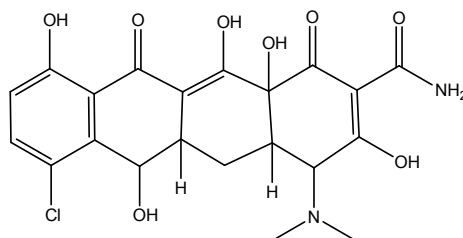
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Rifabutin



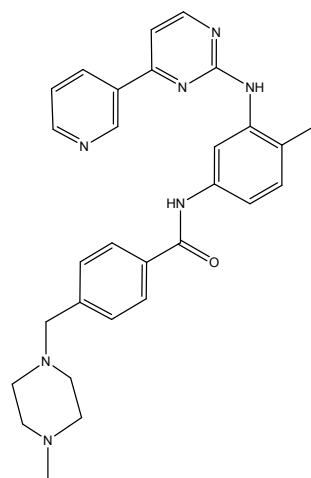
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Demeclocycline



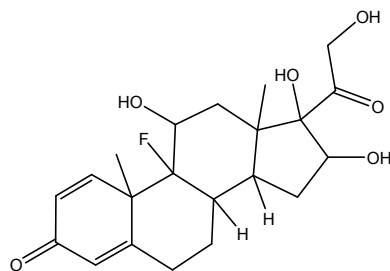
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Imatinib



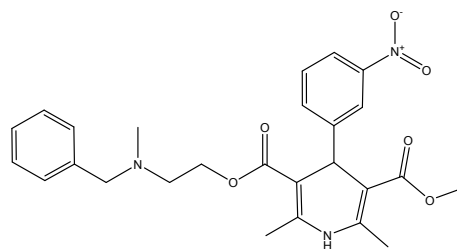
-10.3 -9.3 -11 -10.7 -9 -9.9 -12.1

Triamcinolone



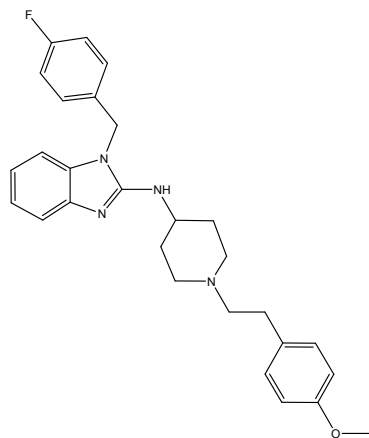
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Nicardipine



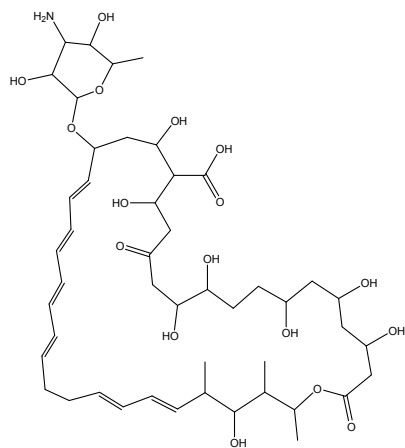
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Astemizole



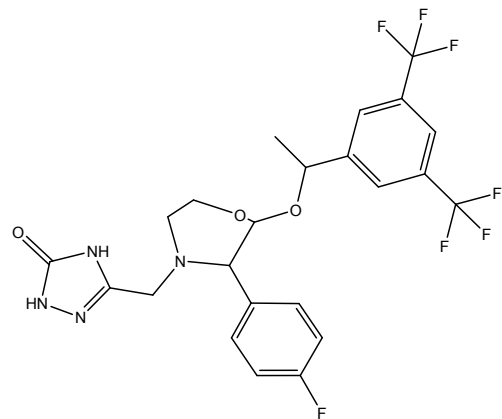
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Nystatin



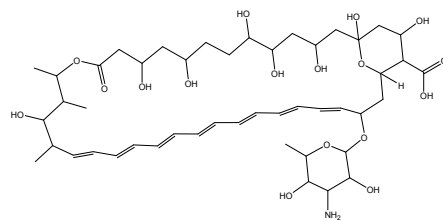
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Aprepitant



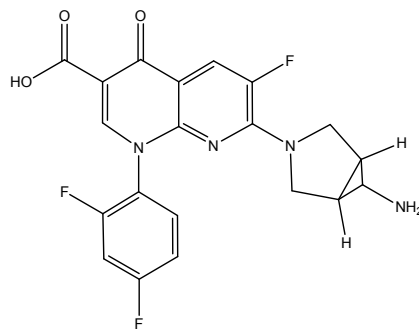
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Amphotericin B



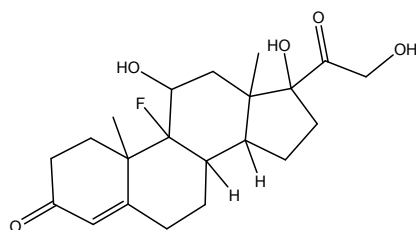
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Trovafloracin



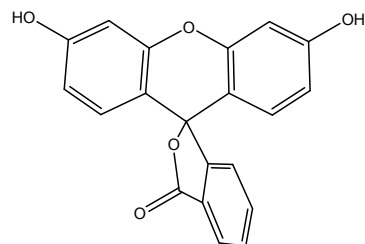
-8 -7.9 -10.5 -8.3 -9.2 -9.9 -9.6

Fludrocortisone



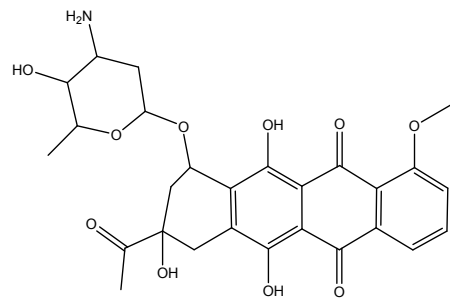
-8.7 -8.1 -10.6 -8.2 -9.1 -9.3 -8.6

Fluorescein



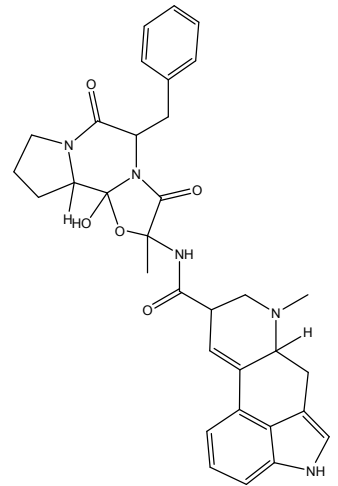
-10.8 -7.9 -11.4 -10 -9.2 -10.5 -10.6

Daunorubicin



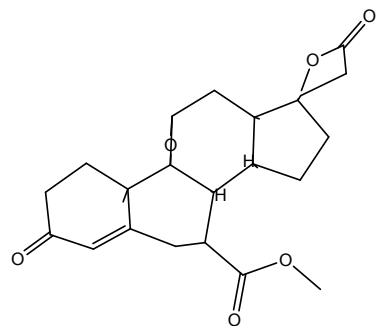
-9.5 -9.2 -10.6 -9.7 -10.3 -10.6 -9.2

Ergotamine



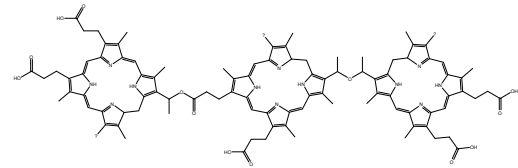
-10.3 -9.6 -13.3 -10.9 -10.7 -11.7 -10.2

Eplerenone



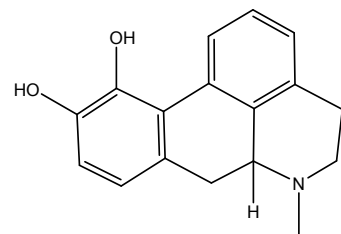
-8.6 -7.6 -11.1 -8.5 -9.4 -9.5 -7.8

Porfimer



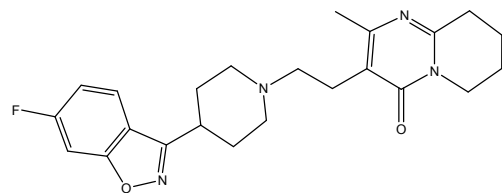
-11.7 -11.8 -11.1 -9.7 -12 -12.8 -12.3

Apomorphine



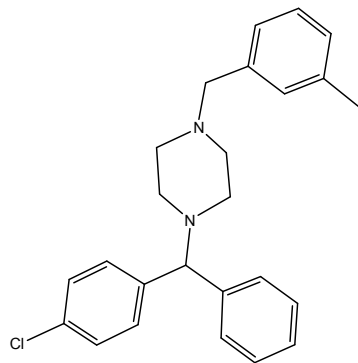
-8.7 -8.9 -9.8 -10.8 -9.2 -9.2 -8.8

Risperidone



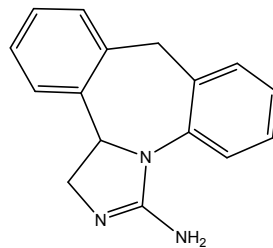
-9.7 -10.6 -10.8 -9.3 -8.9 -9.5 -12.4

Meclizine



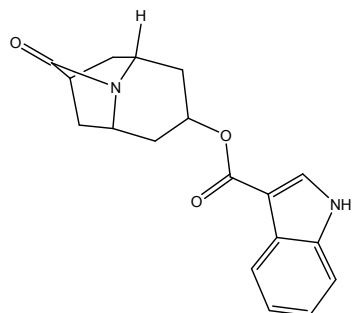
-10.8 -7.9 -10.3 -9.1 -8.5 -9.2 -8.8

Epinastine



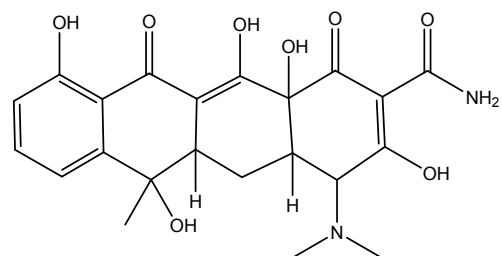
-9.1 -11.2 -10 -10.1 -8.9 -9 -9.6

Dolasetron



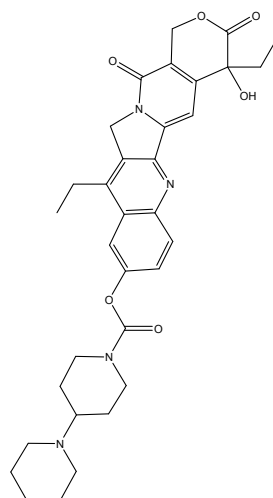
-8.1 -6.8 -10.6 -8 -7.7 -8.4 -10.4

Tetracycline



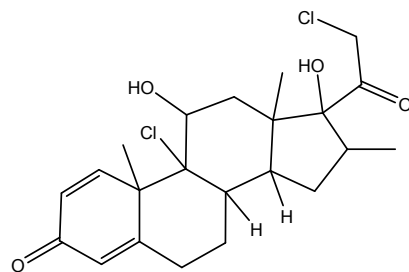
-8.1 -8.5 -11.1 -8.7 -9.7 -11 -8.3

Irinotecan



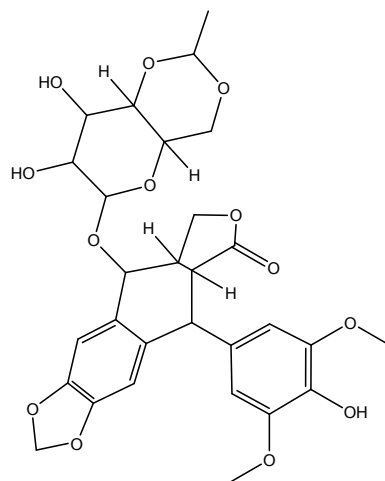
-10.5 -8.9 -11.8 -9.7 -9.8 -11.4 -10.3

Mometasone



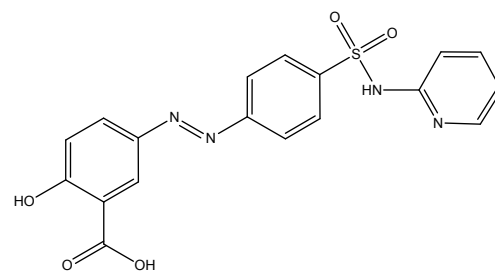
-8.6 -7.8 -10.7 -8 -8.6 -8.8 -8.9

Etoposide



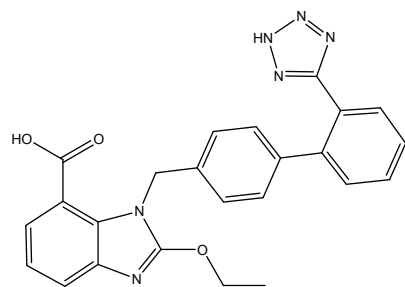
-9.4 -8.3 -11.8 -9.2 -9.6 -10.9 -8.9

Sulfasalazine



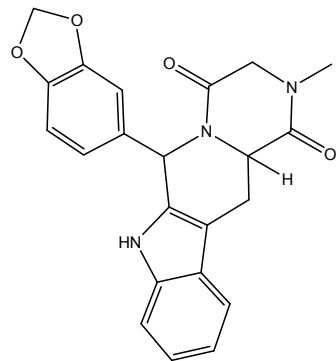
-9.1 -8.9 -9.7 -10.5 -7.5 -8.5 -11.7

Candesartan



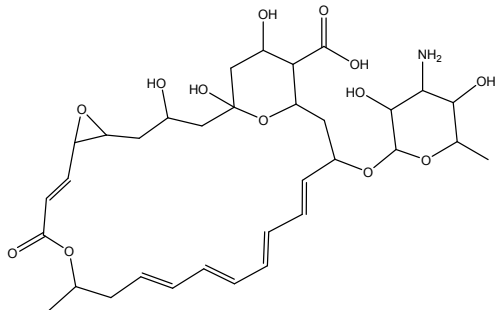
-9.9 -8.2 -11 -9.1 -8.5 -9.7 -10.3

Tadalafil



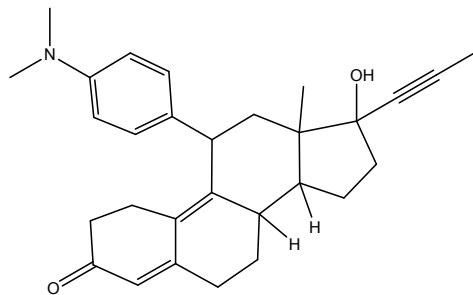
-8.4 -8.1 -11.5 -9 -9.2 -11.4 -9.6

Natamycin



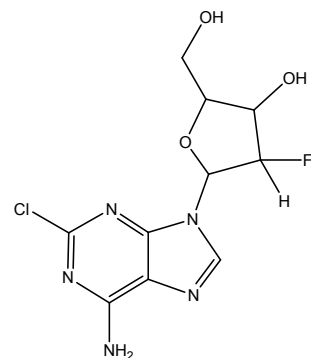
-11.2 -10 -10.8 -10.3 -10.9 -11.7 -11.4

Mifepristone



-10.7 -8.8 -9.8 -10.2 -9.6 -11.2 -10.6

Clofazimine



-8.9

-8.1

-11.8

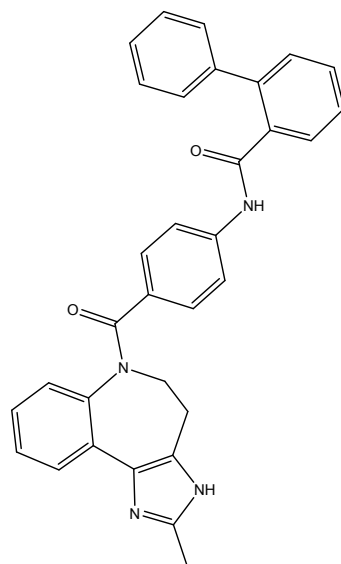
-9.8

-9.4

-10

-10.4

Conivaptan



-12.8

-10.2

-12.7

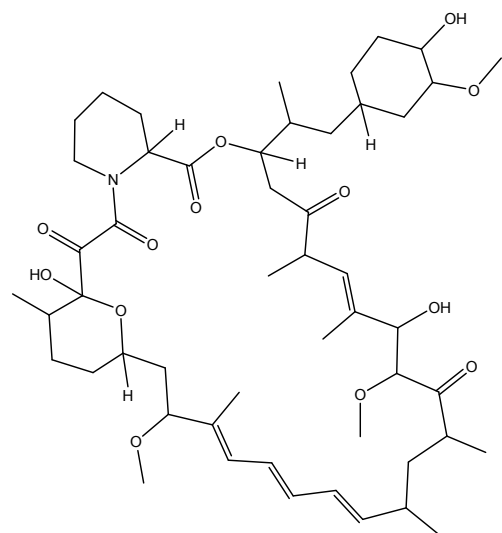
-10.4

-10.6

-10.4

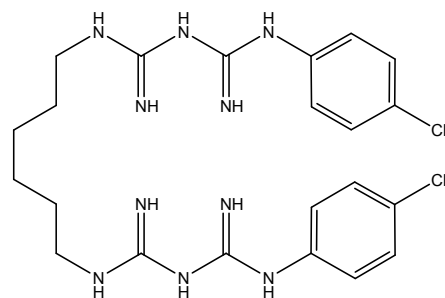
-10.3

Sirolimus



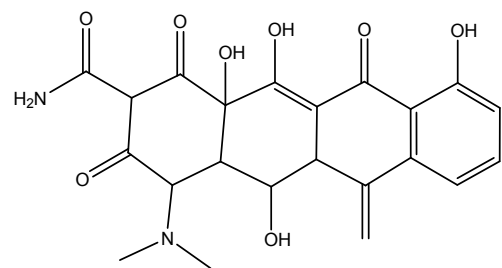
-11.2 -9.5 -10.6 -10.3 -11.3 -9.2 -9.8

Chlorhexidine



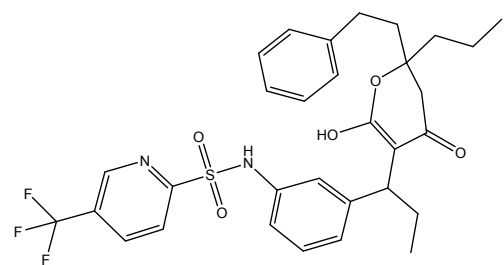
-10.6 -7.9 -7.7 -6.6 -6.8 -7.8 -8.5

Methacycline



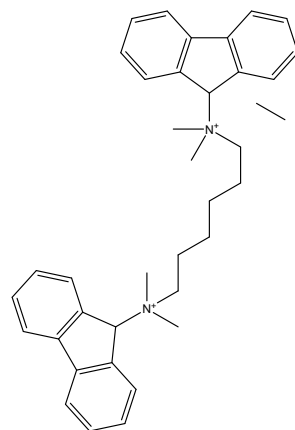
-10 -8.4 -10.5 -10.7 -9.6 -10.8 -9.1

Tipranavir



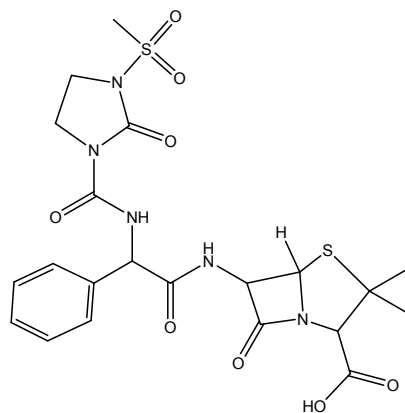
-9.9 -8.9 -11.1 -9.6 -8.3 -9.5 -10

Hexafluronium



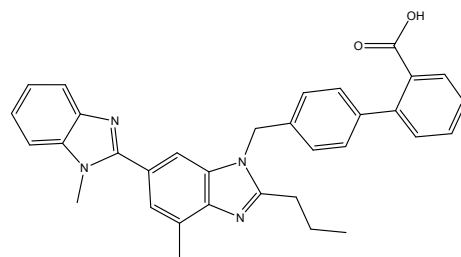
-10 -4.8 -10.5 -6.8 -8.2 -9.8 -9.4

Mezlocillin



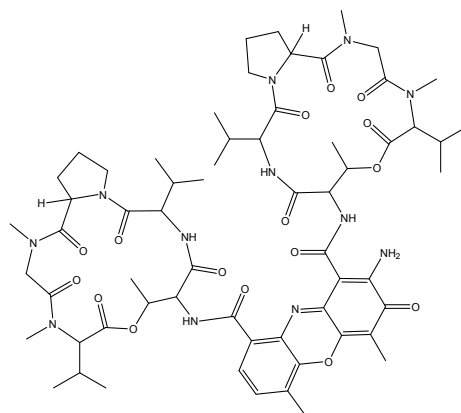
-8.5 -7.5 -10.9 -8.9 -9.1 -9.8 -9.2

Telmisartan



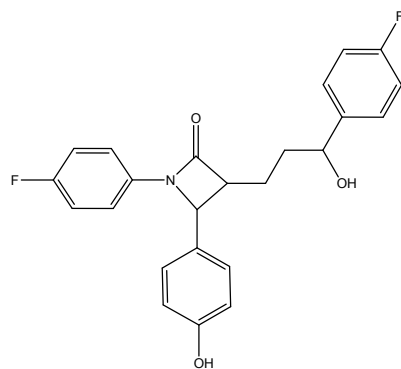
-11 -9 -13.2 -10.4 -9.6 -11.1 -10.6

Dactinomycin



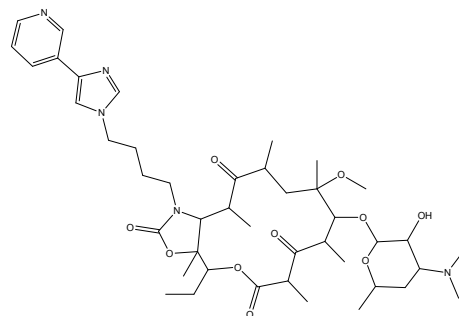
-10.9 -9.4 -10.7 -10.3 -12.3 -11.8 -10.3

Ezetimibe



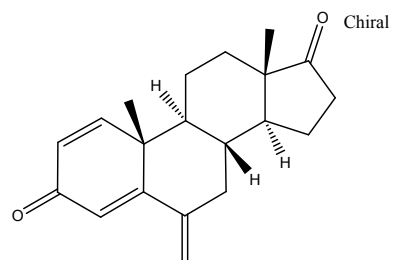
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Telithromycin



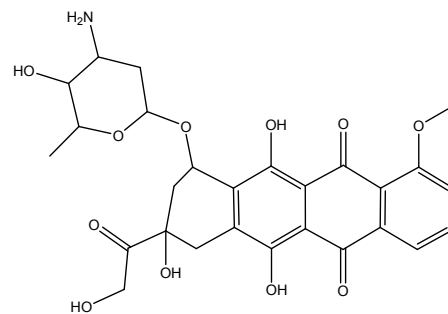
-9.1 -8.5 -10.5 -7.8 -9.3 -9.6 -9.1

Exemestane



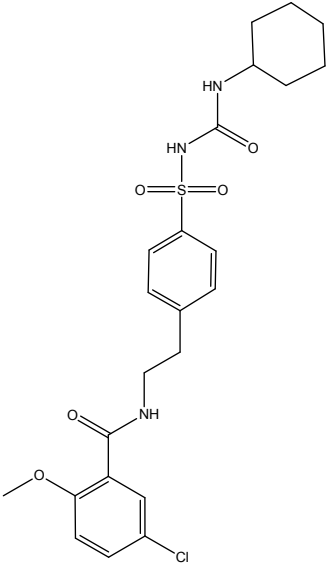
-8.8 -8.1 -10.5 -10.4 -10 -9.6 -9.2

Doxorubicin



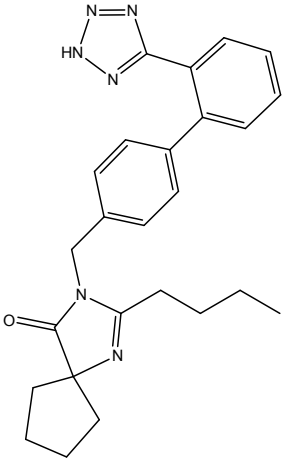
-9.2 -8 -10.9 -9.3 -10.1 -10.4 -9.5

Glyburide



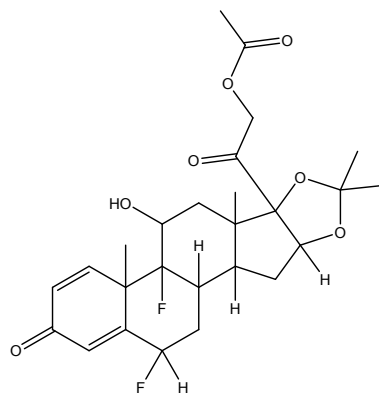
-9.1 -7.9 -9.3 -10.6 -8.2 -8.7 -9.9

Irbesartan



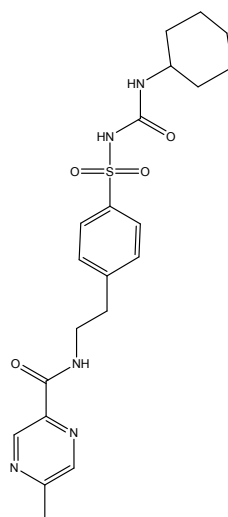
-11.5 -8.6 -10.6 -9 -9.4 -9.3 -10.4

Fluocinonide



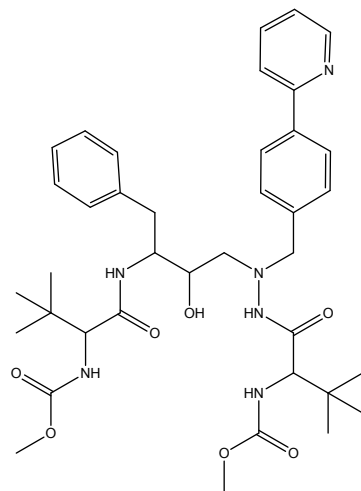
-8.7 -7.9 -10.8 -9.1 -10 -9.5 -9.1

Glipizide



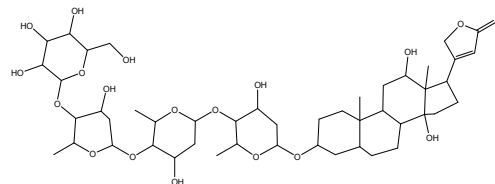
-10.2 -7.9 -10.8 -9.3 -8.2 -8.8 -12.5

Atazanavir



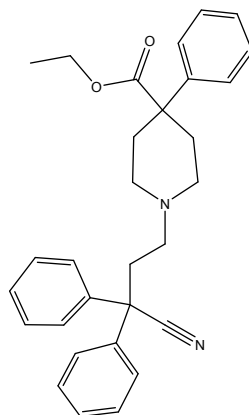
-9.4 -7.5 -11.1 -6.9 -8.3 -9 -8.1

Deslanoside



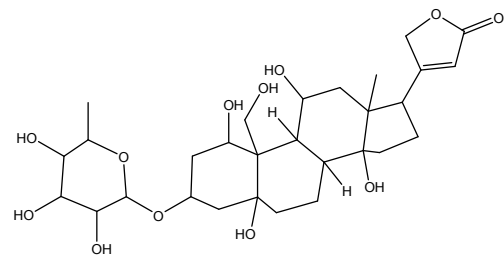
-11 -9.7 -11.7 -11.2 -11.9 -11.3 -11.3

Diphenoxylate



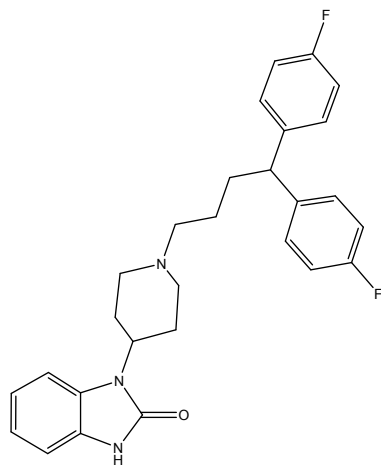
-11 -8.3 -11.5 -10.6 -9.1 -9.6 -9.1

Ouabain



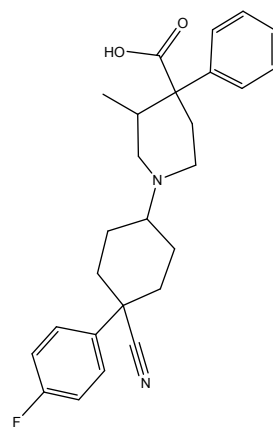
-9.8 -8.7 -12.2 -9.7 -10.3 -10.1 -10.8

Pimozide



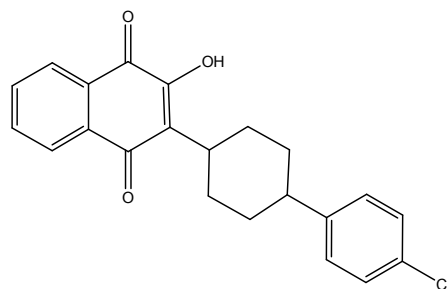
-8.7 -8.8 -11.1 -9.1 -8.8 -9.6 -9.9

Levocabastine



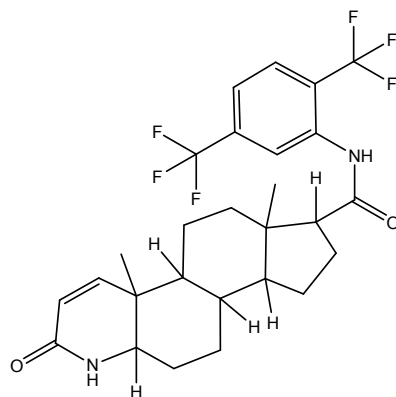
-8.4 -10.1 -12.5 -10.6 -8.6 -9.9 -9.6

Atovaquone



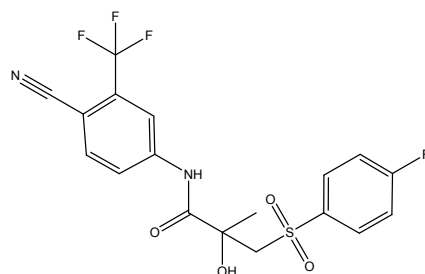
-12.6 -10.6 -10.6 -9.7 -9.3 -9.7 -13.5

Dutasteride



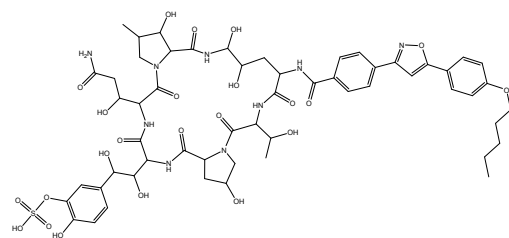
-9.3 -9 -11.9 -10.9 -9.6 -10.3 -10.8

Bicalutamide



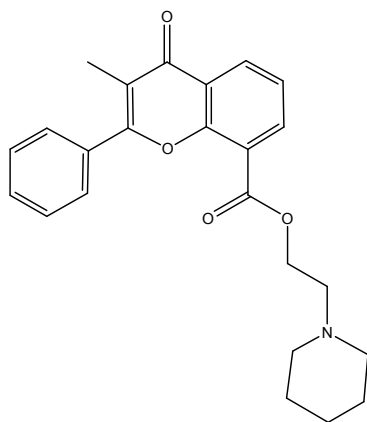
-8.7 -8.1 -10.9 -9.4 -7.9 -9.6 -9.8

Micafungin



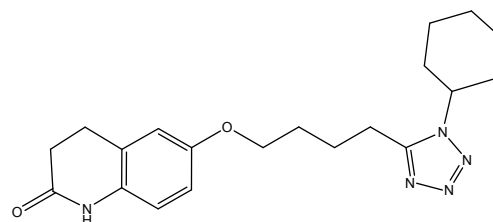
-9.6 -8.8 -8.5 -8.9 -11.1 -8.8 -10.4

Flavoxate



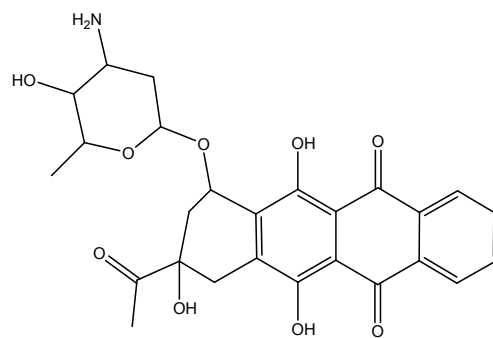
-9.5 -8.3 -11.6 -8.5 -8.8 -9.1 -8.4

Cilostazol



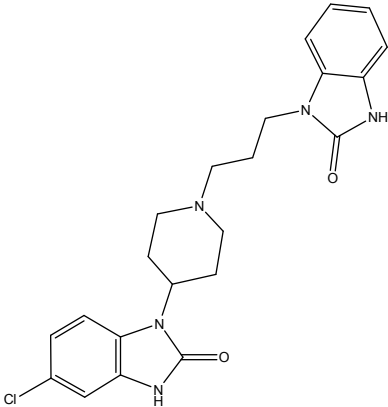
-9.5 -8.6 -9.8 -8.5 -7.7 -8.5 -11.2

Idarubicin



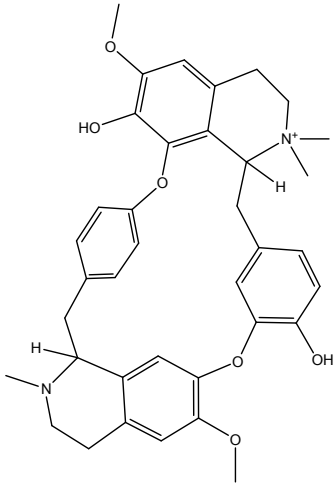
-9.5 -9.3 -11.6 -10.7 -10.3 -11.1 -10.5

Domperidone



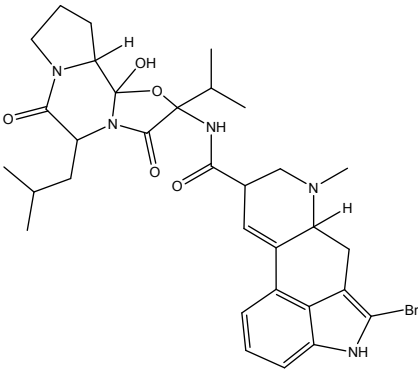
-10.7 -8.5 -9.5 -8.4 -8.3 -9.2 -11.8

Tubocurarine



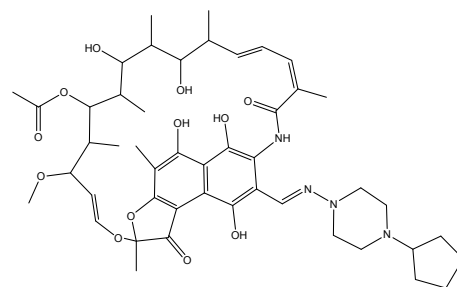
-11.1 -8.8 -10.1 -10.4 -11.9 -11.7 -11.1

Bromocriptine



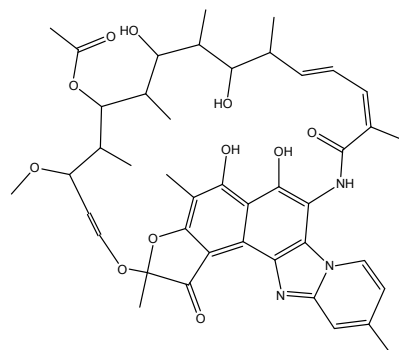
-9.3 -9.1 -11.6 -9.2 -10.6 -10.8 -8.8

Rifapentine



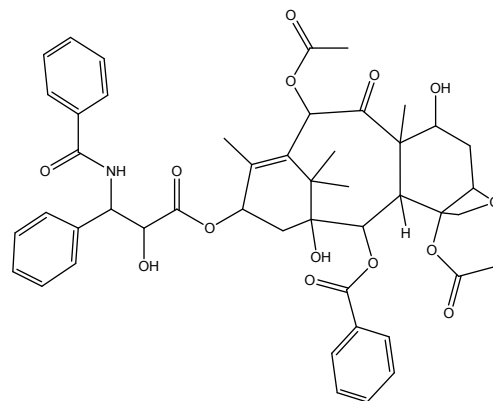
-11 -9.8 -10.4 -10.3 -11.9 -9.5 -10.6

Rifaximin



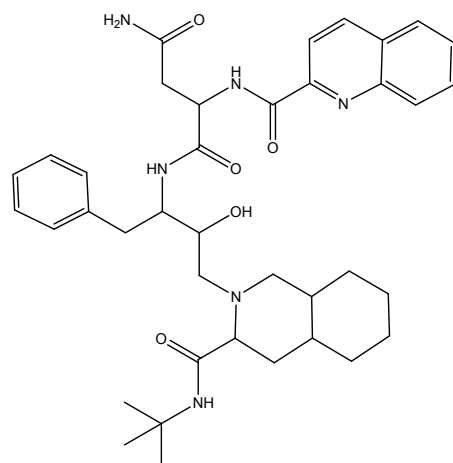
-10.1 -9.1 -11.2 -11.1 -11.5 -9.5 -9.8

Paclitaxel



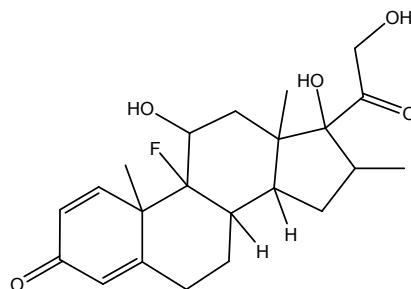
-9.2 -8.8 -11.1 -9.5 -8.7 -10.7 -9.1

Saquinavir



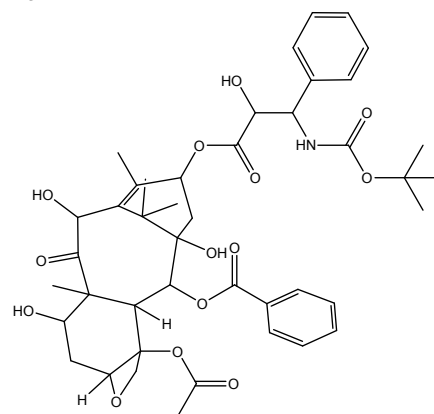
-9.4 -8 -11.9 -9.8 -8.8 -10.3 -9.5

Dexamethasone



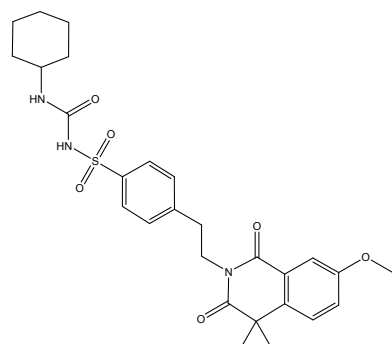
-8.7 -7.8 -10.9 -8.2 -8.9 -8.9 -9.1

Docetaxel



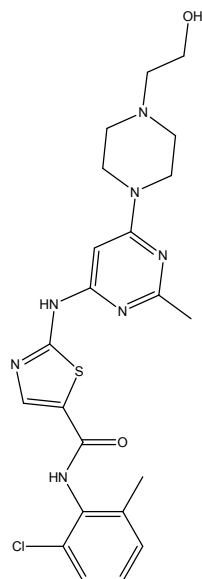
-9.3 -8.7 -11.1 -10.2 -8.3 -10.2 -7.3

Gliquidone



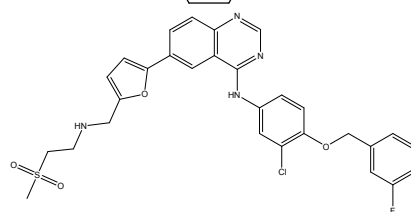
-11.3 -9 -12 -9.6 -9.1 -10.5 -9.8

Dasatinib



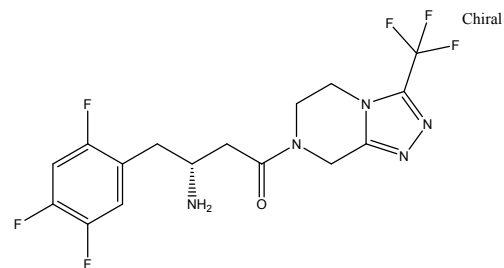
-9.5 -7.8 -9.3 -9 -8.2 -8.7 -10.7

Lapatinib



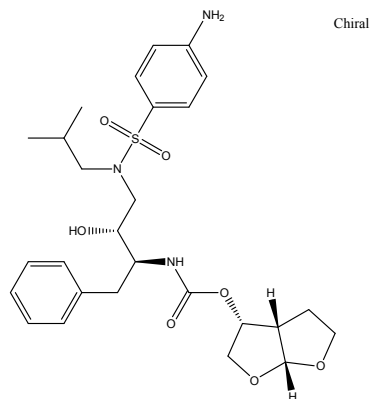
-11.2 -8.5 -9.7 -9 -8.9 -9.4 -10.1

Sitagliptin



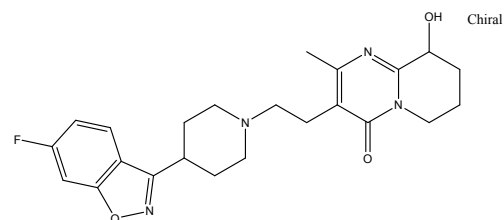
-8.2 -8.3 -10.1 -8.8 -8.1 -9.3 -11.1

Darunavir



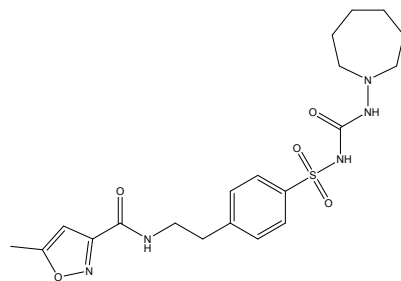
-9 -7.9 -10.5 -8.2 -8.2 -9.1 -8.5

Paliperidone



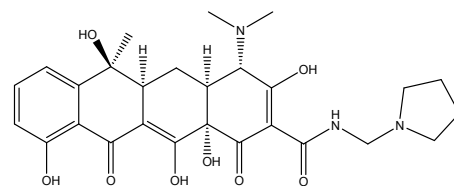
-9.3 -9.2 -11 -9.3 -8.7 -9.9 -13.2

Glisoxepide



-9.5 -8.3 -10.6 -9.2 -8.2 -8.4 -11.7

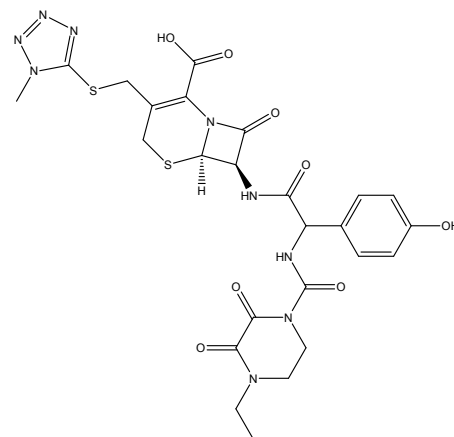
Rolitetracline



Chiral

-8.6 -8.6 -11.1 -9.2 -9.4 -9.7 -8.6

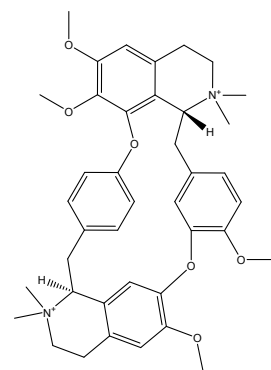
Cefoperazone



Chiral

-10 -8 -10.6 -9 -8.7 -9.5 -9.2

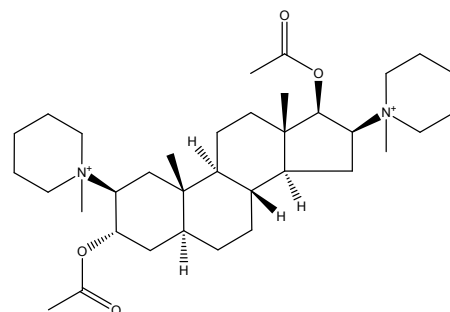
Metocurine



Chiral

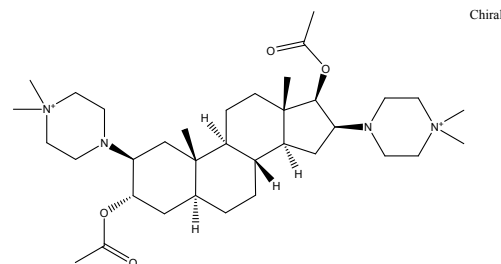
-8.8 -8.3 -9.2 -9.1 -10.1 -10.5 -10.6

Pancuronium



-8.9 -8.1 -10.5 -8 -9.6 -10.3 -7.7

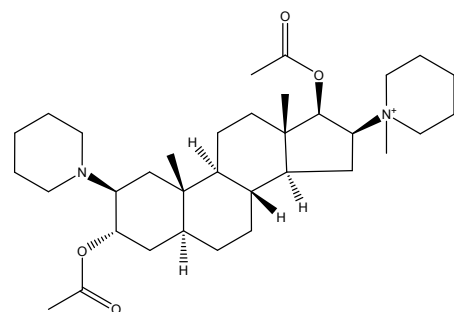
Pipecuronium



Chiral

-8.6 -7.2 -10.7 -8.5 -9.1 -9.7 -7.8

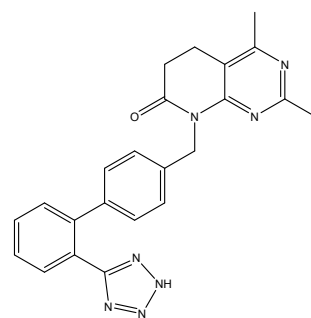
Vecuronium



Chiral

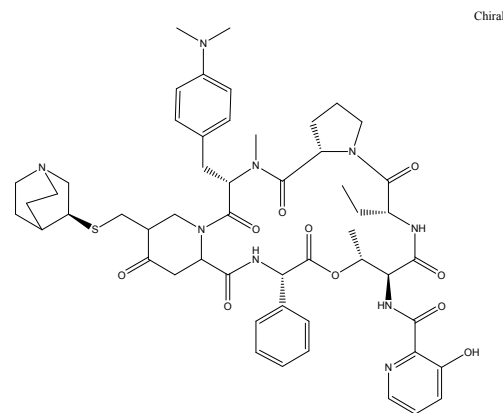
-8.9 -7.7 -10.8 -9 -9.4 -9.8 -7.6

Tasosartan



-9.7 -10.3 -11.5 -10.4 -9.3 -10.1 -9.4

Quinupristin



-9.8

-8.5

-10.4

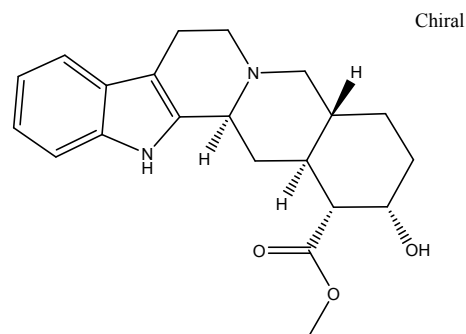
-10.3

-10.4

-10.9

-9.8

Yohimbine



-9.4

-7.4

-10.6

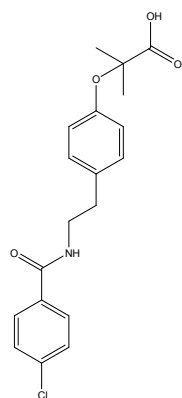
-9.1

-9

-9.2

-8.6

Bezafibrate



-8.9

-7.7

-9.1

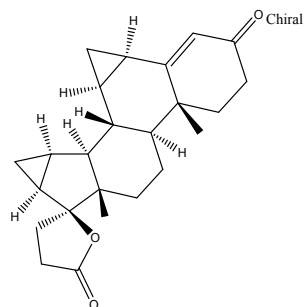
-8.1

-7.5

-7.6

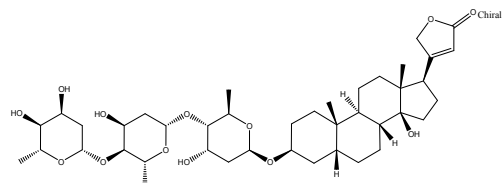
-10.5

Drospirenone



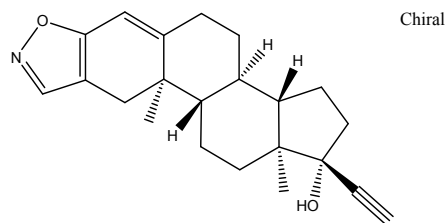
-9.2 -8.5 -10.9 -9.6 -9.8 -11.8 -9.4

Digitoxin



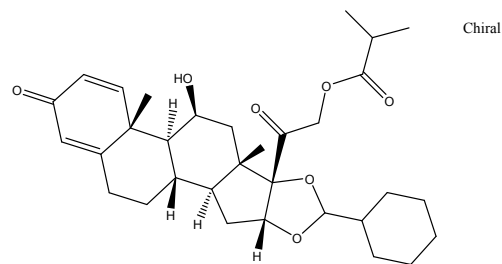
-10.6 -9.1 -11.9 -10.6 -12.1 -12.8 -10.4

Danazol



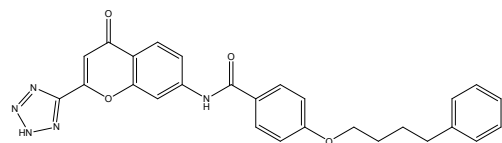
-9.1 -9.1 -10.3 -10.1 -10 -11.2 -9.1

Ciclesonide



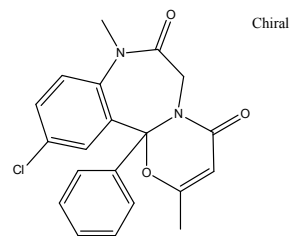
-8.7 -8.4 -11.5 -9.2 -9.6 -10.5 -9.6

Pranlukast



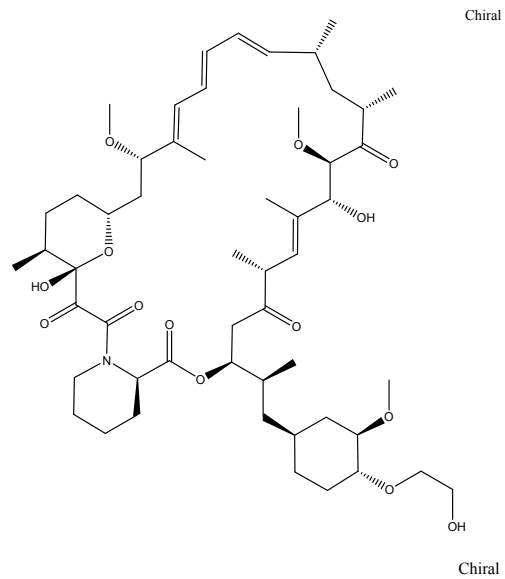
-10.8 -9.2 -9.2 -9 -8.6 -9.8 -12.4

Ketazolam



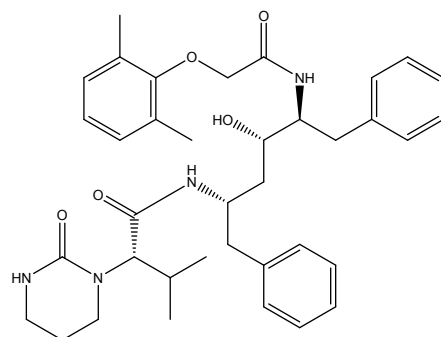
-7.5 -6.8 -10.8 -9.4 -8.3 -8.6 -7.9

Everolimus



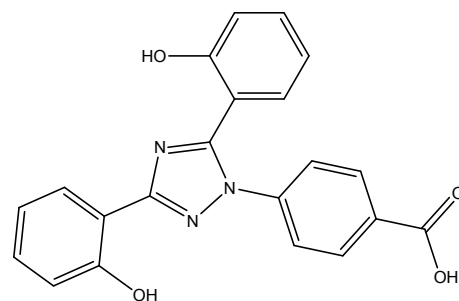
-9.3 -9.1 -10.1 -9.8 -11 -10.9 -9.2

Lopinavir



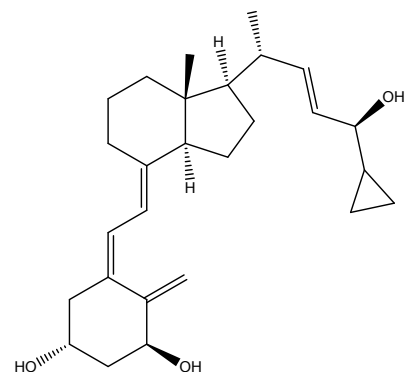
-9.6 -7.2 -11.1 -8 -8.8 -9.4 -8.4

Deferasirox



-9.4 -8.2 -11.6 -10.2 -9 -9.9 -11.1

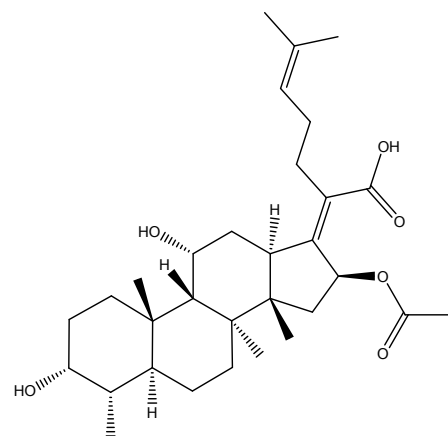
Calcipotriol



Chiral

-8.7 -8.6 -10.3 -8.1 -9 -9 -11.6

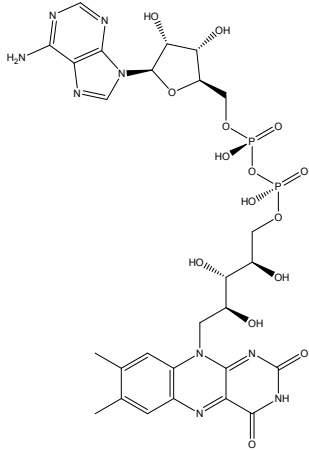
Fusidic Acid



Chiral

-8.2 -7.7 -10.9 -8.5 -8.9 -9.3 -8.7

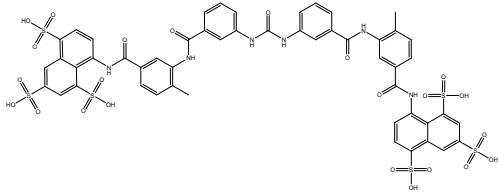
Flavin adenine dinucleotide



Chiral

-9.2 -8.7 -10.7 -9.8 -9.8 -10 -10

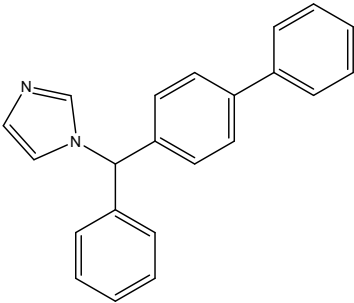
Suramin



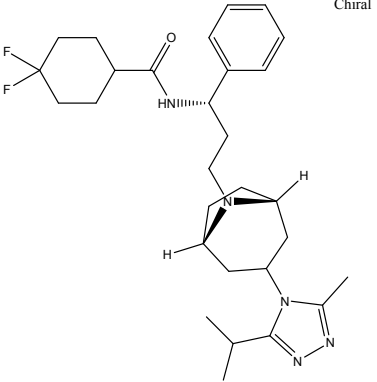
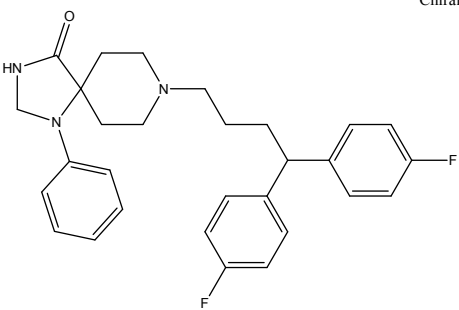
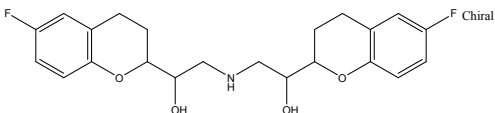
Chiral

-12.1 -10.5 -12.6 -10.8 -11.1 -12.1 -12.5

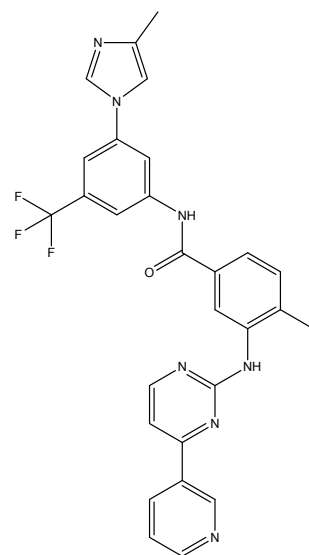
Bifonazole



-8.8 -7.9 -9.9 -9.8 -8.2 -8.9 -11.6

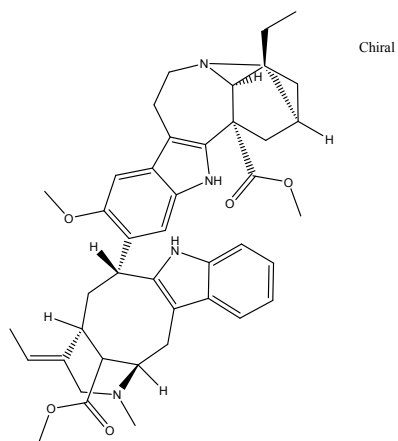
Maraviroc		-8.7	-7	-11.3	-9	-8.7	-9.8	-9.4
Fluspirilene		-11.6	-8.5	-10.2	-9	-10	-9.6	-9.6
Nebivolol		-7.1	-7.5	-10.4	-9	-7.9	-8.7	-12.2

Nilotinib

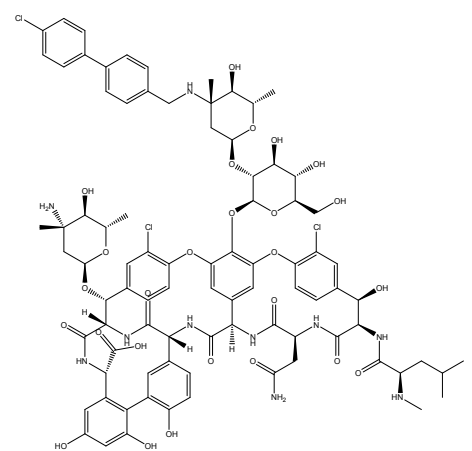
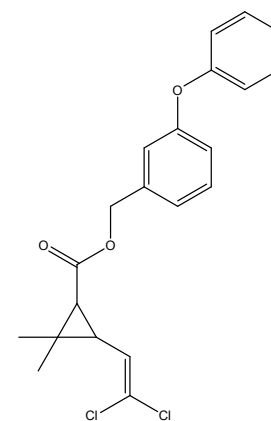
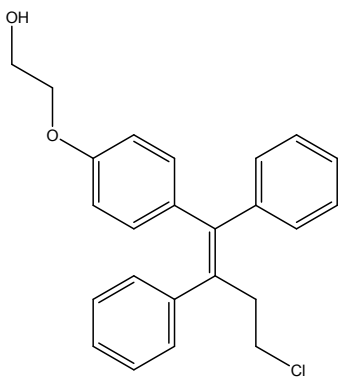


-10.9 -9.4 -12 -10.5 -9.7 -10.7 -10.9

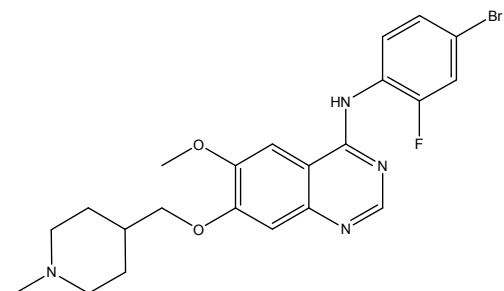
Voacamine



-9.3 -7.6 -11.6 -8.8 -9.6 -8.2 -9

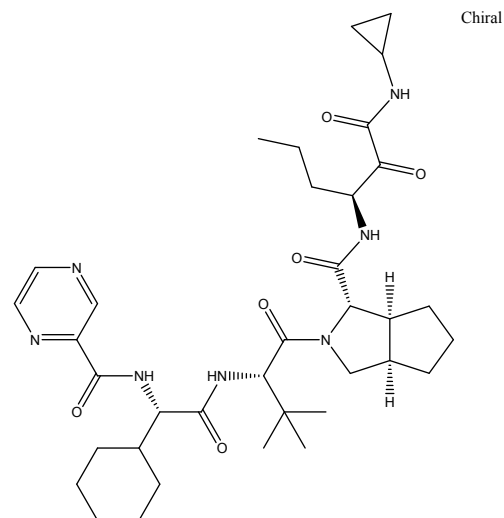
Oritavancin		Chiral	-11	-10.8	-11	-9.4	-12.1	-10.2	-11.4
Permethrin		Chiral	-9.2	-7.6	-8.6	-7.4	-7.6	-8.8	-11
Ospemifene			-8.6	-8	-10.7	-9.9	-8.9	-9.6	-9.6

Vandetanib



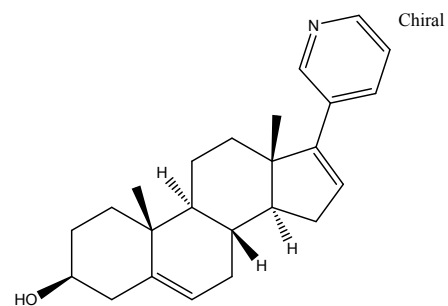
-9.6 -8 -9.6 -8.3 -8.2 -8.4 -11.2

Telaprevir



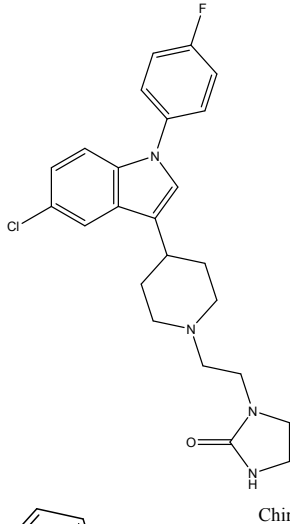
-8.6 -7.2 -10.7 -8.8 -8.6 -9.3 -8.2

Abiraterone



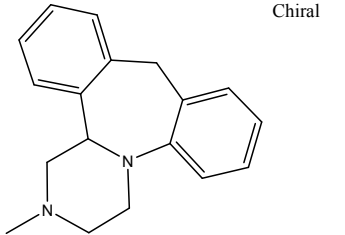
-8.9 -9 -10.1 -10.9 -9.7 -10.3 -8.5

Sertindole



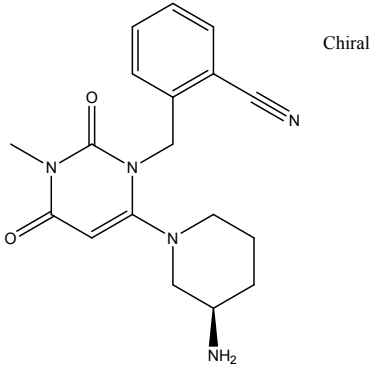
-7.8 -7.9 -10.6 -10.3 -9.2 -9.1 -9.6

Mianserin



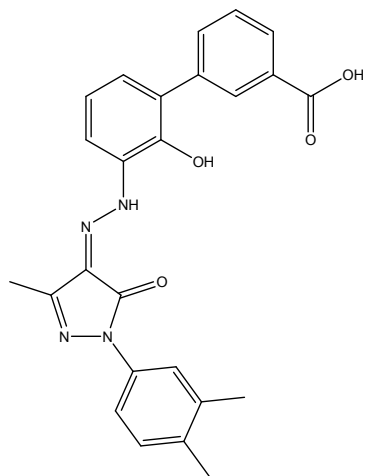
-7.6 -11.1 -10.2 -9.1 -9.3 -9.1 -9.9

Alogliptin



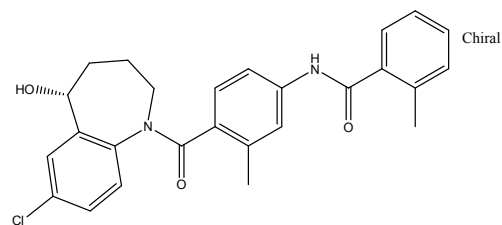
-6.7 -6.6 -10.5 -7.9 -8.1 -8.4 -9

Eltrombopag



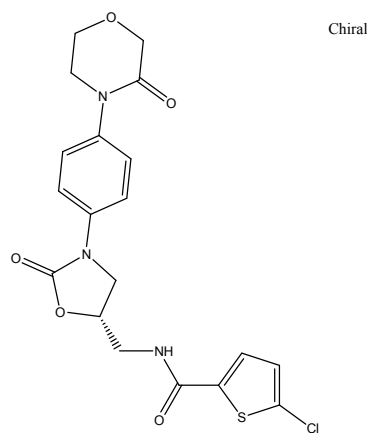
-11.7 -9.7 -11.4 -10.8 -9.9 -10.2 -10.4

Tolvaptan



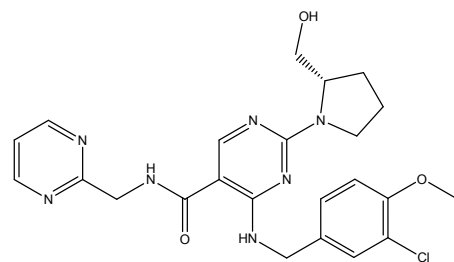
-10.9 -8.7 -10.6 -9.6 -9.1 -9.8 -11.7

Rivaroxaban



-9.8 -7.7 -8.7 -8.6 -7.7 -9.1 -11.5

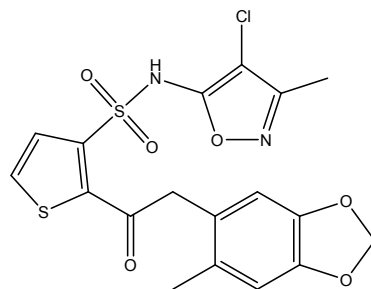
Avanafil



Chiral

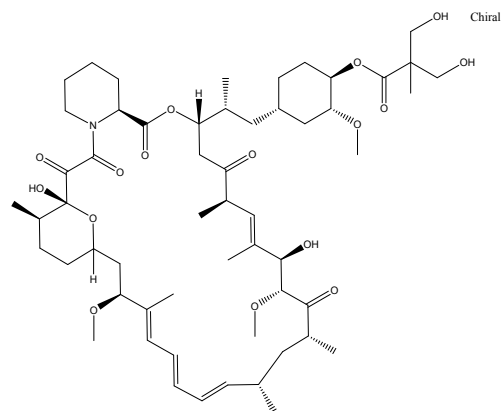
-10.1 -7.8 -9.7 -7.8 -8.1 -9.1 -10.5

Sitaxentan



-9.7 -6.7 -10.6 -9 -7.9 -8.9 -7.8

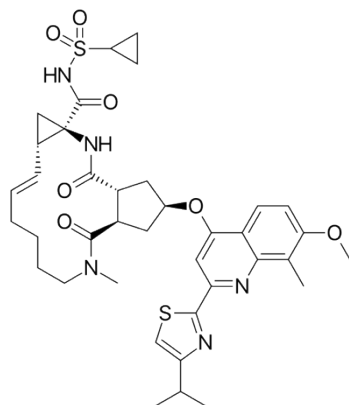
Temsirolimus



Chiral

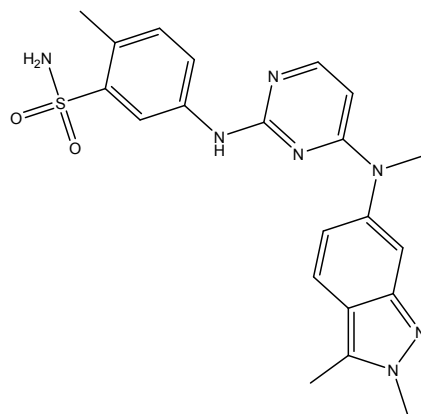
-9.6 -9.5 -10.1 -8.8 -10.8 -9.6 -9.9

Simeprevir



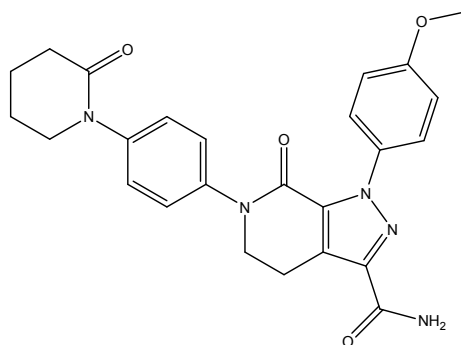
-9.8 -9.4 -11.6 -10.6 -9.6 -11 -9.3

Pazopanib



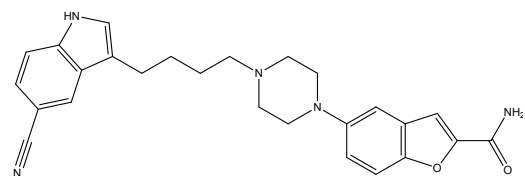
-8.5 -8.2 -11.4 -9.1 -8.9 -9.2 -8.1

Apixaban



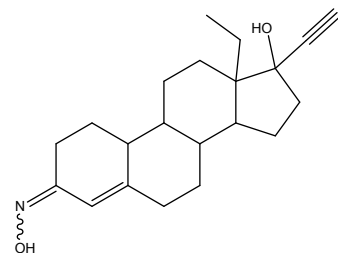
-11.3 -7.7 -10.2 -9.1 -8.5 -10 -10.2

Vilazodone



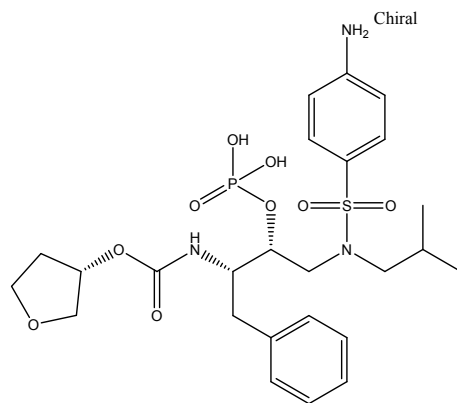
-7.9 -8.3 -9.9 -8.7 -8.3 -9 -11.8

Norelgestromin



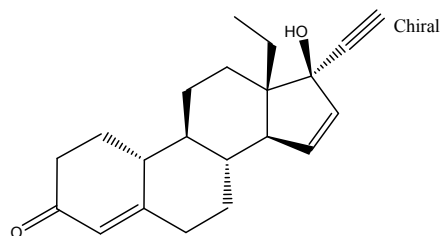
-10.2 -9.4 -9.2 -10.8 -9.2 -9.9 -12.4

Fosaprepitant



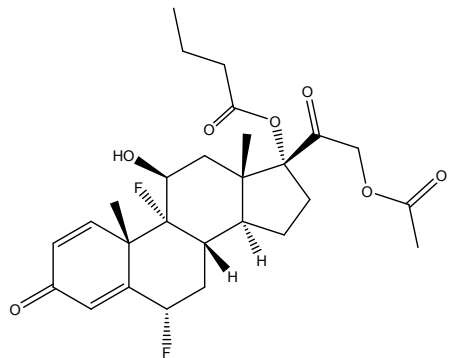
-8.5 -8.8 -11.5 -9.5 -9.5 -10 -9.2

Gestodene



-8.3 -7.9 -9.5 -9.9 -9.2 -9.4 -11

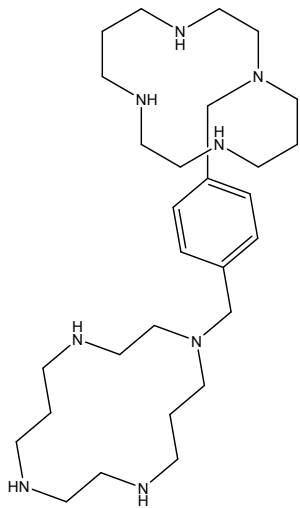
Difluprednate



Chiral

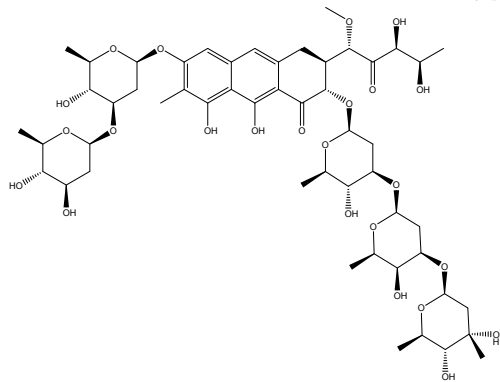
-8.1 -7.3 -10.6 -8.2 -8.4 -9 -8.5

Plerixafor



-8.1 -7.5 -10.7 -9.2 -8.9 -9.3 -8.2

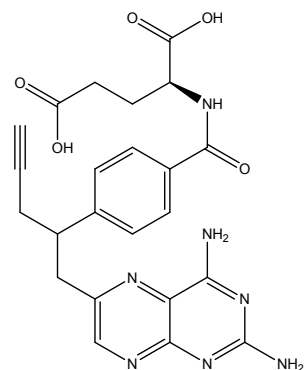
Plicamycin



Chiral

-11.6 -8.8 -12.7 -10.5 -11 -11.8 -10.8

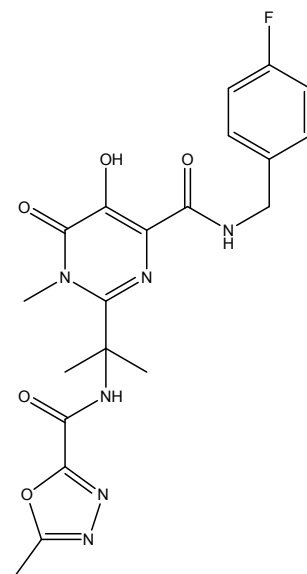
Pralatrexate



Chiral

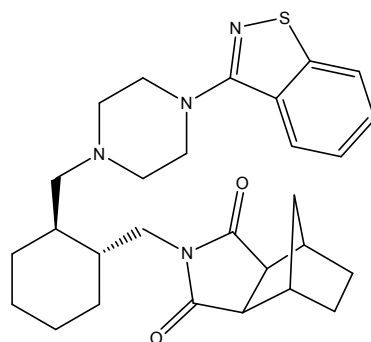
-9.3 -7.8 -10.3 -9.3 -8.6 -9.5 -10.5

Raltegravir



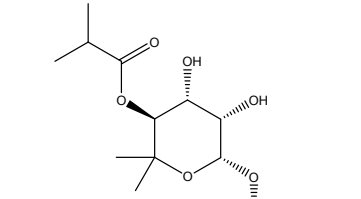
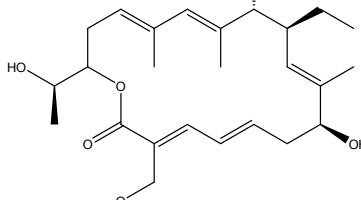
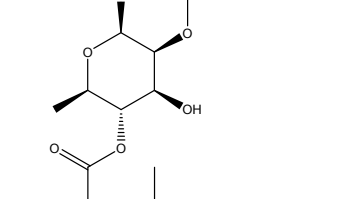
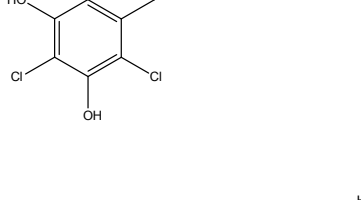
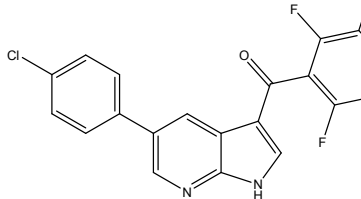
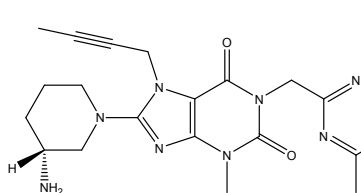
-11.1 -7.4 -10.7 -9.3 -8.6 -9.8 -10.9

Lurasidone

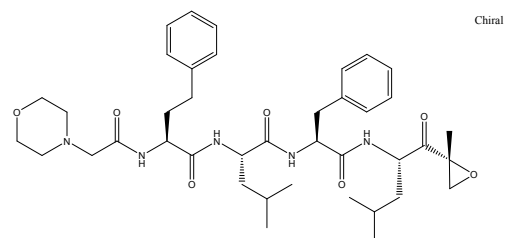


Chiral

-10.5 -8.4 -11.4 -9.3 -9.4 -9.8 -9.9

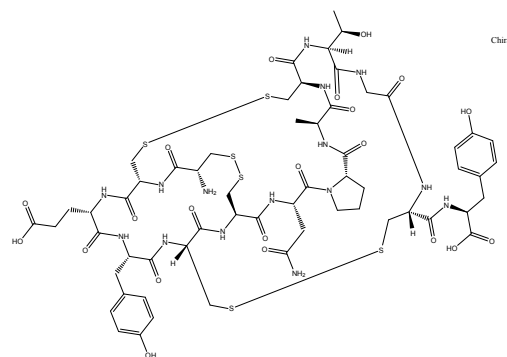
		Chiral							
Fidaxomicin			-10.4	-8.4	-11	-8.7	-9.6	-9.6	-9.8
									
									
Vemurafenib			-8.8	-8.5	-10.7	-9.8	-9.1	-10.2	-10.3
		Chiral							
Linagliptin			-9.4	-8.8	-11.5	-9.5	-8.6	-10.1	-8.9

Carfilzomib



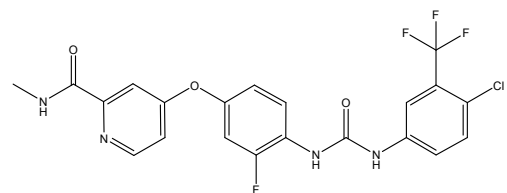
-7.4 -7.6 -10.7 -8.7 -7.9 -8.9 -7.8

Linaclootide



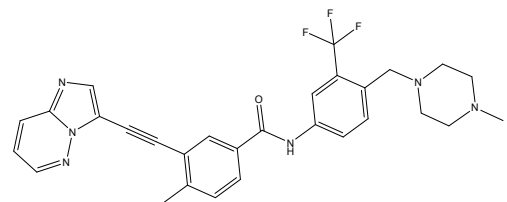
-10.9 -9.4 -9.4 -10.2 -10.6 -9.2 -8.9

Regorafenib



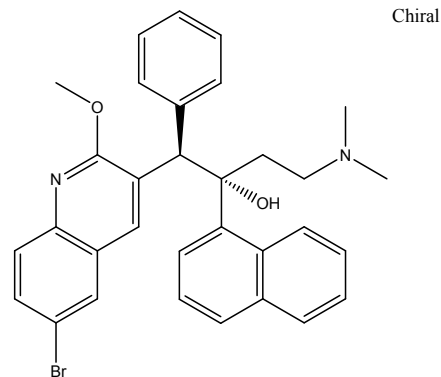
-10 -9.7 -9.9 -10.1 -9 -10.3 -12.7

Ponatinib



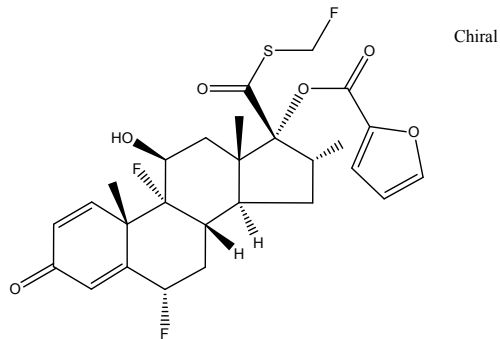
-12.2 -9.8 -10.7 -9.7 -10.2 -10.8 -12.5

Bedaquiline



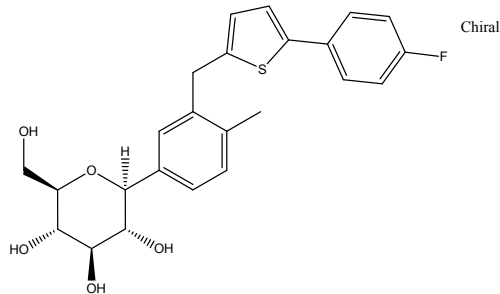
-9.6 -9.1 -12.7 -9.2 -10.4 -11.3 -9.4

Fluticasone furoate

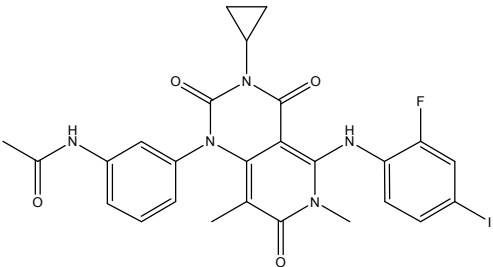
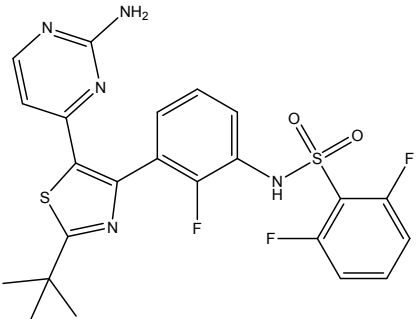
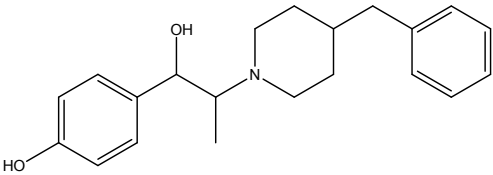
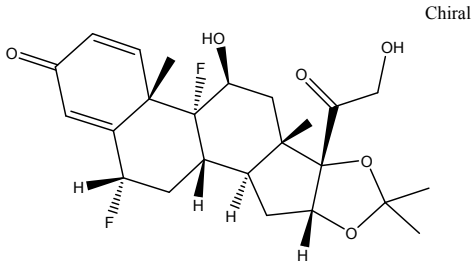
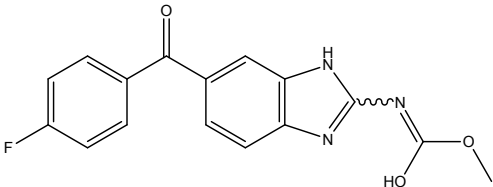


-8.2 -7.4 -11.2 -8.1 -8.1 -8.7 -7.8

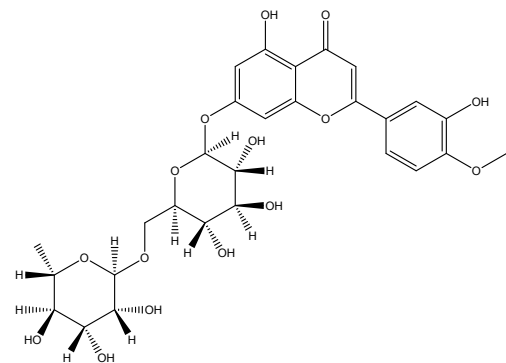
Canagliflozin



-11.8 -9.3 -10.5 -9.5 -10.1 -9.8 -9.1

Trametinib		-8.7	-7.8	-11.9	-8.7	-9.2	-9.8	-10.1
Dabrafenib		-9.7	-8.7	-11.8	-9.7	-9.4	-10.5	-10.6
Ifenprodil		-8	-7.6	-9.9	-8.3	-8.5	-8.8	-10.8
Fluprednidene Acetate	 Chiral	-8.8	-7	-10.8	-8.2	-8.8	-9	-9.1
Flubendazole		-9.4	-7.8	-8.5	-8.5	-8.4	-8.3	-10.9

Diosmin



-10.6

-9

-11.6

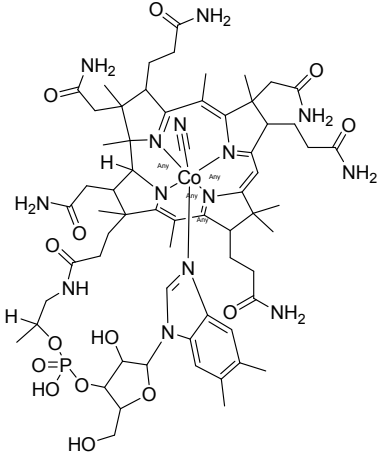
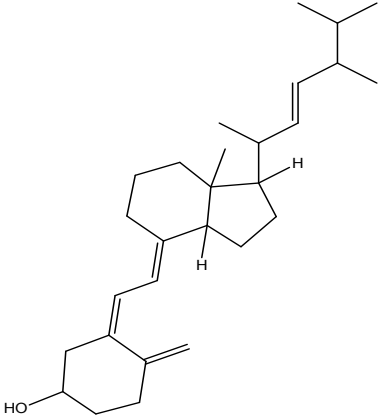
-10.8

-9.8

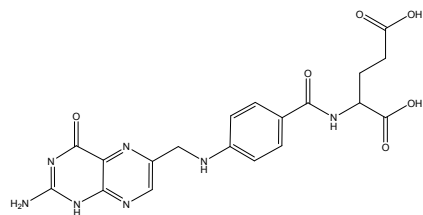
-11.8

-11.7

Table S2 The docking results of 74 drugs with corresponding data in the CMap dataset

Drugs	Docking results (kcal/mol)						
	NMDA	CDK5	BChE	AChE	GSK-3β	BACE1	MAO-B
Cyanocobalamin 	-9.3	-9.4	-7.8	-8.4	-10.9	-8.1	-8.9
Ergocalciferol 	-8.8	-8.4	-10.2	-8.3	-9	-9.9	-11.6

Folic Acid



-9.3

-8.5

-9.3

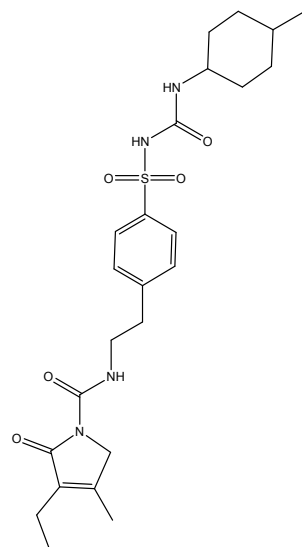
-8.4

-7.7

-8.6

-11.2

Glimepiride



-9.2

-8.9

-9.9

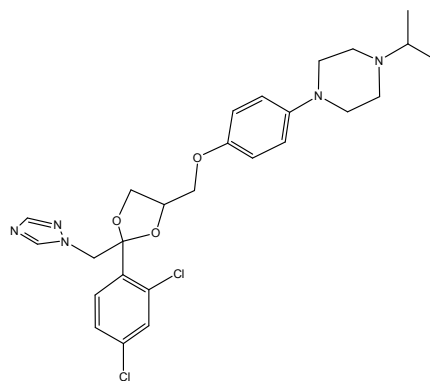
-10

-8.4

-9.1

-12.9

Terconazole



-9

-8.2

-9.7

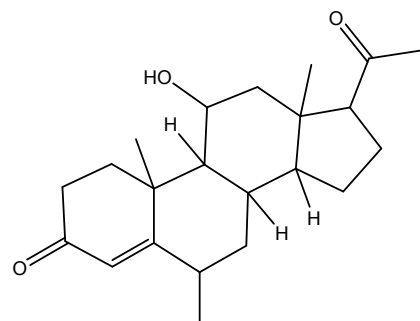
-8.6

-8.1

-8.1

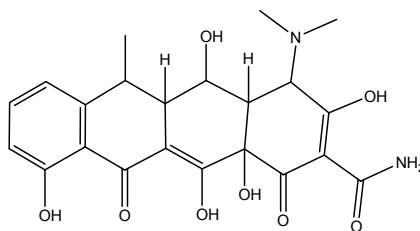
-10.8

Medrysone



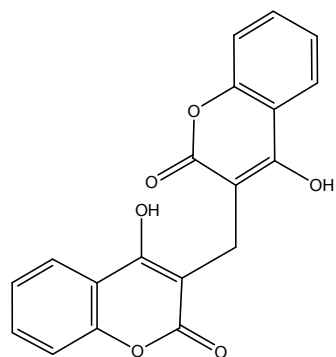
-8.4 -8.2 -10.5 -9.6 -9.2 -9.6 -8.7

Doxycycline



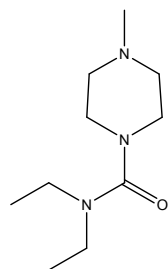
-8.9 -8.3 -11.5 -10 -9.3 -11.3 -8.9

Dicoumarol



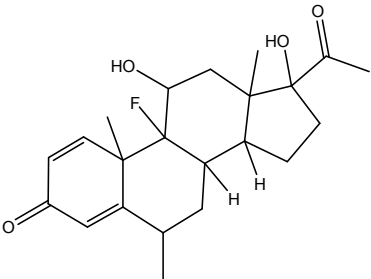
-9.9 -8.2 -12 -9.2 -8.7 -9.5 -10.9

Dihydroergotamine



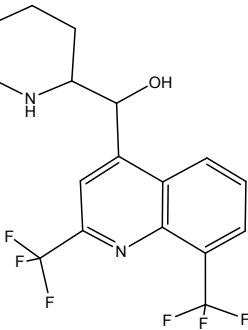
-9.8 -9.3 -13.3 -11.4 -10.8 -11.9 -10.2

Fluorometholone



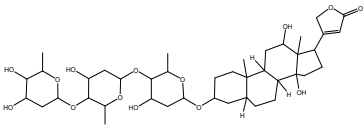
-8.7 -8.6 -10.5 -8.4 -9.1 -9.7 -9.3

Mefloquine



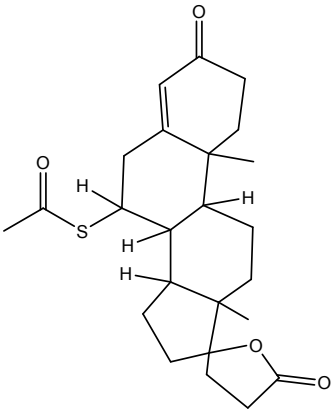
-9.4 -7.2 -9.9 -7.8 -8.7 -8.8 -10.6

Digoxin



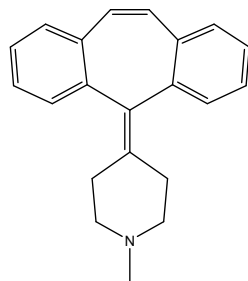
-10 -9.4 -12 -10.5 -12.2 -12.2 -10.4

Spirolactone



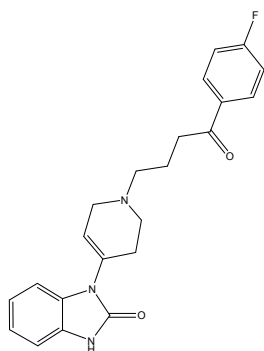
-8.3 -7.8 -10.7 -8.4 -9.4 -8.7 -8.4

Cyproheptadine



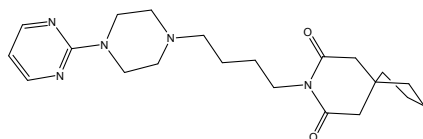
-8 -7.9 -10.8 -9.7 -10.3 -10.3 -10

Droperidol



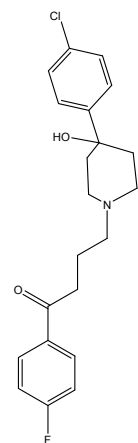
-8.4 -8.4 -10.4 -9.3 -8.5 -8.8 -10.7

Buspirone



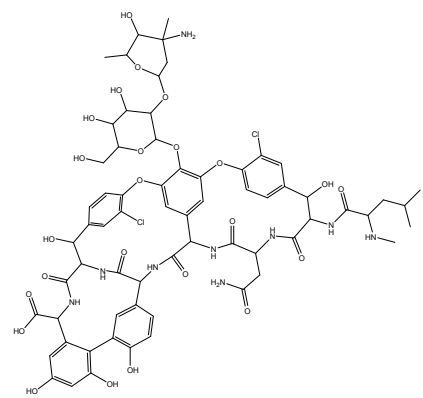
-7.9 -8.1 -9 -7.7 -7.6 -7.4 -10.5

Haloperidol



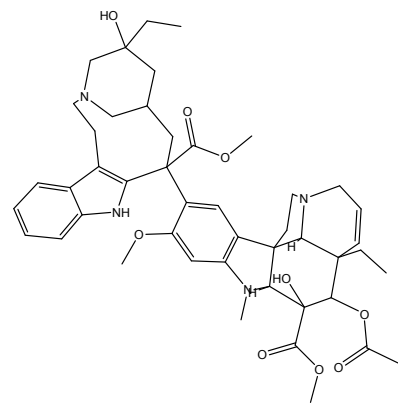
-8.3 -8.5 -9.4 -8.4 -8 -8.5 -11.2

Vancomycin



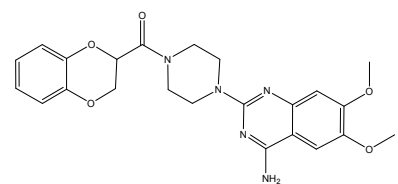
-10.4 -9.9 -11.4 -10.1 -13.1 -10.5 -10.1

Vinblastine



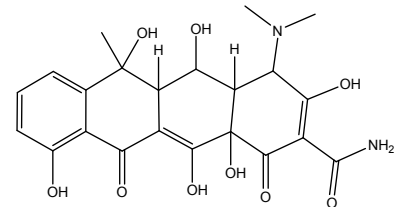
-7.7 -7.3 -11.5 -9.7 -7.8 -7.5 -8

Doxazosin



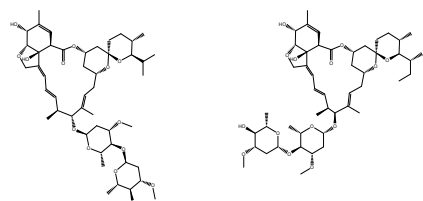
-10.2 -8.5 -10.4 -8.8 -8.6 -9.6 -11.4

Oxytetracycline



-9 -8.6 -11.3 -9.2 -9.5 -11 -9.1

Ivermectin



-11.8

-9.7

-11.6

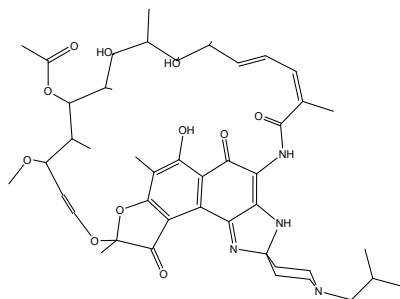
-10.3

-9.8

-10.9

-11.2

Rifabutin



-9.4

-8.9

-8.6

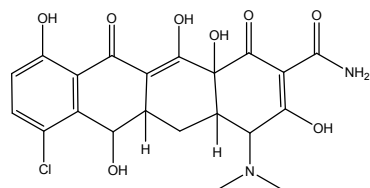
-9.6

-10.5

-8.9

-9.9

Demeclocycline



-8.7

-8.3

-10.2

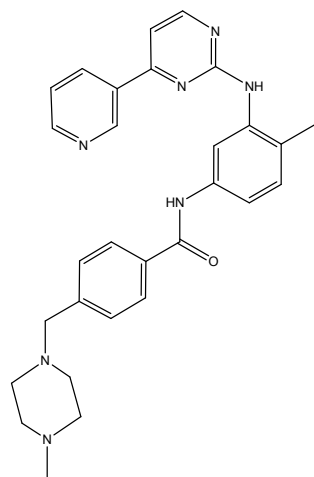
-9

-9.2

-10.8

-8.4

Imatinib



-10.3

-9.3

-11

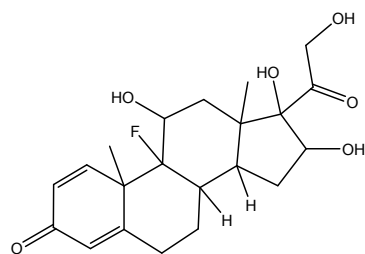
-10.7

-9

-9.9

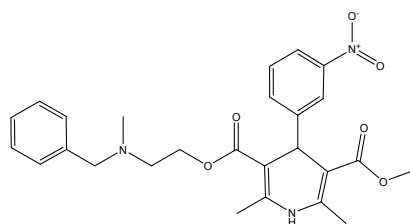
-12.1

Triamcinolone



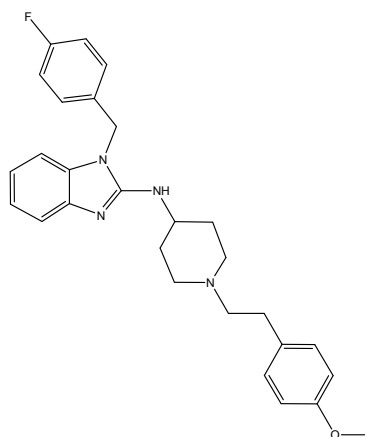
-8.6 -7.4 -10.8 -8.2 -9.2 -9 -8.8

Nicardipine

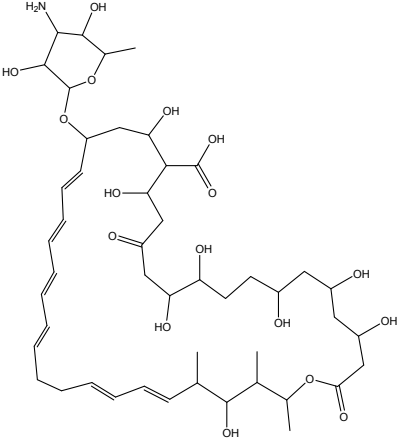
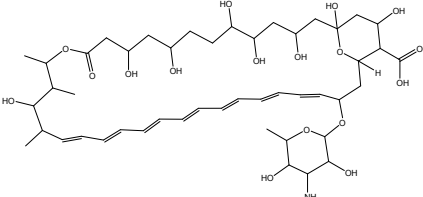
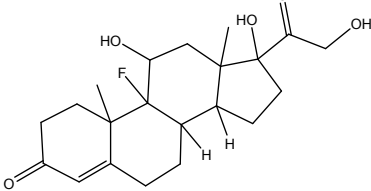
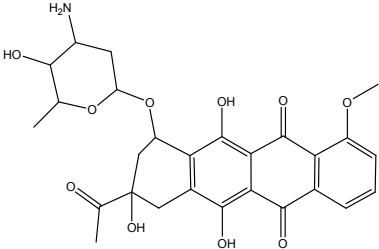


-6.9 -6.7 -10.6 -7.4 -7 -8.8 -8.7

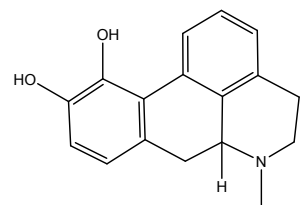
Astemizole



-11.2 -9.6 -10.5 -9.6 -8.4 -8.9 -10

Nystatin		-11.2	-9.4	-11	-10.4	-12.5	-9.6	-10.6
Amphotericin B		-11.9	-10.3	-11.4	-11.3	-12.8	-14.3	-10.9
Fludrocortisone		-8.7	-8.1	-10.6	-8.2	-9.1	-9.3	-8.6
Daunorubicin		-9.5	-9.2	-10.6	-9.7	-10.3	-10.6	-9.2

Apomorphine



-8.7

-8.9

-9.8

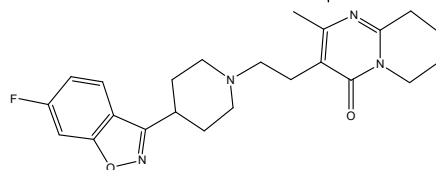
-10.8

-9.2

-9.2

-8.8

Risperidone



-9.7

-10.6

-10.8

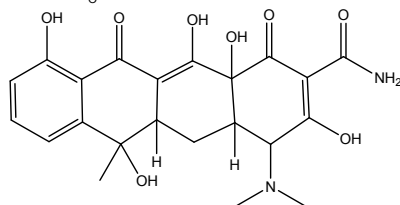
-9.3

-8.9

-9.5

-12.4

Tetracycline



-8.1

-8.5

-11.1

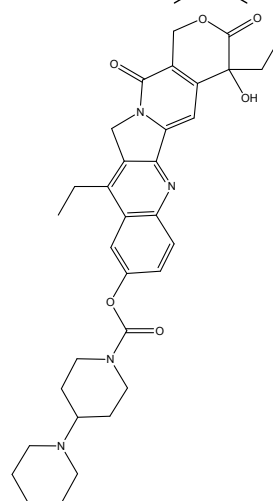
-8.7

-9.7

-11

-8.3

Irinotecan



-10.5

-8.9

-11.8

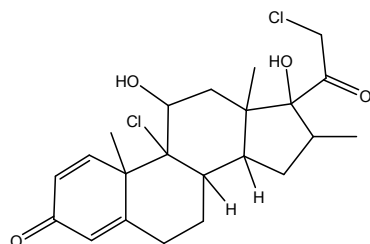
-9.7

-9.8

-11.4

-10.3

Mometasone



-8.6

-7.8

-10.7

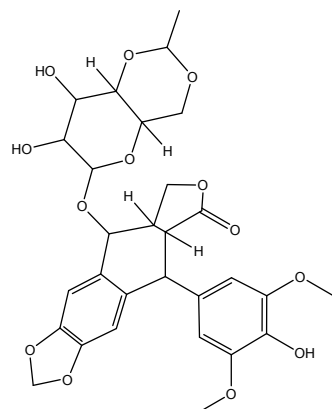
-8

-8.6

-8.8

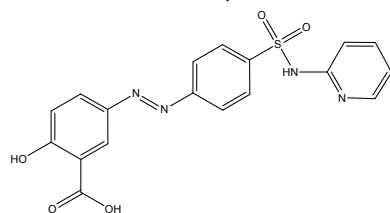
-8.9

Etoposide



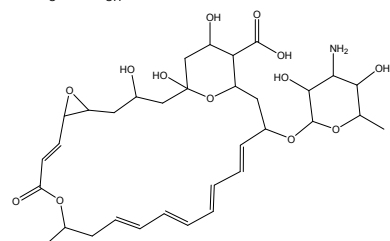
-9.4 -8.3 -11.8 -9.2 -9.6 -10.9 -8.9

Sulfasalazine



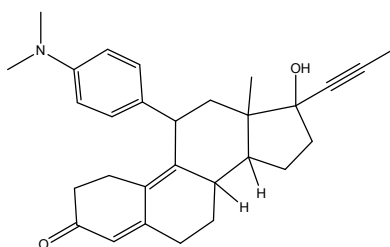
-9.1 -8.9 -9.7 -10.5 -7.5 -8.5 -11.7

Natamycin



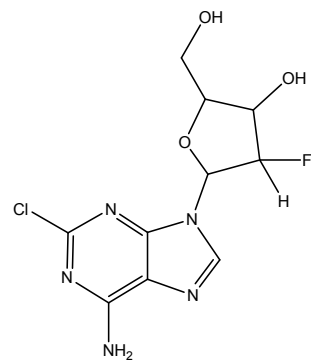
-11.2 -10 -10.8 -10.3 -10.9 -11.7 -11.4

Mifepristone



-10.7 -8.8 -9.8 -10.2 -9.6 -11.2 -10.6

Clofazimine



-8.9

-8.1

-11.8

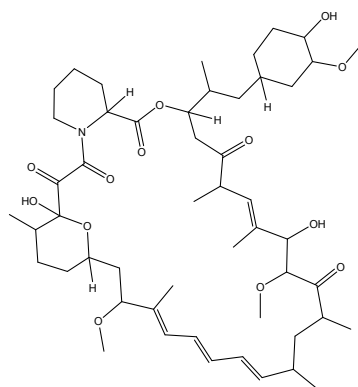
-9.8

-9.4

-10

-10.4

Sirolimus



-11.2

-9.5

-10.6

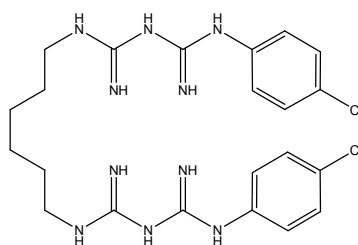
-10.3

-11.3

-9.2

-9.8

Chlorhexidine



-10.6

-7.9

-7.7

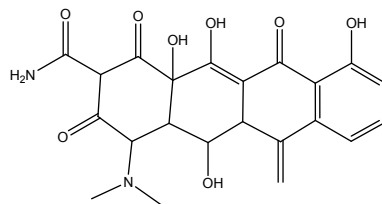
-6.6

-6.8

-7.8

-8.5

Methacycline



-10

-8.4

-10.5

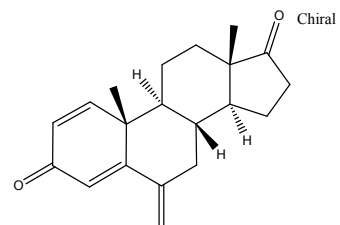
-10.7

-9.6

-10.8

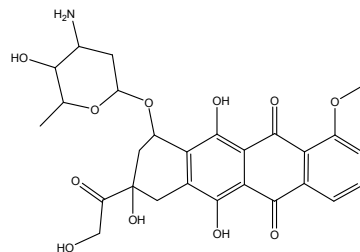
-9.1

Exemestane



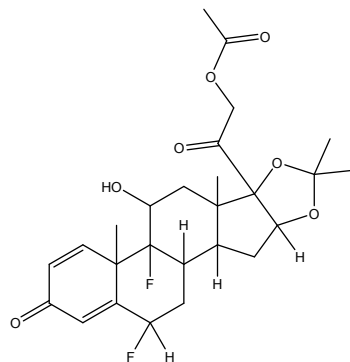
-8.8 -8.1 -10.5 -10.4 -10 -9.6 -9.2

Doxorubicin



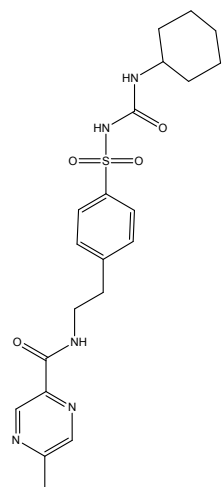
-9.2 -8 -10.9 -9.3 -10.1 -10.4 -9.5

Fluocinonide



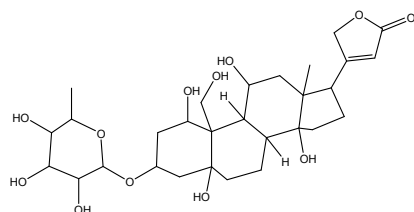
-8.7 -7.9 -10.8 -9.1 -10 -9.5 -9.1

Glipizide



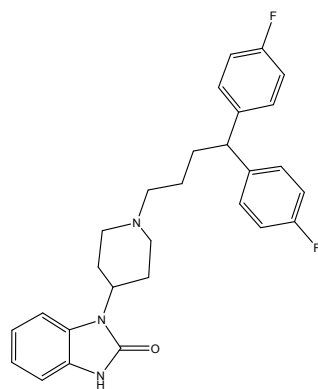
-10.2 -7.9 -10.8 -9.3 -8.2 -8.8 -12.5

Ouabain



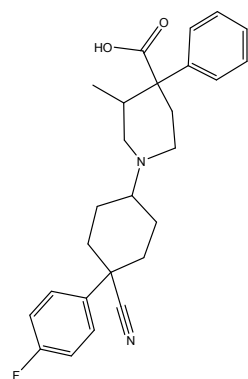
-9.8 -8.7 -12.2 -9.7 -10.3 -10.1 -10.8

Pimozide



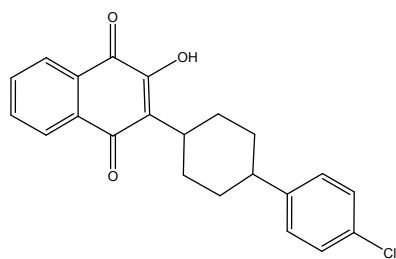
-8.7 -8.8 -11.1 -9.1 -8.8 -9.6 -9.9

Levocabastine



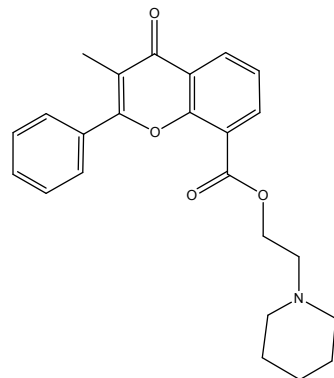
-8.4 -10.1 -12.5 -10.6 -8.6 -9.9 -9.6

Atovaquone



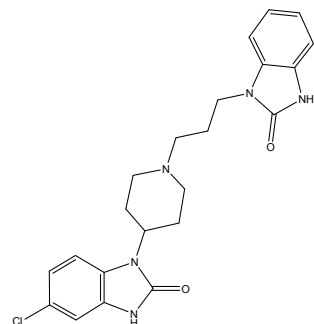
-12.6 -10.6 -10.6 -9.7 -9.3 -9.7 -13.5

Flavoxate



-9.5 -8.3 -11.6 -8.5 -8.8 -9.1 -8.4

Domperidone



-10.7

-8.5

-9.5

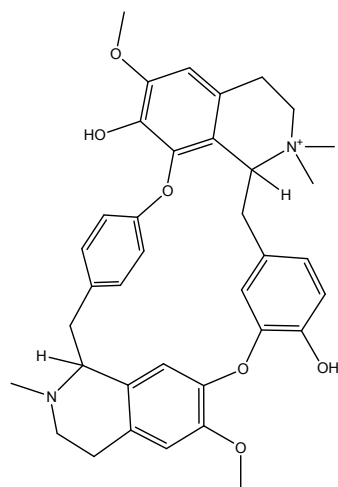
-8.4

-8.3

-9.2

-11.8

Tubocurarine



-11.1

-8.8

-10.1

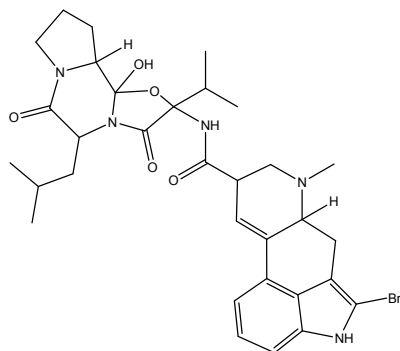
-10.4

-11.9

-11.7

-11.1

Bromocriptine



-9.3

-9.1

-11.6

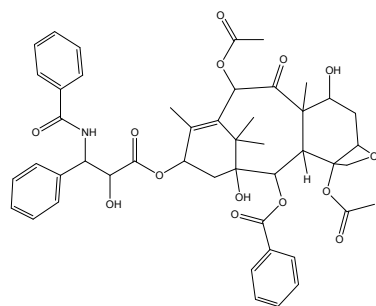
-9.2

-10.6

-10.8

-8.8

Paclitaxel



-9.2

-8.8

-11.1

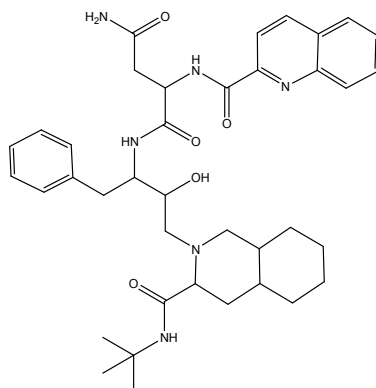
-9.5

-8.7

-10.7

-9.1

Saquinavir



-9.4

-8

-11.9

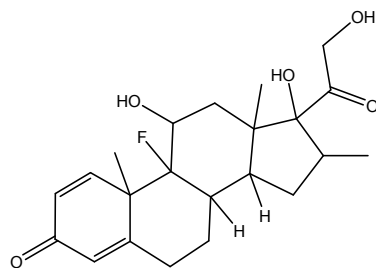
-9.8

-8.8

-10.3

-9.5

Dexamethasone



-8.7

-7.8

-10.9

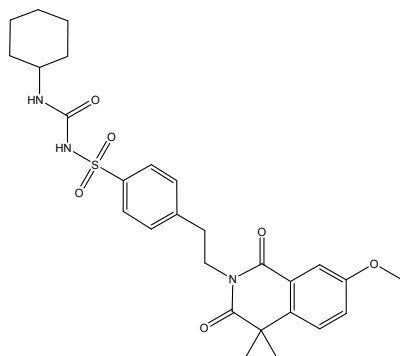
-8.2

-8.9

-8.9

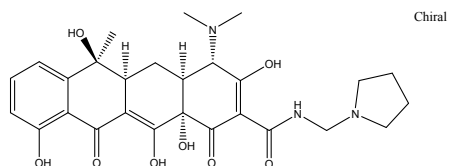
-9.1

Gliquidone



-11.3 -9 -12 -9.6 -9.1 -10.5 -9.8

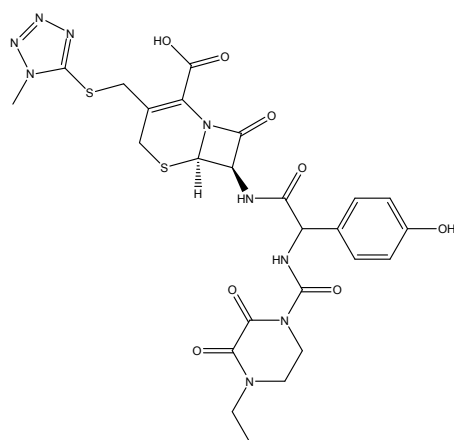
Rolitetracycline



Chiral

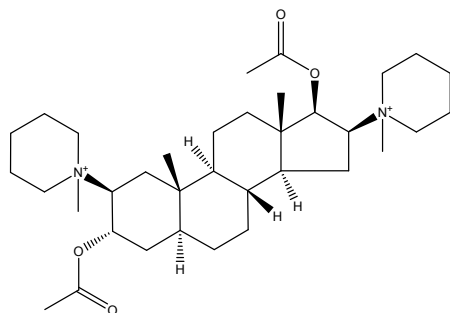
-8.6 -8.6 -11.1 -9.2 -9.4 -9.7 -8.6

Cefoperazone



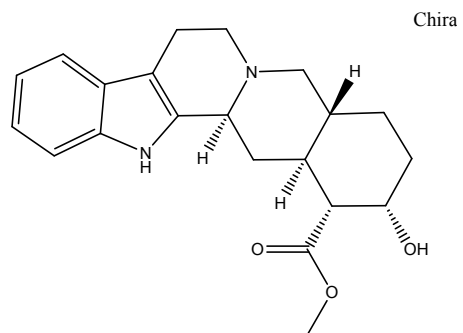
-10 -8 -10.6 -9 -8.7 -9.5 -9.2

Pancuronium



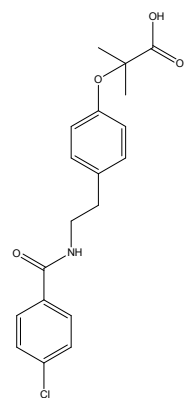
-8.9 -8.1 -10.5 -8 -9.6 -10.3 -7.7

Yohimbine



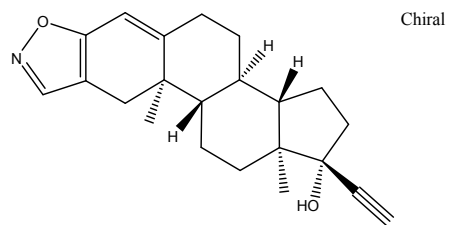
-9.4 -7.4 -10.6 -9.1 -9 -9.2 -8.6

Bezafibrate



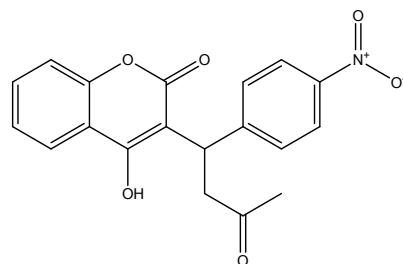
-8.9 -7.7 -9.1 -8.1 -7.5 -7.6 -10.5

Danazol



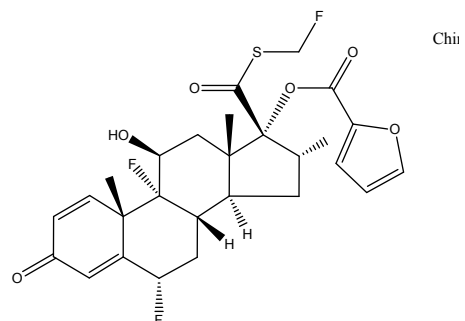
-9.1 -9.1 -10.3 -10.1 -10 -11.2 -9.1

Acenocoumarol



-8 -7.8 -10.9 -8.5 -8.5 -8.2 -8.7

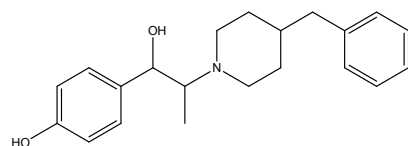
Fluticasone furoate



Chiu

-8.2 -7.4 -11.2 -8.1 -8.1 -8.7 -7.8

Ifenprodil



-8 -7.6 -9.9 -8.3 -8.5 -8.8 -10.8
