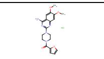
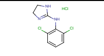
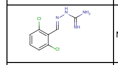
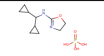
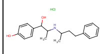
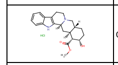
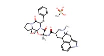
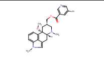
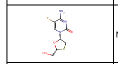
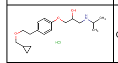
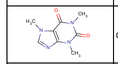
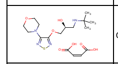
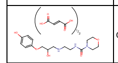
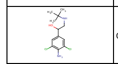
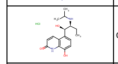
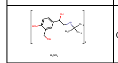
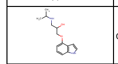
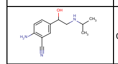
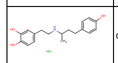
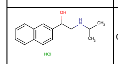
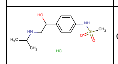
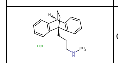
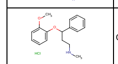
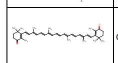
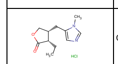
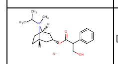
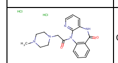
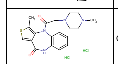
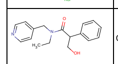
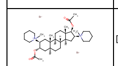
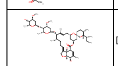
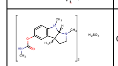
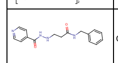
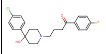
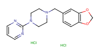
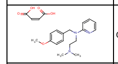
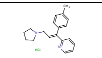
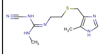
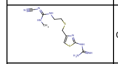
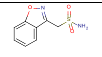
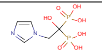
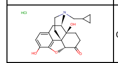
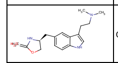
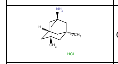
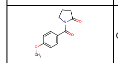
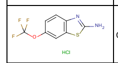
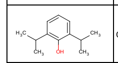
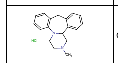
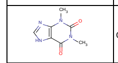
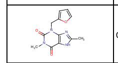
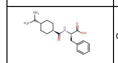
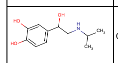
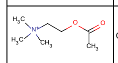
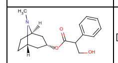
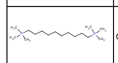
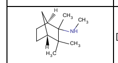
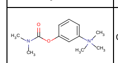
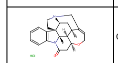
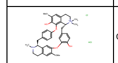
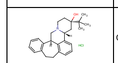
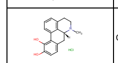
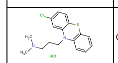
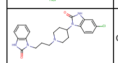
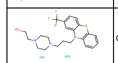
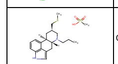
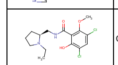
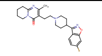
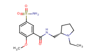
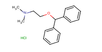
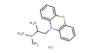
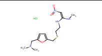
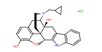
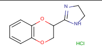
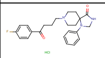
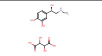
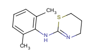
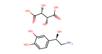
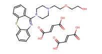
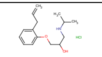
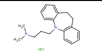
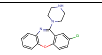
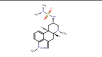
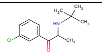
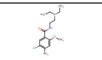
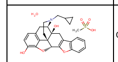
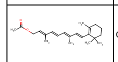
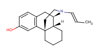
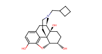
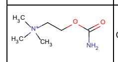
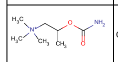
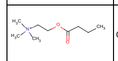
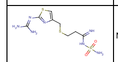
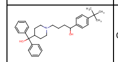
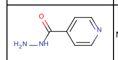
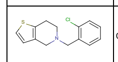
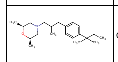
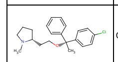
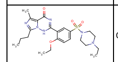
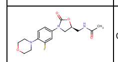
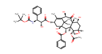
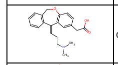
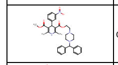
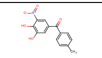
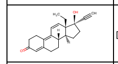
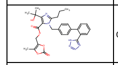
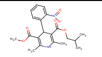
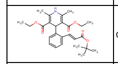
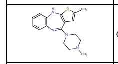
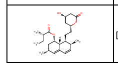
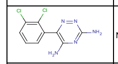
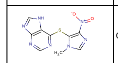
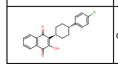
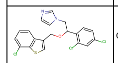
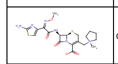
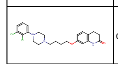
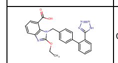
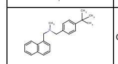
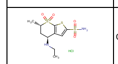
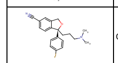
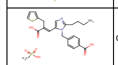
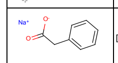
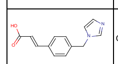
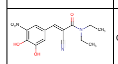
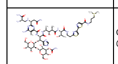
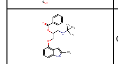
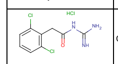
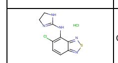
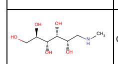
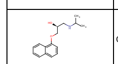
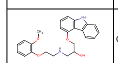
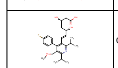
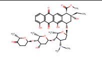
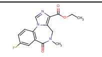
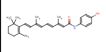
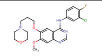
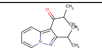
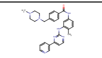
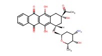
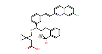
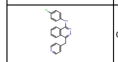
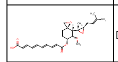
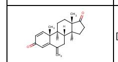
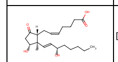
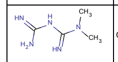
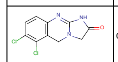
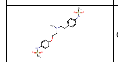
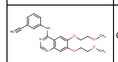
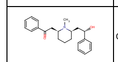
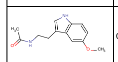
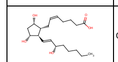
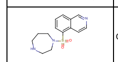
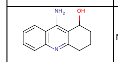
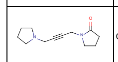
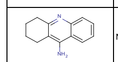
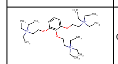
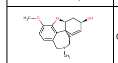
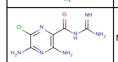
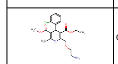
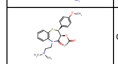
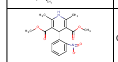
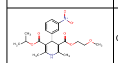
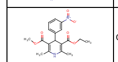
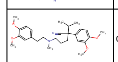
Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	Cl.NC(=N)NC(=N.N1CCOCC1	1-[(morpholin-4-yl)carboximidoyl]guanidine hydrochloride	Moroxydine HCl	207.7	1	FDA Approved Drug Library	3160-91-6	DL-552	2mg/ml	DMSO	2841J
	Cl.CCC[C@@H]1C[C@H](N(C)C1)C(=O)N[C@H]([C@H](C)Cl)[C@H]1O[C@H](SC)[C@H](O)[C@@H](O)[C@H]1O	(2S,4R)-N-[(1S,2S)-2-chloro-1-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(methylsulfanyl)oxan-2-yl]propyl]-1-methyl-4-propylpyrrolidine-2-carboxamide hydrochloride	Clindamycin HCl	461.4	1	FDA Approved Drug Library	21462-39-5	A-190	2mg/ml	DMSO	2841J
	NC(=O)OCC(COC(N)=O)C1=CC=CC=C1	3-(carbamoyloxy)-2-phenylpropyl carbamate	Felbamate	238.2	1	FDA Approved Drug Library	25451-15-4	DL-567	2mg/ml	DMSO	2841J
	CC[C@@H]1NC(=O)[C@H]([C@H](O)[C@H](C)C/C=C/C)N(C)C(=O)[C@H](C(C)C)N(C)C(=O)[C@H](CC(C)C)N(C)C(=O)[C@H](CC(C)C)N(C)C(=O)[C@@H](C)N(C=O)[C@H](CC(C)C)N(C)C(=O)[C@@H](N(C=O)[C@H](CC(C)C)N(C)C(=O)CN(C)C1=O)C(C)C	(3S,6S,9S,12R,15S,18S,21S,24S,30S,33S)-30-ethyl-33-[(1R,2R,4E)-1-hydroxy-2-methylhex-4-en-1-yl]-1,4,7,10,12,15,19,25,28-nonamethyl-6,9,18,24-tetrakis(2-methylpropyl)-3,21-bis(propan-2-yl)-1,4,7,10,13,16,19,22,25,28,31-undecaazacyclotritriacontan-2,5,8,11,14,17,20,23,26,29,32-undecone	Cyclosporin A	1202.6	1	FDA Approved Drug Library	59865-13-3	A-195	2mg/ml	DMSO	2841J
	Cl.Cl.COC1=C(OC)C=C2C(=O)C(CC3CCN(CC4=CC=CC=C4)CC3)C2=C1	2-[(1-benzylpiperidin-4-yl)methyl]-5,6-dimethoxy-2,3-dihydro-1H-inden-1-one dihydrochloride	Donepezil HCl	452.4	1	FDA Approved Drug Library	120011-70-3	DL-568	2mg/ml	DMSO	2841J
	CCC[C@@H]1C[C@H](N(C)C1)C(=O)N[C@H]([C@H](C)O)[C@H]1O[C@H](SC)[C@H](O)[C@@H](O)[C@H]1O	(2S,4R)-N-[(1R,2R)-2-hydroxy-1-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(methylsulfanyl)oxan-2-yl]propyl]-1-methyl-4-propylpyrrolidine-2-carboxamide	Lincomycin	406.5	1	FDA Approved Drug Library	154-21-2	A-240	2mg/ml	DMSO	2841J
	COC(=O)C1=CC=C(O)C2=NC3=C(C=O)C(O)=CC(O)=C3N=C12	methyl 6-formyl-4,7,9-trihydroxyphenazine-1-carboxylate	Lomofungin	314.2	1	FDA Approved Drug Library	26786-84-5	A-245	2mg/ml	DMSO	2841J
	COC1=C(C)C2=C(C(=O)OC2)C(O)=C1C\C=C/(C)CCC(O)=O	(4E)-6-(4-hydroxy-6-methoxy-7-methyl-3-oxo-1,3-dihydro-2-benzofuran-5-yl)-4-methylhex-4-enoic acid	Mycophenolic Acid	320.3	1	FDA Approved Drug Library	24280-93-1	A-249	2mg/ml	DMSO	2841J
	[Na].CO[C@@H]1[C@@H](OC(N)=O)[C@H](O)[C@H](OC2=C(C)C3=C(C=C2)C(O)=C(NC(=O)C2=CC(CC=C(C)C)=C(O)C=C2)C(=O)O3)OC1(C)C	(3R,4S,5S,6R)-5-hydroxy-6-[(4-hydroxy-3-[[4-hydroxy-3-(3-methylbut-2-en-1-yl)benzene]amido]-8-methyl-2-oxo-2H-chromen-7-yl)oxy]-3-methoxy-2,2-dimethyloxan-4-yl carbamate sodium	Novobiocin Na	635.6	1	FDA Approved Drug Library	1476-53-5	A-256	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@@H](C)[C@@](O)(O1)C(=O)C(=O)N1CCCC[C@@]1([H])C(=O)O[C@@]([H])(CC(=O)[C@H](C)/C=C(/C)[C@@H](O)[C@@H](OC)C(=O)[C@H](C)C[C@H](C)/C=C/C=C/C=C(/C)[C@H](C2)OC)[C@H](C)C[C@@H]1CC[C@@H](O)[C@@H](C1)OC	(1R,9S,12S,15R,16E,18R,19R,21R,23S,24E,26E,28E,30S,32S,35R)-1,18-dihydroxy-12-[(2R)-1-[(1S,3R,4R)-4-hydroxy-3-methoxycyclohexyl]propan-2-yl]-19,30-dimethoxy-15,17,21,23,29,35-hexamethyl-11,36-dioxa-4-azatricyclo[30.3.1.0⁴,⁹]hexatriaconta-16,24,26,28-tetraene-2,3,10,14,20-pentone	Rapamycin	914.2	1	FDA Approved Drug Library	53123-88-9	A-275	2mg/ml	DMSO	2841J
	Cl.Cl.[H][C@@]12O[C@@]3([H])O[C@H](C)CC(=O)[C@]3(O)O[C@]1([H])[C@@H](NC)[C@@H](O)[C@@H](NC)[C@@H]2O	(1R,3S,5R,8R,10R,11S,12S,13R,14S)-8,12,14-trihydroxy-5-methyl-11,13-bis(methylamino)-2,4,9-trioxatricyclo[8.4.0.0⁵,¹³]tetradecan-7-one dihydrochloride	Spectinomycin 2HCl	405.3	1	FDA Approved Drug Library	21736-83-4	A-280	2mg/ml	DMSO	2841J
	Cl.CC(C)COCC(CN(CC1=CC=CC=C1)C1=CC=CC=C1)N1CCCC1	N-benzyl-N-[3-(2-methylpropoxy)-2-(pyrrolidin-1-yl)propyl]aniline hydrochloride	Bepridil HCl	403.0	1	FDA Approved Drug Library	74764-40-2	AC-104	2mg/ml	DMSO	2841J
	Cl.CCCCC1=C(C(=O)C2=CC(I)=C(OCCN(CC)CC)C(I)=C2)C2=C(O1)C=CC=C2	(2-[4-[(2-butyl-1-benzofuran-3-yl)carbonyl]-2,6-diiodophenoxy]ethyl)diethylamine hydrochloride	Amiodarone HCl	681.8	1	FDA Approved Drug Library	19774-82-4	AC-105	2mg/ml	DMSO	2841J
	Cl.COC(=O)C1=C(C)NC(C)=C(C1C1=CC(=CC=C1)[N+][O-])=C(O)C(=O)OCCN(C)CC1=CC=CC=C1	3-[2-[benzyl(methyl)amino]ethyl] 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate hydrochloride	Nicardipine HCl	516.0	1	FDA Approved Drug Library	54527-84-3	AC-108	2mg/ml	DMSO	2841J
	FC1=CC=C(C=C1)C(CCCN1CCC(CC1)N1C(=O)NC2=C1C=CC=C2)C1=CC=C(F)C=C1	1-[1-[4,4-bis(4-fluorophenyl)butyl]piperidin-4-yl]-2,3-dihydro-1H-1,3-benzodiazol-2-one	Pimozide	461.5	1	FDA Approved Drug Library	2062-78-4	AC-109	2mg/ml	DMSO	2841J
	Cl.CN(C)C(=O)C(CCN1CCC(O)(CC1)C1=CC=C(Cl)C=C1)(C1=CC=CC=C1)C1=CC=CC=C1	4-[4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl]-N,N-dimethyl-2,2-diphenylbutanamide hydrochloride	Loperamide HCl	513.5	1	FDA Approved Drug Library	34552-83-5	ALX-550-253	2mg/ml	DMSO	2841J
	FC1=CC=C(C=C1)C(CCCN1CCC2(CC1)N(CNC2=O)C1=CC=CC=C1)C1=CC=C(F)C=C1	8-[4,4-bis(4-fluorophenyl)butyl]-1-phenyl-1,3,8-triazaspiro[4.5]decan-4-one	Fluspirilene	475.6	1	FDA Approved Drug Library	1841-19-6	AC-116	2mg/ml	DMSO	2841J
	CCCCNC(=O)NS(=O)(=O)C1=CC=C(C)C=C1	3-butyl-1-[(4-methylbenzene)sulfonyl]urea	Tolbutamide	270.3	1	FDA Approved Drug Library	64-77-7	ALX-550-301	2mg/ml	DMSO	2841J
	CC(NC)NC1=CC=NC=C1)=N/C#N)C(C)(C)C	(Z)-2-cyano-1-(3,3-dimethylbutan-2-yl)-3-(pyridin-4-yl)guanidine	Pinacidil	245.3	1	FDA Approved Drug Library	85371-64-8	ALX-550-285	2mg/ml	DMSO	2841J
	CC1=CN=C(C=N1)C(=O)NCCC1=CC=C(C=C1)S(=O)(=O)N(C(=O)NC1CCCCC1	N-[2-(4-[[(cyclohexylcarbamoyl)amino]sulfonyl]phenyl)ethyl]-5-methylpyrazine-2-carboxamide	Glipizide	445.5	1	FDA Approved Drug Library	29094-61-9	AC-120	2mg/ml	DMSO	2841J
	CC1=CC=C(C=C1)N(CC1=NCCN1)C1=CC=CC(O)=C1	3-[(4,5-dihydro-1H-imidazol-2-ylmethyl)(4-methylphenyl)amino]phenol	Phentolamine	281.4	1	FDA Approved Drug Library	73-05-2	AC-121	2mg/ml	DMSO	2841J
	Cl.[H][O][H].[H][O][H].[H][C@@]12CCN(C)[C@@H]1C=C)[C@@]3([H])(C2)[C@H](O)C1=CC=NC2=C1C=C(OC)C=C2	(R)-[(2S,4S,5R)-5-ethenyl-1-azabicyclo[2.2.2]octan-2-yl](6-methoxyquinolin-4-yl)methanol dihydrate hydrochloride	Quinine HCl·2H₂O	396.9	1	FDA Approved Drug Library	6119-47-7	AC-122	2mg/ml	DMSO	2841J
	OC(=O)C1=C(NC2=CC(=CC=C2)C(F)(F)F)C=CC=C1	2-[[3-(trifluoromethyl)phenyl]amino]benzoic acid	Flufenamic acid	281.2	1	FDA Approved Drug Library	530-78-9	AC-123	2mg/ml	DMSO	2841J
	CCCNCC(O)COC1=C(C=CC=C1)C(=O)CCC1=CC=CC=C1	1-[2-[2-hydroxy-3-(propylamino)propoxy]phenyl]-3-phenylpropan-1-one	Propafenone	341.4	1	FDA Approved Drug Library	54063-53-5	AC-124	2mg/ml	DMSO	2841J
	O=C1NC(=O)C(/N1)(C1=CC=CC=C1)C1=CC=CC=C1	5,5-diphenylimidazolidine-2,4-dione	Phenytoin	252.3	1	FDA Approved Drug Library	57-41-0	AC-125	2mg/ml	DMSO	2841J
	Cl.CCN(CC)CCNC(=O)C1=CC=C(N)C=C1	4-amino-N-[2-(diethylamino)ethyl]benzamide hydrochloride	Procainamide HCl	271.8	1	FDA Approved Drug Library	614-39-1	AC-127	2mg/ml	DMSO	2841J
	Cl.[H][O][H].CCN(CC)CC(=O)NC1=C(C)C=CC=C1C	2-(diethylamino)-N-(2,6-dimethylphenyl)acetamide hydrate hydrochloride	Lidocaine HCl·H₂O	288.8	1	FDA Approved Drug Library	6108-05-0	ALX-550-251	2mg/ml	DMSO	2841J
	CC(O)=O.FC(F)(F)COC1=C(C(=O)NCC2CCCCN2)=C(OCC(F)(F)F)C=C1	N-(piperidin-2-ylmethyl)-2,5-bis(2,2,2-trifluoroethoxy)benzamide; acetic acid	Flecainide acetate	474.4	1	FDA Approved Drug Library	54143-56-5	AC-130	2mg/ml	DMSO	2841J
	OC(=O)/C=C/C(O)=O.CN(CCOC1=CC=C(CC2SC(=O)NC2=O)C=C1)C1=CC=CC=N1	(2Z)-but-2-enedioic acid; 5-[[4-[2-[methyl(pyridin-2-yl)amino]ethoxy]phenyl]methyl]-1,3-thiazolidine-2,4-dione	Rosiglitazone maleate	473.5	1	FDA Approved Drug Library	155141-29-0	DL-569	2mg/ml	DMSO	2841J
	Cl.[H][C@@]12C[C@@]3([H])C[C@@]([H])(C[C@@]([H])(C1)C[C@@]N)(C2)C3	adamantan-1-amine hydrochloride	Amantadine HCl	187.7	1	FDA Approved Drug Library	665-66-7	DL-570	2mg/ml	DMSO	2841J
	Cl.CC1=C(CC2=NCCN2)C(=O)C(O)C(=C1)C(C)(C)C	6-tert-butyl-3-(4,5-dihydro-1H-imidazol-2-ylmethyl)-2,4-dimethylphenol hydrochloride	Oxymetazoline HCl	296.8	1	FDA Approved Drug Library	2315-02-8	AC-138	2mg/ml	DMSO	2841J
	OC(C(O)C(O)=O)C(O)=O.CC(C(O)C1CCC(O)CC1)N1CCC(CC2CCCCC2)CC1	2,3-dihydroxybutanedioic acid; 4-[2-[4-(cyclohexylmethyl)piperidin-1-yl]-1-hydroxypropyl]cyclohexan-1-ol	Ifenprodil tartrate	487.6	1	FDA Approved Drug Library	23210-56-2	AC-142	2mg/ml	DMSO	2841J
	Cl.Cl.COC1=C(C=CC=C1)N1CCN(CC(O)COC2=C3C=CC=CC3=CC=CC2)CC1	1-[4-(2-methoxyphenyl)piperazin-1-yl]-3-(naphthalen-1-yloxy)propan-2-ol dihydrochloride	Naftopidil·2HCl	465.4	1	FDA Approved Drug Library	57149-07-2	AC-144	2mg/ml	DMSO	2841J

Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	Cl.COC1=CC2=NC(=NC(N)=C2C=C1OC)N1CCN(CC1)C(=O)C1=CC=CO1	2-{4-[(furan-2-yl)carbonyl]piperazin-1-yl}-6,7-dimethoxyquinazolin-4-amine hydrochloride	Prazosin·HCl	419.9	1	FDA Approved Drug Library	19237-84-4	AC-146	2mg/ml	DMSO	2841J
	Cl.ClC1=CC=CC(Cl)=C1NC1=NCCN1	N-(2,6-dichlorophenyl)-4,5-dihydro-1H-imidazol-2-amine hydrochloride	Clonidine·HCl	266.6	1	FDA Approved Drug Library	4205-91-8	AC-152	2mg/ml	DMSO	2841J
	NC(=N)N\N=C\C1=C(Cl)C=CC=C1Cl	1-[(E)-[(2,6-dichlorophenyl)methylidene]amino]guanidine	Guanabenz	231.1	1	FDA Approved Drug Library	5051-62-7	AC-153	2mg/ml	DMSO	2841J
	OP(O)(O)=O.C1CC1C(NC1=NCCO1)C1CC1	N-(dicyclopropylmethyl)-4,5-dihydro-1,3-oxazol-2-amine; phosphoric acid	Rilmenidine phosphate	278.2	1	FDA Approved Drug Library	85409-38-7	AC-154	2mg/ml	DMSO	2841J
	Cl.CC(CCC1=CC=CC=C1)NC(C)C(O)C1=CC=C(O)C=C1	4-{1-hydroxy-2-[(4-phenylbutan-2-yl)amino]propyl}phenol hydrochloride	Buphenine·HCl	335.9	1	FDA Approved Drug Library	849-55-8	DL-571	2mg/ml	DMSO	2841J
	Cl.[H][C@@]12CC[C@H](O)[C@H](C(=O)OC)[C@@]1([H])C[C@]1([H])N(CCC3=C1NC1=CC=CC=C31)C2	methyl (1S,15R,18S,19R,20S)-18-hydroxy-3,13-diazapentacyclo[11.8.0.$0^{2,10}$.$0^{4,9}$.$0^{15,20}$]henicosa-2(10),4,6,8-tetraene-19-carboxylate hydrochloride	Yohimbine·HCl	390.9	1	FDA Approved Drug Library	146-48-5	AC-161	2mg/ml	DMSO	2841J
	CS(O)(=O)=O.[H][C@@]12CCCN1C(=O)[C@H](CC1=CC=CC=C1)N1C(=O)[C@](C)(NC(=O)[C@@H]3CC4C5=C6C(C[C@@]4([H])N(C)C3)=CNC6=CC=C5)O[C@@]21O	(4R,7R)-N-[(1S,2S,4R,7S)-7-benzyl-2-hydroxy-4-methyl-5,8-dioxo-3-oxa-6,9-diazatricyclo[7.3.0.$0^{2,6}$]dodecan-4-yl]-6-methyl-6,11-diazatetracyclo[7.6.1.$0^{2,7}$.$0^{12,16}$]hexadeca-1(16),9,12,14-tetraene-4-carboxamide; methanesulfonic acid	Dihydroergotamine mesylate	679.8	1	FDA Approved Drug Library	11032-41-0	AC-164	2mg/ml	DMSO	2841J
	[H][C@@]12CC3=CN(C)C4=CC=CC(=C34)[C@]1(C[C@@H](COC(=O)C1=CN=CC(Br)=C1)CN2C)OC	[(2S,4R,7R)-2-methoxy-6,11-dimethyl-6,11-diazatetracyclo[7.6.1.$0^{2,7}$.$0^{12,16}$]hexadeca-1(16),9,12,14-tetraen-4-yl]methyl 5-bromopyridine-3-carboxylate	Nicergoline	484.4	1	FDA Approved Drug Library	27848-84-6	AC-165	2mg/ml	DMSO	2841J
	NC1=NC(=O)N(C=C1F)[C@@H]1CS[C@H](CO)O1	4-amino-5-fluoro-1-[(2R,5S)-2-(hydroxymethyl)-1,3-oxathiolan-5-yl]-1,2-dihydropyrimidin-2-one	Emtricitabine	247.2	1	FDA Approved Drug Library	143491-57-0	DL-564	2mg/ml	DMSO	2841J
	Cl.CC(C)NCC(O)COC1=CC=C(CCOCC2CC2)C=C1	(3-{4-[2-(cyclopropylmethoxy)ethyl]phenoxy}-2-hydroxypropyl)(propan-2-yl)amine hydrochloride	Betaxolol·HCl	343.9	1	FDA Approved Drug Library	63659-19-8	AC-169	2mg/ml	DMSO	2841J
	CN1C=NC2=C1C(=O)N(C)C(=O)N2C	1,3,7-trimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione	Caffeine	194.2	1	FDA Approved Drug Library	58-08-2	ALX-550-322	2mg/ml	DMSO	2841J
	OC(=O)\C=C/C(O)=O.CC(C)(C)NC[C@H](O)COC1=NSN=C1N1CCOCC1	(2Z)-but-2-enedioic acid; tert-butyl[(2S)-2-hydroxy-3-{[4-(morpholin-4-yl)-1,2,5-thiadiazol-3-yl]oxy}propyl]amine	(S)-Timolol maleate	432.5	1	FDA Approved Drug Library	26921-17-5	AC-172	2mg/ml	DMSO	2841J
	OC(=O)\C=C\C(O)=O.OC(CNCCNC(=O)N1CCOCC1)COC1=CC=C(O)C=C1	(2E)-but-2-enedioic acid; N-(2-{[2-hydroxy-3-(4-hydroxyphenoxy)propyl]amino}ethyl)morpholine-4-carboxamide	Xamoterol hemifumarate	455.5	1	FDA Approved Drug Library	73210-73-8	AC-173	2mg/ml	DMSO	2841J
	CC(C)(C)NCC(O)C1=CC(Cl)=C(N)C(Cl)=C1	1-(4-amino-3,5-dichlorophenyl)-2-(tert-butylamino)ethan-1-ol	Clenbuterol	277.2	1	FDA Approved Drug Library	37148-27-9	AC-174	2mg/ml	DMSO	2841J
	Cl.CC[C@H](NC(C)C)[C@H](O)C1=CC=C(O)C2=C1C=CC(=O)N2	8-hydroxy-5-[(1R,2S)-1-hydroxy-2-[(propan-2-yl)amino]butyl]-1,2-dihydroquinolin-2-one hydrochloride	Procaterol·HCl	326.8	1	FDA Approved Drug Library	62929-91-3	AC-175	2mg/ml	DMSO	2841J
	OS(O)(=O)=O.CC(C)(C)NCC(O)C1=CC=C(O)C(CO)=C1.CC(C)(C)NCC(O)C1=CC=C(O)C(CO)=C1	bis(4-[2-(tert-butylamino)-1-hydroxyethyl]-2-(hydroxymethyl)phenol); sulfuric acid	Salbutamol hemisulfate	576.7	1	FDA Approved Drug Library	51022-70-9	AC-176	2mg/ml	DMSO	2841J
	CC(C)NCC(O)COC1=CC=CC2=C1C=CN2	[2-hydroxy-3-(1H-indol-4-yloxy)propyl](propan-2-yl)amine	Pindolol	248.3	1	FDA Approved Drug Library	13523-86-9	AC-181	2mg/ml	DMSO	2841J
	CC(C)NCC(O)C1=CC(C#N)=C(N)C=C1	2-amino-5-{1-hydroxy-2-[(propan-2-yl)amino]ethyl}benzonitrile	Cimaterol	219.3	1	FDA Approved Drug Library	54239-37-1	AC-183	2mg/ml	DMSO	2841J
	Cl.CC(CCC1=CC=C(O)C=C1)NCCC1=CC=C(O)C(O)=C1	4-(2-{[4-(4-hydroxyphenyl)butan-2-yl]amino}ethyl)benzene-1,2-diol hydrochloride	Dobutamine·HCl	337.8	1	FDA Approved Drug Library	49745-95-1	AC-185	2mg/ml	DMSO	2841J
	Cl.CC(C)NCC(O)C1=CC2=C(C=CC=C2)C=C1	1-(naphthalen-2-yl)-2-[(propan-2-yl)amino]ethan-1-ol hydrochloride	Pronethalol·HCl	265.8	1	FDA Approved Drug Library	51-02-5	AC-189	2mg/ml	DMSO	2841J
	Cl.CC(C)NCC(O)C1=CC=C(NS(C)(=O)=O)C=C1	N-(4-{1-hydroxy-2-[(propan-2-yl)amino]ethyl}phenyl)methanesulfonamide hydrochloride	Sotalol·HCl	308.8	1	FDA Approved Drug Library	959-24-0	AC-192	2mg/ml	DMSO	2841J
	Cl.[H][C@]12CC[C@](CCCNC)(C3=C1C=CC=C3)C1=C2C=CC=C1	methyl(3-{tetracyclo[6.6.2.$0^{2,7}$.$0^{9,14}$]hexadeca-2(7),3,5,9(14),10,12-hexaen-1-yl}propyl)amine hydrochloride	Maprotiline·HCl	313.9	1	FDA Approved Drug Library	10347-81-6	AR-111	2mg/ml	DMSO	2841J
	Cl.CNCCC(OC1=CC=CC=C1OC)C1=CC=CC=C1	[3-(2-methoxyphenoxy)-3-phenylpropyl](methyl)amine hydrochloride	Nisoxetine·HCl	307.8	1	FDA Approved Drug Library	57754-86-6	AC-194	2mg/ml	DMSO	2841J
	CC(\C=C\C=C(C)\C=C\C1=C(C)C(=O)CCC1(C)C)=C/C=C/C=C(C)/C=C/C=C(C)/C=C/C1=C(C)C(=O)CCC1(C)C	2,4,4-trimethyl-3-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-(2,6,6-trimethyl-3-oxocyclohex-1-en-1-yl)octadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl]cyclohex-2-en-1-one	Canthaxanthin	564.8	1	FDA Approved Drug Library	514-78-3	DL-553	2mg/ml	DMSO	2841J
	Cl.CC[C@H]1[C@@H](CC2=CN=CN2C)COC1=O	(3S,4R)-3-ethyl-4-[(1-methyl-1H-imidazol-5-yl)methyl]oxolan-2-one hydrochloride	Pilocarpine·HCl	244.7	1	FDA Approved Drug Library	54-71-7	AC-214	2mg/ml	DMSO	2841J
	[Br-].[H][C@]12CC[C@]([H])(C[C@@H](C1)OC(=O)C(CO)C1=CC=CC=C1)[N+]2(C)C(C)C	(1R,3R,5S)-3-[(3-hydroxy-2-phenylpropanoyl)oxy]-8-methyl-8-(propan-2-yl)-8-azabicyclo[3.2.1]octan-8-ium bromide	Ipratropium·Br	412.4	1	FDA Approved Drug Library	22254-24-6	AC-218	2mg/ml	DMSO	2841J
	Cl.Cl.CN1CCN(CC(=O)N2C3=NC=CC=C3NC(=O)C3=C2C=CC=C3)CC1	2-[2-(4-methylpiperazin-1-yl)acetyl]-2,4,9-triazatricyclo[9.4.0.$0^{3,8}$]pentadeca-1(11),3,5,7,12,14-hexaen-10-one dihydrochloride	Pirenzepine·2HCl	424.3	1	FDA Approved Drug Library	29868-97-1	AC-220	2mg/ml	DMSO	2841J
	Cl.Cl.CN1CCN(CC(=O)N2C3=C(C)SC=C3C(=O)NC3=C2C=CC=C3)CC1	4-methyl-2-[2-(4-methylpiperazin-1-yl)acetyl]-5-thia-2,9-diazatricyclo[8.4.0.$0^{3,7}$]tetradeca-1(10),3,6,11,13-pentaen-8-one dihydrochloride	Telenzepine·2HCl	443.4	1	FDA Approved Drug Library	147416-96-4	AC-221	2mg/ml	DMSO	2841J
	CCN(CC1=CC=NC=C1)C(=O)C(CO)C1=CC=CC=C1	N-ethyl-3-hydroxy-2-phenyl-N-(pyridin-4-ylmethyl)propanamide	Tropicamide	284.4	1	FDA Approved Drug Library	1508-75-4	AC-222	2mg/ml	DMSO	2841J
	[Br-].[Br-].[H][C@@]12C[C@@H]([C@H](OC(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CC[C@@]2([H])C[C@H](OC(C)=O)[C@H](C[C@]12C)[N+]1(C)CCCCC1)[N+]1(C)CCCCC1	1-[(1S,2S,4S,5S,7S,10R,11S,13S,14R,15S)-5,14-bis(acetyloxy)-2,15-dimethyl-13-(1-methylpiperidin-1-ium-1-yl)tetracyclo[8.7.0.$0^{2,7}$.$0^{11,15}$]heptadecan-4-yl]-1-methylpiperidin-1-ium dibromide	Pancuronium·2Br	732.7	1	FDA Approved Drug Library	15500-66-0	AC-232	2mg/ml	DMSO	2841J
	[H][C@@]12OC\C3=C/C=C/[C@H](C)[C@H](O[C@H]4C[C@H](OC)[C@@H](O[C@H]5C[C@H](OC)[C@@H](O)[C@H](C)O5)[C@H](C)O4)\C(C)=C\C[C@@H]4C[C@@H](C[C@]5(CC[C@H](C)[C@]([H])(O5)[C@@H](C)CC)O4)OC(=O)[C@H](C=C(C)[C@H]1O)[C@@]23O	(1'R,2R,4'S,5S,6R,8'R,10'E,12'S,13'S,14'E,16'E,20'R,21'R,24'S)-6-[(2S)-butan-2-yl]-21',24'-dihydroxy-12'-{[(2R,4S,5S,6S)-5-{[(2S,4S,5S,6S)-5-hydroxy-4-methoxy-6-methyloxan-2-yl]oxy}-4-methoxy-6-methyloxan-2-yl]oxy}-5,11',13',22'-tetramethyl-3',7',19'-trioxaspiro[oxane-2,6'-tetracyclo[15.6.1.$1^{4,8}$.$0^{20,24}$]pentacosane]-10',14',16',22'-tetraen-2'-one	Ivermectin	875.1	1	FDA Approved Drug Library	70288-86-7	AC-238	2mg/ml	DMSO	2841J
	OS(O)(=O)=O.[H][C@]12N(C)CC[C@@]1(C)C1=C(C=CC(OC(=O)NC)=C1)N2C.[H][C@]12N(C)CC[C@@]1(C)C1=C(C=CC(OC(=O)NC)=C1)N2C	bis((3aS,8aR)-1,3a,8-trimethyl-1H,2H,3H,3aH,8H,8aH-pyrrolo[2,3-b]indol-5-yl N-methylcarbamate); sulfuric acid	Physostigmine sulfate	648.8	1	FDA Approved Drug Library	64-47-1	AC-241	2mg/ml	DMSO	2841J
	O=C(CCNNC(=O)C1=CC=NC=C1)NCC1=CC=CC=C1	N-benzyl-3-(pyridin-4-ylformohydrazido)propanamide	Nialamide	298.3	1	FDA Approved Drug Library	51-12-7	DL-554	2mg/ml	DMSO	2841J

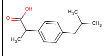
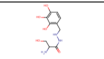
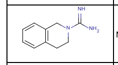
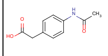
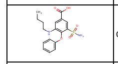
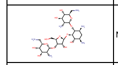
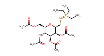
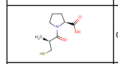
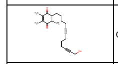
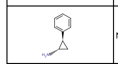
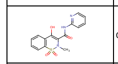
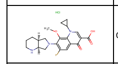
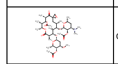
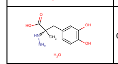
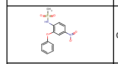
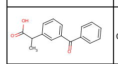
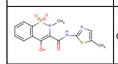
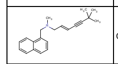
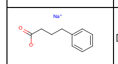
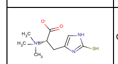
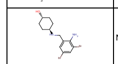
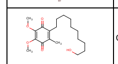
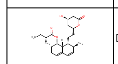
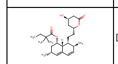
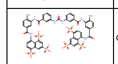
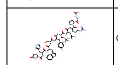
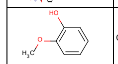
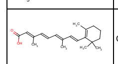
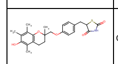
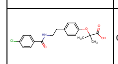
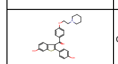
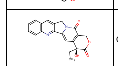
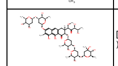
Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	OC1(CCN(CCCC(=O)C2=CC=C(F)C=C2)CC1)C1=CC=C(Cl)C=C1	4-[4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl]-1-(4-fluorophenyl)butan-1-one	Haloperidol	375.9	1	FDA Approved Drug Library	52-86-8	AC-250	2mg/ml	DMSO	2841J
	Cl.Cl.C(N1CCN(CC1)C1=NC=CC=N1)C1=CC2=C(OCO2)C=C1	2-[4-(2H-1,3-benzodioxol-5-ylmethyl)piperazin-1-yl]pyrimidine dihydrochloride	Piribedil·2HCl	371.3	1	FDA Approved Drug Library	78213-63-5	AC-259	2mg/ml	DMSO	2841J
	OC(=O)\C=C/C(O)=O.COC1=CC=C(CN(CCN(C)C)C2=NC=CC=C2)C=C1	(2Z)-but-2-enedioic acid; N-[2-(dimethylamino)ethyl]-N-[(4-methoxyphenyl)methyl]pyridin-2-amine	Mepyramine maleate	401.5	1	FDA Approved Drug Library	59-33-6	AC-277	2mg/ml	DMSO	2841J
	Cl.CC1=CC=C(C=C1)C(=C/CN1CCCC1)\C1=NC=CC=C1	2-[(1E)-1-(4-methylphenyl)-3-(pyrrolidin-1-yl)prop-1-en-1-yl]pyridine hydrochloride	Trans-triprolidine·HCl	314.9	1	FDA Approved Drug Library	6138-79-0	AC-279	2mg/ml	DMSO	2841J
	CN\C(NC#N)=N\CCSCC1=C(C)NC=N1	(Z)-1-cyano-3-methyl-2-(2-{[(5-methyl-1H-imidazol-4-yl)methyl]sulfanyl}ethyl)guanidine	Cimetidine	252.3	1	FDA Approved Drug Library	51481-61-9	AC-280	2mg/ml	DMSO	2841J
	CN\C(NCCSCC1=CSC(NC(N)=N)=N1)=N/C#N	(E)-3-(2-{[(2-carbamimidamido-1,3-thiazol-4-yl)methyl]sulfanyl}ethyl)-2-cyano-1-methylguanidine	Tiotidine	312.4	1	FDA Approved Drug Library	69014-14-8	AC-282	2mg/ml	DMSO	2841J
	NS(=O)(=O)CC1=NOC2=CC=CC=C12	1,2-benzoxazol-3-ylmethanesulfonamide	Zonisamide	212.2	1	FDA Approved Drug Library	68291-97-4	DL-555	2mg/ml	DMSO	2841J
	OC(CN1C=CN=C1)(P(O)(O)=O)P(O)(O)=O	[1-hydroxy-2-(1H-imidazol-1-yl)-1-phosphonoethyl]phosphonic acid	Zoledronic acid	272.1	1	FDA Approved Drug Library	118072-93-8	DL-556	2mg/ml	DMSO	2841J
	Cl.OC1=CC=C2C[C@H]3N(CC4CC4)CC[C@@]45[C@@H](OC1=C24)C(=O)CC[C@@]35O	(1S,5R,13R,17S)-4-(cyclopropylmethyl)-10,17-dihydroxy-12-oxa-4-azapentacyclo$[9.6.1.0^{1,13}.0^{5,17}.0^{7,18}]$octadeca-7,9,11(18)-trien-14-one hydrochloride	Naltrexone·HCl	377.9	1	FDA Approved Drug Library	16676-29-2	AC-322	2mg/ml	DMSO	2841J
	O.CN(C)CCC1=CNC2=CC=C(C[C@H]3COC(=C)N3)C=C12	dimethyl[2-(5-{[(4S)-2-methylidene-1,3-oxazolidin-4-yl]methyl}-1H-indol-3-yl)ethyl]amine hydrate	Zolmitriptan	303.4	1	FDA Approved Drug Library	139264-17-8	DL-560	2mg/ml	DMSO	2841J
	Cl.[H][C@]12C[C@]3(C)C[C@](C)(C1)C[C@](N)(C2)C3	(1R,3R,5S,7R)-3,5-dimethyladamantan-1-amine hydrochloride	Memantine·HCl	215.8	1	FDA Approved Drug Library	19982-08-2	ALX-550-363	2mg/ml	DMSO	2841J
	COC1=CC=C(C=C1)C(=O)N1CCCC1=O	1-[(4-methoxyphenyl)carbonyl]pyrrolidin-2-one	Aniracetam	219.2	1	FDA Approved Drug Library	72432-10-1	AC-439	2mg/ml	DMSO	2841J
	Cl.NC1=NC2=C(S1)C=C(OC(F)(F)F)C=C2	6-(trifluoromethoxy)-1,3-benzothiazol-2-amine hydrochloride	Riluzole·HCl	270.7	1	FDA Approved Drug Library	1744-22-5	ALX-550-344	2mg/ml	DMSO	2841J
	CC(C)C1=CC=CC(C(C)C)=C1O	2,6-bis(propan-2-yl)phenol	Propofol	178.3	1	FDA Approved Drug Library	2078-54-8	AC-508	2mg/ml	DMSO	2841J
	Cl.CN1CCN2C(C1)C1=CC=CC=C1CC1=C2C=CC=C1	5-methyl-2,5-diazatetracyclo$[13.4.0.0^{2,7}.0^{8,13}]$nonadeca-1(15),8,10,12,16,18-hexaene hydrochloride	Mianserin·HCl	300.8	2	FDA Approved Drug Library	21535-47-7	AC-554	2mg/ml	DMSO	2841J
	CN1C2=C(NC=N2)C(=O)N(C)C1=O	1,3-dimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione	Aminophylline	180.2	2	FDA Approved Drug Library	317-34-0	AC-615	2mg/ml	DMSO	2841J
	CN1C(=O)N(CC2=CC=CO2)C2=C(NC(C)=N2)C1=O	3-(furan-2-ylmethyl)-1,8-dimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione	Furafylline	260.2	2	FDA Approved Drug Library	80288-49-9	AC-626	2mg/ml	DMSO	2841J
	CC(C)[C@H]1CC[C@@H](CC1)C(=O)N[C@H](CC1=CC=CC=C1)C(O)=O	(2R)-3-phenyl-2-{[4-(propan-2-yl)cyclohexyl]formamido}propanoic acid	Nateglinide	317.4	2	FDA Approved Drug Library	105816-04-4	DL-561	2mg/ml	DMSO	2841J
	CC(C)NCC(O)C1=CC=C(O)C(O)=C1	4-{1-hydroxy-2-[(propan-2-yl)amino]ethyl}benzene-1,2-diol	DL-Isoproterenol	211.3	2	FDA Approved Drug Library	51-30-9	AC-729	2mg/ml	DMSO	2841J
	CC(=O)OCC[N+](C)(C)C	[2-(acetyloxy)ethyl]trimethylazanium	Acetylcholine	146.2	2	FDA Approved Drug Library	60-31-1	AC-734	2mg/ml	DMSO	2841J
	[H][C@]12CC[C@]([H])(C[C@@H](C1)OC(=O)C(CO)C1=CC=CC=C1)N2C	(1R,3R,5S)-8-methyl-8-azabicyclo[3.2.1]octan-3-yl 3-hydroxy-2-phenylpropanoate	Atropine	289.4	2	FDA Approved Drug Library	55-48-1	AC-735	2mg/ml	DMSO	2841J
	C[N+](C)(C)CCCCCCCCCC[N+](C)(C)C	trimethyl[10-(trimethylazaniumyl)decyl]azanium	Decamethonium	258.5	2	FDA Approved Drug Library	541-22-0	AC-737	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@@]([H])(C1)C(C)(NC)C2(C)C	(1S,4R)-N,2,3,3-tetramethylbicyclo[2.2.1]heptan-2-amine	Mecamylamine	167.3	2	FDA Approved Drug Library	826-39-1	AC-741	2mg/ml	DMSO	2841J
	CN(C)C(=O)OC1=CC(=CC=C1)[N+](C)(C)C	3-[(dimethylcarbamoyl)oxy]-N,N,N-trimethylanilinium	Neostigmine	223.3	2	FDA Approved Drug Library	114-80-7	AC-743	2mg/ml	DMSO	2841J
	Cl.[H][C@@]12N3C4=C(C=CC=C4)[C@@]11CCN4CC5=CCO[C@@]([H])(CC3=O)[C@]2([H])[C@@]5([H])C[C@@H]14	(1R,11S,18S,20R,21R,22S)-12-oxa-8,17-diazaheptacyclo$[15.5.2.0^{1,18}.0^{2,7}.0^{8,22}.0^{11,21}.0^{15,20}]$tetracosa-2(7),3,5,14-tetraen-9-one hydrochloride	Strychnine·HCl	370.9	2	FDA Approved Drug Library	1421-86-9	AC-745	2mg/ml	DMSO	2841J
	Cl.[Cl-].COC1=CC2=C3C=C1OC1=C(O)C=CC(C[C@@H]4C5=C(OC6=CC=C(C[C@@H]3N(C)CC2)C=C6)C(O)=C(OC)C=C5CC[N+]4(C)C)=C1	(1S,16R)-9,21-dihydroxy-10,25-dimethoxy-15,15,30-trimethyl-7,23-dioxa-15,30-diazaheptacyclo$[22.6.2.2^{3,6}.1^{8,12}.1^{18,22}.0^{27,31}.0^{16,34}]$hexatriaconta-3,5,8(34),9,11,18(33),19,21,24(32),25,27(31),35-dodecaen-15-ium hydrochloride chloride	(+)-Tubocuraraine chloride	681.6	2	FDA Approved Drug Library	57-94-3	AC-746	2mg/ml	DMSO	2841J
	Cl.[H][C@]12C[C@](O)(CCN1C[C@]1([H])C3=C(CCC4=C1C2=CC=C4)C=CC=C3)C(C)(C)C	(1R,6R,8R)-6-tert-butyl-3-azapentacyclo$[11.8.1.0^{3,8}.0^{9,22}.0^{16,21}]$docosa-9,11,13(22),16(21),17,19-hexaen-6-ol hydrochloride	(+)-Butaclamol·HCl	398.0	2	FDA Approved Drug Library	55528-07-9	AC-747	2mg/ml	DMSO	2841J
	Cl.[H][C@]12CC3=CC=C(O)C(O)=C3C3=CC=CC(CCN1C)=C23	(9R)-10-methyl-10-azatetracyclo$[7.7.1.0^{2,7}.0^{13,17}]$heptadeca-1(16),2,4,6,13(17),14-hexaene-3,4-diol hydrochloride	(R)-(-)-Apomorphine·HCl	303.8	2	FDA Approved Drug Library	314-19-2	AC-748	2mg/ml	DMSO	2841J
	Cl.CN(C)CCCN1C2=CC(Cl)=CC=C2SC2=C1C=CC=C2	[3-(2-chloro-10H-phenothiazin-10-yl)propyl]dimethylamine hydrochloride	Chlorpromazine·HCl	355.3	2	FDA Approved Drug Library	69-09-0	AC-749	2mg/ml	DMSO	2841J
	ClC1=CC2=C(C=C1)N(C1CCN(CCCN3C(=O)NC4=C3C=CC=C4)CC1)C(=O)N2	5-chloro-1-{1-[3-(2-oxo-2,3-dihydro-1H-1,3-benzodiazol-1-yl)propyl]piperidin-4-yl}-2,3-dihydro-1H-1,3-benzodiazol-2-one	Domperidone	425.9	2	FDA Approved Drug Library	57808-66-9	AC-751	2mg/ml	DMSO	2841J
	Cl.Cl.OCCN1CCN(CCCN2C3=CC(=CC=C3SC3=C2C=CC=C3)C(F)(F)F)CC1	2-(4-{3-[2-(trifluoromethyl)-10H-phenothiazin-10-yl]propyl}piperazin-1-yl)ethan-1-ol dihydrochloride	Fluphenazine·2HCl	510.4	2	FDA Approved Drug Library	146-56-5	AC-753	2mg/ml	DMSO	2841J
	CS(O)(=O)=O.[H][C@@]12CC3=CNC4=C3C(=CC=C4)[C@@]1([H])C[C@@H](CSC)CN2CCC	(2R,4R,7R)-4-[(methylsulfanyl)methyl]-6-propyl-6,11-diazatetracyclo$[7.6.1.0^{2,7}.0^{12,16}]$hexadeca-1(15),9,12(16),13-tetraene; methanesulfonic acid	Pergolide mesylate	410.6	2	FDA Approved Drug Library	66104-23-2	AC-755	2mg/ml	DMSO	2841J
	CCN1CCC[C@H]1CNC(=O)C1=C(OC)C(Cl)=CC(Cl)=C1O	3,5-dichloro-N-{[(2S)-1-ethylpyrrolidin-2-yl]methyl}-2-hydroxy-6-methoxybenzamide	S(-)-Raclopride	347.2	2	FDA Approved Drug Library	84225-95-6	AC-757	2mg/ml	DMSO	2841J

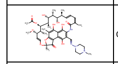
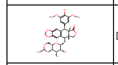
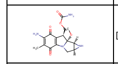
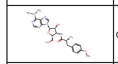
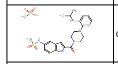
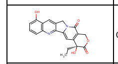
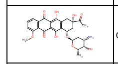
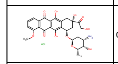
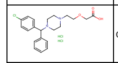
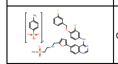
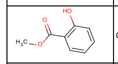
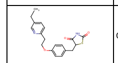
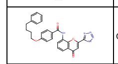
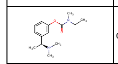
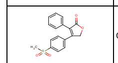
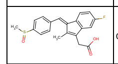
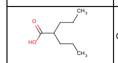
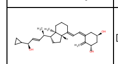
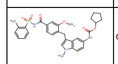
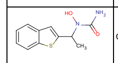
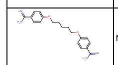
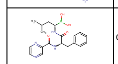
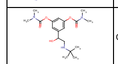
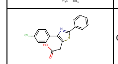
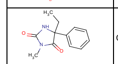
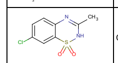
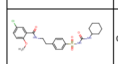
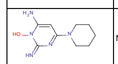
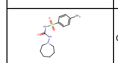
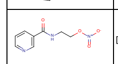
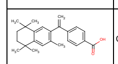
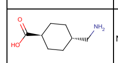
Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	CC1=C(CCN2CCC(CC2)C2=NOC3=C2C=CC(F)=C3)C(=O)N2CCCCC2=N1	3-{2-[4-(6-fluoro-1,2-benzoxazol-3-yl)piperidin-1-yl]ethyl}-2-methyl-4H,6H,7H,8H,9H-pyrido[1,2-a]pyrimidin-4-one	Risperidone	410.5	2	FDA Approved Drug Library	106266-06-2	AC-758	2mg/ml	DMSO	2841J
	CCN1CCC[C@H]1CNC(=O)C1=CC(=CC=C1OC)S(N)(=O)=O	N-{[(2S)-1-ethylpyrrolidin-2-yl]methyl}-2-methoxy-5-sulfamoylbenzamide	(S)-(-)-Sulpiride	341.4	2	FDA Approved Drug Library	23672-07-3	AC-760	2mg/ml	DMSO	2841J
	Cl.CN(C)CCOC(C1=CC=CC=C1)C1=CC=CC=C1	[2-(diphenylmethoxy)ethyl]dimethylamine hydrochloride	Diphenhydramine·HCl	291.8	2	FDA Approved Drug Library	147-24-0	AC-763	2mg/ml	DMSO	2841J
	Cl.CC(CN1C2=CC=CC=C2SC2=C1C=CC=C2)N(C)C	dimethyl[1-(10H-phenothiazin-10-yl)propan-2-yl]amine hydrochloride	Promethazine·HCl	320.9	2	FDA Approved Drug Library	58-33-3	AC-765	2mg/ml	DMSO	2841J
	Cl.CN\C(NCCSCC1=CC=C(CN(C)C)O1)=C\[N+]([O-])=O	dimethyl[(5-{[(2-{[(Z)-1-(methylamino)-2-nitroethenyl]amino}ethyl)sulfanyl]methyl}furan-2-yl)methyl]amine hydrochloride	Ranitidine·HCl	350.9	2	FDA Approved Drug Library	66357-59-3	AC-766	2mg/ml	DMSO	2841J
	Cl.OC1=C2O[C@H]3C4=C(C[C@@]5(O)C6CC(C=C1)=C2[C@@]35CCN6CC1CC1)C1=C(N4)C=CC=C1	(1S,2S,13R)-22-(cyclopropylmethyl)-14-oxa-11,22-diazaheptacyclo$[13.9.1.0^{1,13}.0^{2,21}.0^{4,12}.0^{5,10}.0^{19,25}]$pentacosa-4(12),5(10),6,8,15,17,19(25)-heptaene-2,16-diol hydrochloride	Naltrindole·HCl	451.0	2	FDA Approved Drug Library	111469-81-9	AC-770	2mg/ml	DMSO	2841J
	Cl.C1CN=C(N1)C1COC2=C(O1)C=CC=C2	2-(2,3-dihydro-1,4-benzodioxin-2-yl)-4,5-dihydro-1H-imidazole hydrochloride	Idazoxan·HCl	240.7	2	FDA Approved Drug Library	79944-56-2	AC-806	2mg/ml	DMSO	2841J
	Cl.FC1=CC=C(C=C1)C(=O)CCCN1CCC2(CC1)N(CNC2=O)C1=CC=CC=C1	8-[4-(4-fluorophenyl)-4-oxobutyl]-1-phenyl-1,3,8-triazaspiro[4.5]decan-4-one hydrochloride	Spiperone·HCl	431.9	2	FDA Approved Drug Library	749-02-0	AC-807	2mg/ml	DMSO	2841J
	OC(C(O)C(O)=O)C(O)=O.CNC[C@H](O)C1=CC=C(O)C(O)=C1	2,3-dihydroxybutanedioic acid; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol	L-(+)-Epinephrine tartrate	333.3	2	FDA Approved Drug Library	51-40-1	AC-808	2mg/ml	DMSO	2841J
	CC1=CC=CC(C)=C1NC1=NCCCS1	N-(2,6-dimethylphenyl)-5,6-dihydro-4H-1,3-thiazin-2-amine	Xylazine	220.3	2	FDA Approved Drug Library	7361-61-7	AC-809	2mg/ml	DMSO	2841J
	O[C@H]([C@@H](O)C(O)=O)C(O)=O.NC[C@H](O)C1=CC=C(O)C(O)=C1	(2R,3R)-2,3-dihydroxybutanedioic acid; 4-[(1R)-2-amino-1-hydroxyethyl]benzene-1,2-diol	Norepinephrine-(+)-tartrate L (-)	319.3	2	FDA Approved Drug Library	50-40-1	AC-810	2mg/ml	DMSO	2841J
	OC(=O)\C=C\C(O)=O.OC(=O)\C=C\C(O)=O.OCCOCCN1CCN(CC1)C1=NC2=CC=CC=C2SC2=CC=CC=C12	bis((2E)-but-2-enedioic acid); 2-[2-(4-{2-thia-9-azatricyclo$[9.4.0.0^{3,8}]$pentadeca-1(15),3,5,7,9,11,13-heptaen-10-yl}piperazin-1-yl)ethoxy]ethan-1-ol	Quetiapine Fumarate	615.7	2	FDA Approved Drug Library	111974-72-2	DL-557	2mg/ml	DMSO	2841J
	Cl.CC(C)NCC(O)COC1=CC=CC=C1CC=C	{2-hydroxy-3-[2-(prop-2-en-1-yl)phenoxy]propyl}(propan-2-yl)amine hydrochloride	Alprenolol·HCl	285.8	2	FDA Approved Drug Library	13707-88-5	AC-812	2mg/ml	DMSO	2841J
	Cl.CN(C)CCCN1C2=CC=CC=C2CCC2=C1C=CC=C2	(3-{2-azatricyclo$[9.4.0.0^{3,8}]$pentadeca-1(11),3,5,7,12,14-hexaen-2-yl}propyl)dimethylamine hydrochloride	Imipramine·HCl	316.9	2	FDA Approved Drug Library	113-52-0	AC-813	2mg/ml	DMSO	2841J
	ClC1=CC2=C(OC3=C(C=CC=C3)N=C2N2CCNCC2)C=C1	13-chloro-10-(piperazin-1-yl)-2-oxa-9-azatricyclo$[9.4.0.0^{3,8}]$pentadeca-1(11),3(8),4,6,9,12,14-heptaene	Amoxapine	313.8	2	FDA Approved Drug Library	14028-44-5	AC-814	2mg/ml	DMSO	2841J
	[H][C@@]12CC3=CN(C)C4=C3C(=CC=C4)[C@@]1([H])C[C@@H](CN2C)NS(=O)(=O)N(C)C	{[(2R,4S,7R)-6,11-dimethyl-6,11-diazatetracyclo$[7.6.1.0^{2,7}.0^{12,16}]$hexadeca-1(15),9,12(16),13-tetraen-4-yl]sulfamoyl}dimethylamine	Mesulergine	362.5	2	FDA Approved Drug Library	64795-35-3	AC-834	2mg/ml	DMSO	2841J
	CC(NC(C)(C)C)C(=O)C1=CC=CC(Cl)=C1	2-(tert-butylamino)-1-(3-chlorophenyl)propan-1-one	Amfebutamone	239.7	2	FDA Approved Drug Library	34911-55-2	DL-558	2mg/ml	DMSO	2841J
	CCN(CC)CCNC(=O)C1=CC(Cl)=C(N)C=C1OC	4-amino-5-chloro-N-[2-(diethylamino)ethyl]-2-methoxybenzamide	Metoclopramide	299.8	2	FDA Approved Drug Library	7232-21-5	AC-840	2mg/ml	DMSO	2841J
	O.CS(O)(=O)=O.OC1=C2O[C@H]3C4=C(C[C@@]5(O)[C@H]6CC(C=C1)=C2[C@@]35CCN6CC1CC1)C1=C(O4)C=CC=C1	(1S,2S,13R,21R)-22-(cyclopropylmethyl)-11,14-dioxa-22-azaheptacyclo$[13.9.1.0^{1,13}.0^{2,21}.0^{4,12}.0^{5,10}.0^{19,25}]$pentacosa-4(12),5(10),6,8,15,17,19(25)-heptaene-2,16-diol methanesulfonic acid hydrate	Naltriben methanesulfonate hydrate	529.6	2	FDA Approved Drug Library	111555-58-9	AC-858	2mg/ml	DMSO	2841J
	CC(=O)OC\C=C(C)\C=C\C=C(C)\C=C\C1=C(C)CCCC1(C)C	(2E,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraen-1-yl acetate	Vitamin A acetate	328.5	2	FDA Approved Drug Library	127-47-9	DL-124	2mg/ml	DMSO	2841J
	[H][C@@]12CCCC[C@@]11CCN(\C=C\C)[C@@H]2CC2=C1C=C(O)C=C2	(1R,9R,10R)-17-[(1E)-prop-1-en-1-yl]-17-azatetracyclo$[7.5.3.0^{1,10}.0^{2,7}]$heptadeca-2(7),3,5-trien-4-ol	Levallorphan	283.4	2	FDA Approved Drug Library	71-82-9	AC-891	2mg/ml	DMSO	2841J
	O[C@H]1CC[C@@]2(O)[C@H]3CC4=CC=C(O)C5=C4[C@@]2(CCN3CC2CCC2)[C@H]1O5	(1S,5R,13R,14S,17S)-4-(cyclobutylmethyl)-12-oxa-4-azapentacyclo$[9.6.1.0^{1,13}.0^{5,17}.0^{7,18}]$octadeca-7,9,11(18)-triene-10,14,17-triol	Nalbuphine	357.4	2	FDA Approved Drug Library	59052-16-3	AC-893	2mg/ml	DMSO	2841J
	C[N+](C)(C)CCOC(N)=O	2-(trimethylazaniumyl)ethyl carbamate	Carbamylcholine	147.2	2	FDA Approved Drug Library	51-83-2	AC-911	2mg/ml	DMSO	2841J
	CC(C[N+](C)(C)C)OC(N)=O	1-(trimethylazaniumyl)propan-2-yl carbamate	Carbamyl-beta-methylcholine	161.2	2	FDA Approved Drug Library	590-63-6	AC-912	2mg/ml	DMSO	2841J
	CCCC(=O)OCC[N+](C)(C)C	[2-(butanoyloxy)ethyl]trimethylazanium	Butyrylcholine	174.3	2	FDA Approved Drug Library	2963-78-2	AC-915	2mg/ml	DMSO	2841J
	NC(N)=NC1=NC(CSCCC(=N)NS(N)(=O)=O)=CS1	3-[({2-[(diaminomethylidene)amino]-1,3-thiazol-4-yl}methyl)sulfanyl]-N-sulfamoylpropanimidamide	FAMOTIDINE	337.4	2	FDA Approved Drug Library	76824-35-6	AC-925	2mg/ml	DMSO	2841J
	CC(C)(C)C1=CC=C(C=C1)C(O)CCCN1CCC(CC1)C(O)(C1=CC=CC=C1)C1=CC=CC=C1	1-(4-tert-butylphenyl)-4-[4-(hydroxydiphenylmethyl)piperidin-1-yl]butan-1-ol	Terfenadine	471.7	2	FDA Approved Drug Library	50679-08-8	AC-928	2mg/ml	DMSO	2841J
	NNC(=O)C1=CC=NC=C1	pyridine-4-carbohydrazide	Isoniazid	137.1	2	FDA Approved Drug Library	54-85-3	AC-986	2mg/ml	DMSO	2841J
	ClC1=C(CN2CCC3=C(C2)C=CS3)C=CC=C1	5-[(2-chlorophenyl)methyl]-4H,5H,6H,7H-thieno[3,2-c]pyridine	Ticlopidine	263.8	2	FDA Approved Drug Library	53885-35-1	AC-993	2mg/ml	DMSO	2841J
	CCC(C)(C)C1=CC=C(CC(C)CN2C[C@H](C)O[C@H](C)C2)C=C1	(2R,6S)-2,6-dimethyl-4-{2-methyl-3-[4-(2-methylbutan-2-yl)phenyl]propyl}morpholine	Amorolfine	317.5	2	FDA Approved Drug Library	78613-35-1	DL-246	2mg/ml	DMSO	2841J
	CN1CCC[C@@H]1CCO[C@](C)(C1=CC=CC=C1)C1=CC=C(Cl)C=C1	(2R)-2-{2-[(1R)-1-(4-chlorophenyl)-1-phenylethoxy]ethyl}-1-methylpyrrolidine	Clemastine	343.9	2	FDA Approved Drug Library	14976-57-9	DL-247	2mg/ml	DMSO	2841J
	CCCC1=NC(C)=C2N1NC(=NC2=O)C1=CC(=CC=C1OCC)S(=O)(=O)N1CCN(CC)CC1	2-[2-ethoxy-5-(4-ethylpiperazine-1-sulfonyl)phenyl]-5-methyl-7-propyl-1H,4H-imidazo[4,3-f][1,2,4]triazin-4-one	Vardenafil	488.6	2	FDA Approved Drug Library	224785-90-4	DL-248	2mg/ml	DMSO	2841J
	CC(=O)NC[C@H]1CN(C(=O)O1)C1=CC=C(N2CCOCC2)C(F)=C1	N-{[(5S)-3-[3-fluoro-4-(morpholin-4-yl)phenyl]-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide	Linezolid	337.3	2	FDA Approved Drug Library	165800-03-3	DL-249	2mg/ml	DMSO	2841J

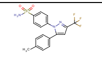
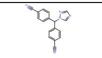
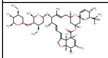
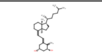
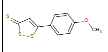
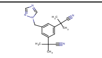
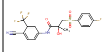
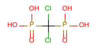
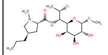
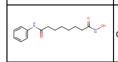
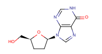
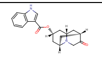
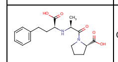
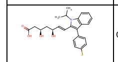
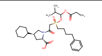
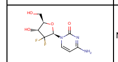
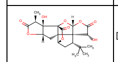
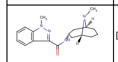
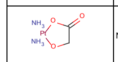
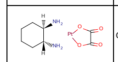
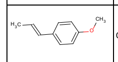
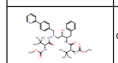
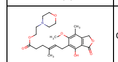
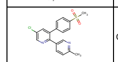
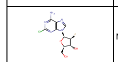
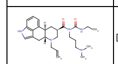
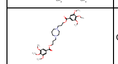
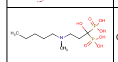
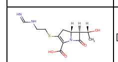
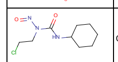
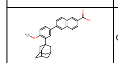
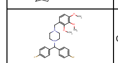
Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	[H][C@@]12C[C@H](O)[C@@]3(C)C(=O)[C@H](O)C4=C(C)[C@H](C[C@@](O)([C@@H](OC(=O)C5=CC=CC=C5)[C@]3([H])[C@@]1(CO2)OC(C)=O)C4(C)C)OC(=O)[C@H](O)[C@@H](NC(=O)OC(C)(C)C)C1=CC=CC=C1	(1S,2S,3R,4S,7R,9S,10S,12R,15S)-4-(acetyloxy)-15-{[(2R,3S)-3-{[(tert-butoxy)carbonyl]amino}-2-hydroxy-3-phenylpropanoyl]oxy}-1,9,12-trihydroxy-10,14,17,17-tetramethyl-11-oxo-6-oxatetracyclo[11.3.1.0^{3,10}.0^{4,7}]heptadec-13-en-2-yl benzoate	Docetaxil	807.9	2	FDA Approved Drug Library	114977-28-5	DL-250	2mg/ml	DMSO	2841J
	CN(C)CC\C=C1\C2=C(COC3=C1C=C(CC(O)=O)C=C3)C=CC=C2	2-[(2Z)-2-[3-(dimethylamino)propylidene]-9-oxatricyclo[9.4.0.0^{3,8}]pentadeca-1(11),3(8),4,6,12,14-hexaen-5-yl]acetic acid	Olopatadine	337.4	2	FDA Approved Drug Library	113806-05-6	DL-251	2mg/ml	DMSO	2841J
	COC(=O)C1=C(C)NC(C)=C(C1C1=CC=CC(=C1)[N+]([O-])=O)C(=O)OCCN1CCN(CC1)C(C1=CC=CC=C1)C1=CC=CC=C1	3-{2-[4-(diphenylmethyl)piperazin-1-yl]ethyl} 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate	Manidipine	610.7	2	FDA Approved Drug Library	120092-68-4	DL-258	2mg/ml	DMSO	2841J
	CC1=CC=C(C=C1)C(=O)C1=CC(O)=C(O)C(=C1)[N+]([O-])=O	5-[(4-methylphenyl)carbonyl]-3-nitrobenzene-1,2-diol	Tolcapone	273.2	2	FDA Approved Drug Library	134308-13-7	DL-252	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@@](O)(C#C)[C@@]1(CC)C=CC1=C3CCC(=O)C=C3CC[C@@]21[H]	(10S,11S,14R,15S)-15-ethyl-14-ethynyl-14-hydroxytetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadeca-1,6,16-trien-5-one	Gestrinone	308.4	2	FDA Approved Drug Library	16320-04-0	DL-253	2mg/ml	DMSO	2841J
	CCCC1=NC(=C(N1CC1=CC=C(C=C1)C1=CC=CC=C1C1=NN=NN1)C(=O)OCC1=C(C)OC(=O)O1)C(C)(C)O	(5-methyl-2-oxo-2H-1,3-dioxol-4-yl)methyl 4-(2-hydroxypropan-2-yl)-2-propyl-1-({4-[2-(1H-1,2,3,4-tetrazol-5-yl)phenyl]phenyl}methyl)-1H-imidazole-5-carboxylate	Olmesartan	558.6	2	FDA Approved Drug Library	144689-63-4	DL-254	2mg/ml	DMSO	2841J
	COC(=O)C1=C(C)NC(C)=C(C1C1=CC=CC=C1[N+]([O-])=O)C(=O)OCC(C)C	3-methyl 5-(2-methylpropyl) 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate	Nisoldipine	388.4	2	FDA Approved Drug Library	63675-72-9	DL-255	2mg/ml	DMSO	2841J
	CCOC(=O)C1=C(C)NC(C)=C(C1C1=CC=CC=C1\C=C\C(=O)OC(C)(C)C)C(=O)OCC	3,5-diethyl 4-{2-[(1E)-3-(tert-butoxy)-3-oxoprop-1-en-1-yl]phenyl}-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate	Lacidipine	455.5	2	FDA Approved Drug Library	103890-78-4	DL-256	2mg/ml	DMSO	2841J
	CN1CCN(CC1)C1=NC2=C(NC3=C1C=C(C)S3)C=CC=C2	5-methyl-8-(4-methylpiperazin-1-yl)-4-thia-2,9-diazatricyclo[8.4.0.0^{3,7}]tetradeca-1(10),3(7),5,8,11,13-hexaene	Olanzapine	312.4	2	FDA Approved Drug Library	132539-06-1	DL-257	2mg/ml	DMSO	2841J
	[H][C@]12[C@H](C[C@@H](C)C=C1C=C[C@H](C)[C@@H]2CC[C@@H]1C[C@@H](O)CC(=O)O1)OC(=O)[C@@H](C)CC	(1S,3R,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxooxan-2-yl]ethyl}-3,7-dimethyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl (2S)-2-methylbutanoate	Lovastatin	404.5	2	FDA Approved Drug Library	75330-75-5	G-226	2mg/ml	DMSO	2841J
	NC1=NC(N)=C(N=N1)C1=CC=CC(Cl)=C1Cl	6-(2,3-dichlorophenyl)-1,2,4-triazine-3,5-diamine	Lamotrigine	256.1	2	FDA Approved Drug Library	84057-84-1	NA-137	2mg/ml	DMSO	2841J
	CN1C=NC(=C1SC1=NC=NC2=C1NC=N2)[N+]([O-])=O	6-[(1-methyl-4-nitro-1H-imidazol-5-yl)sulfanyl]-7H-purine	Azathioprine	277.3	2	FDA Approved Drug Library	446-86-6	DL-572	2mg/ml	DMSO	2841J
			Blank		2	FDA Approved Drug Library			2mg/ml		2841J
	OC1=C([C@H]2CC[C@@H](CC2)C2=CC=C(Cl)C=C2)C(=O)C2=C(C=CC=C2)C1=O	2-[4-(4-chlorophenyl)cyclohexyl]-3-hydroxy-1,4-dihydronaphthalene-1,4-dione	Atovaquone	366.8	2	FDA Approved Drug Library	95233-18-4	DL-262	2mg/ml	DMSO	2841J
	ClC1=CC(Cl)=C(C=C1)C(CN1C=CN=C1)OCC1=CSC2=C1C=CC=C2Cl	1-{2-[(7-chloro-1-benzothiophen-3-yl)methoxy]-2-(2,4-dichlorophenyl)ethyl}-1H-imidazole	Sertaconazole	437.8	2	FDA Approved Drug Library	99592-32-2	DL-208	2mg/ml	DMSO	2841J
	CO\N=C(C(=O)N[C@H]1[C@H]2SCC(C[N+]3(C)CCCC3)=C(N2C1=O)C([O-])=O)\C1=CSC(N)=N1	1-{[(6R,7R)-7-[(2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-(methoxyimino)acetamido]-2-carboxylato-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl}-1-methylpyrrolidin-1-ium	Cefepime	480.6	2	FDA Approved Drug Library	88040-23-7	DL-191	2mg/ml	DMSO	2841J
	ClC1=C(Cl)C(=CC=C1)N1CCN(CCCCOC2=CC3=C(CCC(=O)N3)C=C2)CC1	7-{4-[4-(2,3-dichlorophenyl)piperazin-1-yl]butoxy}-1,2,3,4-tetrahydroquinolin-2-one	Aripiprazole	448.4	2	FDA Approved Drug Library	129722-12-9	DL-178	2mg/ml	DMSO	2841J
	CCOC1=NC2=C(N1CC1=CC=C(C=C1)C1=CC=CC=C1C1=NN=NN1)C(=CC=C2)C(O)=O	2-ethoxy-1-({4-[2-(1H-1,2,3,4-tetrazol-5-yl)phenyl]phenyl}methyl)-1H-1,3-benzodiazole-7-carboxylic acid	Candesartan	440.5	2	FDA Approved Drug Library	139481-59-7	DL-264	2mg/ml	DMSO	2841J
	CN(CC1=CC=C(C=C1)C(C)(C)C)CC1=CC=CC2=C1C=CC=C2	[(4-tert-butylphenyl)methyl](methyl)(naphthalen-1-ylmethyl)amine	Butenafine	317.5	2	FDA Approved Drug Library	101828-21-1	DL-101	2mg/ml	DMSO	2841J
	Cl.CCN[C@H]1C[C@H](C)S(=O)(=O)C2=C1C=C(S2)S(N)(=O)=O	(2S,4S)-4-(ethylamino)-2-methyl-1,1-dioxo-2H,3H,4H-1λ^{6},7-thieno[2,3-b][1λ^{6}]thiopyran-6-sulfonamide hydrochloride	Dorzolamide·HCl	360.9	2	FDA Approved Drug Library	120279-96-1	DL-200	2mg/ml	DMSO	2841J
	CN(C)CCC[C@]1(OCC2=CC(=CC=C12)C#N)C1=CC=C(F)C=C1	(1S)-1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-2-benzofuran-5-carbonitrile	Escitalopram	324.4	2	FDA Approved Drug Library	128196-01-0	DL-212	2mg/ml	DMSO	2841J
	CS(O)(=O)=O.CCCCC1=NC=C(\C=C(/CC2=CC=CS2)C(O)=O)N1CC1=CC=C(C=C1)C(O)=O	4-({2-butyl-5-[(1E)-2-carboxy-2-(thiophen-2-ylmethyl)eth-1-en-1-yl]-1H-imidazol-1-yl}methyl)benzoic acid; methanesulfonic acid	Eprosartan mesylate	520.6	2	FDA Approved Drug Library	144143-96-4	DL-209	2mg/ml	DMSO	2841J
	[Na+].[O-]C(=O)CC1=CC=CC=C1	sodium 2-phenylacetate	Sodium Phenylacetate	158.1	2	FDA Approved Drug Library	114-70-5	DL-119	2mg/ml	DMSO	2841J
	OC(=O)\C=C\C1=CC=C(CN2C=CN=C2)C=C1	(2E)-3-[4-(1H-imidazol-1-ylmethyl)phenyl]prop-2-enoic acid	Ozagrel	228.2	2	FDA Approved Drug Library	82571-53-7	EI-378	2mg/ml	DMSO	2841J
	CCN(CC)C(=O)C(\C#N)=C\C1=CC(=C(O)C(O)=C1)[N+]([O-])=O	(2E)-2-cyano-3-(3,4-dihydroxy-5-nitrophenyl)-N,N-diethylprop-2-enamide	Entacapone	305.3	2	FDA Approved Drug Library	130929-57-6	DL-217	2mg/ml	DMSO	2841J
	C[C@@H](O)[C@@H](NC(=O)[C@@H](C)[C@H](O)[C@@H](C)NC(=O)[C@H](NC(=O)C1=C(C)C(N)=NC(=N1)[C@H](CC(N)=O)NC[C@H](N)C(N)=O)[C@@H](O[C@@H]1O[C@@H](CO)[C@@H](O)[C@H](O)[C@@H]1O[C@@H]1O[C@H](CO)[C@@H](O)[C@@H](OC(N)=O)[C@@H]1O)C1=CNC=N1)C(=O)NCCC1=NC(=CS1)C1=NC=C(S1)C(=O)NCCC[S+](C)C	(3-{[2-(2-{2-[(2R,3R)-2-[(2S,3S,4R)-4-[(2R,3R)-2-({6-amino-2-[(1S)-1-{[(2S)-2-amino-2-carbamoylethyl]amino}-2-carbamoylethyl]-5-methylpyrimidin-4-yl}formamido)-3-{[(2R,3S,4S,5S,6S)-3-{[(2S,3S,4R,5R,6R)-4-(carbamoyloxy)-3,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-3-(1H-imidazol-4-yl)propanamido]-3-hydroxy-2-methylpentanamido]-3-hydroxybutanamido]ethyl}-1,3-thiazol-4-yl)-1,3-thiazol-5-yl]formamido}propyl)dimethylsulfanium	Bleomycin	1415.6	2	FDA Approved Drug Library	9041-93-4	AP-302	2mg/ml	DMSO	2841J
	CC1=CC2=C(OCC(CNC(C)(C)C)OC(=O)C3=CC=CC=C3)C=CC=C2N1	1-(tert-butylamino)-3-[(2-methyl-1H-indol-4-yl)oxy]propan-2-yl benzoate	Bopindolol	380.5	2	FDA Approved Drug Library	62658-64-4	AR-100	2mg/ml	DMSO	2841J
	Cl.NC(=N)NC(=O)CC1=C(Cl)C=CC=C1Cl	N-carbamimidoyl-2-(2,6-dichlorophenyl)acetamide hydrochloride	Guanfacine·HCl	282.6	2	FDA Approved Drug Library	29520-14-7	AR-102	2mg/ml	DMSO	2841J
	Cl.ClC1=C(NC2=NCCN2)C2=NSN=C2C=C1	5-chloro-N-(4,5-dihydro-1H-imidazol-2-yl)-2,1,3-benzothiadiazol-4-amine hydrochloride	Tizanidine·HCl	290.2	3	FDA Approved Drug Library	51322-75-9	AR-103	2mg/ml	DMSO	2841J
	CNC[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO	(2R,3R,4R,5S)-6-(methylamino)hexane-1,2,3,4,5-pentol	Meglumine	195.2	3	FDA Approved Drug Library	6284-40-8	DL-549	2mg/ml	DMSO	2841J
	CC(C)NC[C@H](O)COC1=C2C=CC=CC2=CC=C1	[(2S)-2-hydroxy-3-(naphthalen-1-yloxy)propyl](propan-2-yl)amine	Propranolol S(-)	259.3	3	FDA Approved Drug Library	4199-10-4	AR-107	2mg/ml	DMSO	2841J
	COC1=C(OCCNCC(O)COC2=CC=CC3=C2C2=C(N3)C=CC=C2)C=CC=C1	[3-(9H-carbazol-4-yloxy)-2-hydroxypropyl][2-(2-methoxyphenoxy)ethyl]amine	Carvedilol	406.5	3	FDA Approved Drug Library	72656-09-3	AR-112	2mg/ml	DMSO	2841J
	COCC1=C(N=C(C(C)C)C(\C=C\[C@@H](O)C[C@@H](O)CC(O)=O)=C1C1=CC=C(F)C=C1)C(C)C	(3R,5S,6E)-7-[4-(4-fluorophenyl)-5-(methoxymethyl)-2,6-bis(propan-2-yl)pyridin-3-yl]-3,5-dihydroxyhept-6-enoic acid	Cerivastatin	459.6	3	FDA Approved Drug Library	145599-86-6	DL-223	2mg/ml	DMSO	2841J

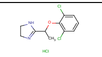
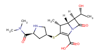
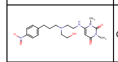
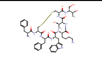
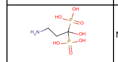
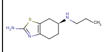
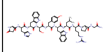
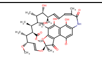
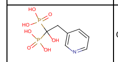
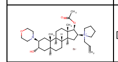
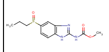
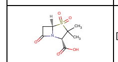
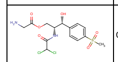
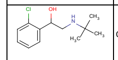
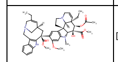
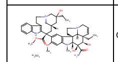
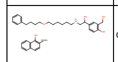
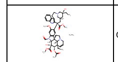
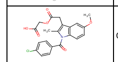
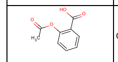
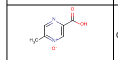
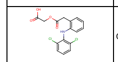
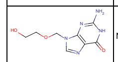
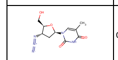
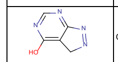
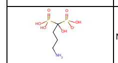
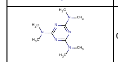
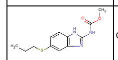
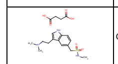
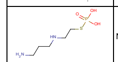
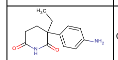
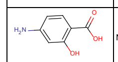
Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	CC[C@@]1(O)C[C@H](O[C@H]2C[C@@H]([C@H](O[C@H]3C[C@H](O)[C@H](O[C@H]4CCC(=O)[C@H](C)O4)[C@H](C)O3)[C@H](C)O2)N(C)C)C2=C(O)C3=C(C=C2[C@H]1C(=O)OC)C(=O)C1=C(C(O)=CC=C1)C3=O	methyl (1R,2R,4S)-4-{[(2R,4S,5S,6S)-4-(dimethylamino)-5-{[(2S,4S,5S,6S)-4-hydroxy-6-methyl-5-{[(2R,6S)-6-methyl-5-oxooxan-2-yl]oxy}oxan-2-yl]oxy}-6-methyloxan-2-yl]oxy}-2-ethyl-2,5,7-trihydroxy-6,11-dioxo-1,2,3,4,6,11-hexahydrotetracene-1-carboxylate	Aclarubicin	811.9	3	FDA Approved Drug Library	57576-44-0	AW-8655	2mg/ml	DMSO	2841J
	CCOC(=O)C1=C2CN(C)C(=O)C3=C(C=CC(F)=C3)N2C=N1	ethyl 12-fluoro-8-methyl-9-oxo-2,4,8-triazatricyclo[8.4.0.0^{2,6}]tetradeca-1(10),3,5,11,13-pentaene-5-carboxylate	Flumazenil	303.3	3	FDA Approved Drug Library	78755-81-4	B-100	2mg/ml	DMSO	2841J
	CC(/C=C/C1=C(C)CCCC1(C)C)=C\C=C\C(C)=C\C(=O)NC1=CC=C(O)C=C1	(2E,4E,6E,8E)-N-(4-hydroxyphenyl)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraenamide	Fenretinide	391.5	3	FDA Approved Drug Library	65646-68-6	GR-103	2mg/ml	DMSO	2841J
	COC1=CC2=C(C=C1OCCCN1CCOCC1)C(NC1=CC(Cl)=C(F)C=C1)=NC=N2	N-(3-chloro-4-fluorophenyl)-7-methoxy-6-[3-(morpholin-4-yl)propoxy]quinazolin-4-amine	Gefitinib	446.9	3	FDA Approved Drug Library	184475-35-2	DL-269	2mg/ml	DMSO	2841J
	CC(C)C(=O)C1=C2C=CC=CN2N=C1C(C)C	2-methyl-1-[2-(propan-2-yl)pyrazolo[1,5-a]pyridin-3-yl]propan-1-one	Ibudilast	230.3	3	FDA Approved Drug Library	50847-11-5	DL-270	2mg/ml	DMSO	2841J
	CN1CCN(CC2=CC=C(C=C2)C(=O)NC2=CC(NC3=NC(=CC=N3)C3=CN=CC=C3)=C(C)C=C2)CC1	N-(4-methyl-3-{[4-(pyridin-3-yl)pyrimidin-2-yl]amino}phenyl)-4-[(4-methylpiperazin-1-yl)methyl]benzamide	Imatinib	493.6	3	FDA Approved Drug Library	152459-95-5	DL-271	2mg/ml	DMSO	2841J
	[H][C@@]1(C[C@@](O)(CC2=C(O)C3=C(C(=O)C4=C(C=CC=C4)C3=O)C(O)=C12)C(C)=O)O[C@H]1C[C@H](N)[C@H](O)[C@H](C)O1	(7S,9S)-9-acetyl-7-{[(2R,4S,5S,6S)-4-amino-5-hydroxy-6-methyloxan-2-yl]oxy}-6,9,11-trihydroxy-5,7,8,9,10,12-hexahydrotetracene-5,12-dione	Idarubicin	497.5	3	FDA Approved Drug Library	58957-92-9	DL-548	2mg/ml	DMSO	2841J
	CC(C)(O)C1=CC=CC=C1CC[C@@H](SCC1(CC(O)=O)CC1)C1=CC=CC(\C=C\C2=NC3=C(C=CC(Cl)=C3)C=C2)=C1	2-[1-({[(1R)-1-{3-[(E)-2-(7-chloroquinolin-2-yl)ethenyl]phenyl}-3-[2-(2-hydroxypropan-2-yl)phenyl]propyl]sulfanyl}methyl)cyclopropyl]acetic acid	Montelukast	586.2	3	FDA Approved Drug Library	158966-92-8	DL-273	2mg/ml	DMSO	2841J
			Blank		3	FDA Approved Drug Library			2mg/ml		2841J
	ClC1=CC=C(NC2=NN=C(CC3=CC=NC=C3)C3=C2C=CC=C3)C=C1	N-(4-chlorophenyl)-4-(pyridin-4-ylmethyl)phthalazin-1-amine	Vatalanib	346.8	3	FDA Approved Drug Library	212141-54-3	DL-275	2mg/ml	DMSO	2841J
	[H][C@]1([C@H](OC)[C@@H](CC[C@]11CO1)OC(=O)\C=C\C=C\C=C\C=C\C(O)=O)[C@@]1(C)O[C@@H]1CC=C(C)C	(2E,4E,6E,8E)-10-{[(3R,4R,5S,6R)-5-methoxy-4-[(2R,3R)-2-methyl-3-(3-methylbut-2-en-1-yl)oxiran-2-yl]-1-oxaspiro[2.5]octan-6-yl]oxy}-10-oxodeca-2,4,6,8-tetraenoic acid	Fumagillin	458.5	3	FDA Approved Drug Library	23110-15-8	CT-100	2mg/ml	DMSO	2841J
	[H][C@@]12CCC(=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CC(=C)C2=CC(=O)C=C[C@]12C	(1S,2R,10R,11S,15S)-2,15-dimethyl-8-methylidenetetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadeca-3,6-diene-5,14-dione	Exemestane	296.4	3	FDA Approved Drug Library	107868-30-4	DL-573	2mg/ml	DMSO	2841J
	[H][C@]1(\C=C\[C@@H](O)CCCCC)[C@H](O)CC(=O)[C@]1([H])C\C=C/CCCC(O)=O	(5Z)-7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]hept-5-enoic acid	Dinoprostone	352.5	3	FDA Approved Drug Library	363-24-6	PG-007	2mg/ml	DMSO	2841J
	CN(C)C(=N)NC(N)=N	1-carbamimidamido-N,N-dimethylmethanimidamide	Metformin	129.2	3	FDA Approved Drug Library	657-24-9	DL-276	2mg/ml	DMSO	2841J
	ClC1=C(Cl)C2=C(C=C1)N=C1NC(=O)CN1C2	6,7-dichloro-1H,2H,3H,5H-imidazolidino[2,1-b]quinazolin-2-one	Anagrelide	256.1	3	FDA Approved Drug Library	68475-42-3	DL-277	2mg/ml	DMSO	2841J
	CN(CCOC1=CC=C(NS(C)(=O)=O)C=C1)CCC1=CC=C(NS(C)(=O)=O)C=C1	N-[4-(2-{[2-(4-methanesulfonamidophenoxy)ethyl](methyl)amino}ethyl)phenyl]methanesulfonamide	Dofetilide	441.6	3	FDA Approved Drug Library	115256-11-6	DL-278	2mg/ml	DMSO	2841J
	COCCOC1=CC2=C(C=C1OCCOC)C(NC1=CC(=CC=C1)C#C)=NC=N2	N-(3-ethynylphenyl)-6,7-bis(2-methoxyethoxy)quinazolin-4-amine	Erlotinib	393.4	3	FDA Approved Drug Library	183321-74-6	DL-279	2mg/ml	DMSO	2841J
	CN1[C@@H](C[C@H](O)C2=CC=CC=C2)CCC[C@H]1CC(=O)C1=CC=CC=C1	2-[(2S,6R)-6-[(2S)-2-hydroxy-2-phenylethyl]-1-methylpiperidin-2-yl]-1-phenylethan-1-one	Lobeline	337.5	3	FDA Approved Drug Library	90-69-7	AC-227	2mg/ml	DMSO	2841J
	COC1=CC2=C(NC=C2CCNC(C)=O)C=C1	N-[2-(5-methoxy-1H-indol-3-yl)ethyl]acetamide	Melatonin	232.3	3	FDA Approved Drug Library	73-31-4	NS-520	2mg/ml	DMSO	2841J
	CCCCC[C@H](O)\C=C\[C@H]1[C@H](O)C[C@H](O)[C@@H]1C\C=C/CCCC(O)=O	(5Z)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoic acid	Dinoprost	354.5	3	FDA Approved Drug Library	551-11-1	PG-008	2mg/ml	DMSO	2841J
	O=S(=O)(N1CCCNCC1)C1=C2C=CN=CC2=CC=C1	5-(1,4-diazepane-1-sulfonyl)isoquinoline	HA1077	291.4	3	FDA Approved Drug Library	103745-39-7	EI-233	2mg/ml	DMSO	2841J
	NC1=C2C(O)CCCC2=NC2=C1C=CC=C2	9-amino-1,2,3,4-tetrahydroacridin-1-ol	Hydroxytacrine	214.3	3	FDA Approved Drug Library	112964-99-5	C-106	2mg/ml	DMSO	2841J
	O=C1CCCN1CC#CCN1CCCC1	1-[4-(pyrrolidin-1-yl)but-2-yn-1-yl]pyrrolidin-2-one	Oxotremorine	206.3	3	FDA Approved Drug Library	17360-35-9	C-109	2mg/ml	DMSO	2841J
	NC1=C2CCCCC2=NC2=CC=CC=C12	1,2,3,4-tetrahydroacridin-9-amine	Tacrine	198.3	3	FDA Approved Drug Library	1684-40-8	C-110	2mg/ml	DMSO	2841J
	CC[N+](CC)(CC)CCOC1=CC=CC(OCC[N+](CC)(CC)CC)=C1OCC[N+](CC)(CC)CC	(2-{2,6-bis[2-(triethylazaniumyl)ethoxy]phenoxy}ethyl)triethylazanium	Gallamine	510.8	3	FDA Approved Drug Library	65-29-2	C-112	2mg/ml	DMSO	2841J
	COC1=CC=C2CN(C)CC[C@@]34C=C[C@H](O)C[C@@H]3OC1=C24	(1S,12S,14R)-9-methoxy-4-methyl-11-oxa-4-azatetracyclo[8.6.1.0^{1,12}.0^{6,17}]heptadeca-6,8,10(17),15-tetraen-14-ol	Galanthamine	287.4	3	FDA Approved Drug Library	1953-04-4	C-115	2mg/ml	DMSO	2841J
	NC(=N)NC(=O)C1=C(N)N=C(N)C(Cl)=N1	3,5-diamino-N-carbamimidoyl-6-chloropyrazine-2-carboxamide	Amiloride	229.6	3	FDA Approved Drug Library	2016-88-8	CA-200	2mg/ml	DMSO	2841J
	CCOC(=O)C1=C(COCCN)NC(C)=C(C1C1=CC=CC=C1Cl)C(=O)OC	3-ethyl 5-methyl 2-[(2-aminoethoxy)methyl]-4-(2-chlorophenyl)-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate	Amlodipine	408.9	3	FDA Approved Drug Library	88150-42-9	CA-202	2mg/ml	DMSO	2841J
	COC1=CC=C(C=C1)[C@@H]1SC2=C(C=CC=C2)N(CCN(C)C)C(=O)[C@@H]1OC(C)=O	(2S,3S)-5-[2-(dimethylamino)ethyl]-2-(4-methoxyphenyl)-4-oxo-2,3,4,5-tetrahydro-1,5-benzothiazepin-3-yl acetate	Diltiazem	414.5	3	FDA Approved Drug Library	33286-22-5	CA-205	2mg/ml	DMSO	2841J
	COC(=O)C1=C(C)NC(C)=C(C1C1=CC=CC=C1[N+]([O-])=O)C(=O)OC	3,5-dimethyl 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate	Nifedipine	346.3	3	FDA Approved Drug Library	21829-25-4	CA-210	2mg/ml	DMSO	2841J
	COCCOC(=O)C1=C(C)NC(C)=C(C1C1=CC(=CC=C1)[N+]([O-])=O)C(=O)OC(C)C	3-(2-methoxyethyl) 5-propan-2-yl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate	Nimodipine	418.4	3	FDA Approved Drug Library	66085-59-4	ALX-550-277	2mg/ml	DMSO	2841J
	CCOC(=O)C1=C(C)NC(C)=C(C1C1=CC=CC(=C1)[N+]([O-])=O)C(=O)OC	3-ethyl 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate	Nitrendipine	360.4	3	FDA Approved Drug Library	39562-70-4	ALX-550-278	2mg/ml	DMSO	2841J
	COC1=CC=C(CCN(C)CCCC(C#N)(C(C)C)C2=CC=C(OC)C(OC)=C2)C=C1OC	2-(3,4-dimethoxyphenyl)-5-{[2-(3,4-dimethoxyphenyl)ethyl](methyl)amino}-2-(propan-2-yl)pentanenitrile	Verapamil	454.6	3	FDA Approved Drug Library	23313-68-0	ALX-550-306	2mg/ml	DMSO	2841J

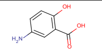
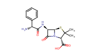
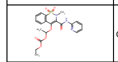
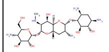
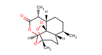
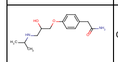
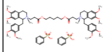
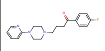
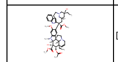
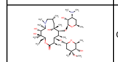
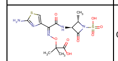
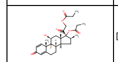
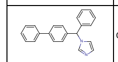
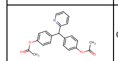
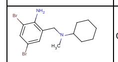
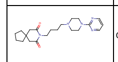
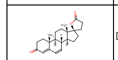
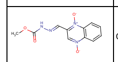
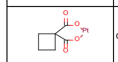
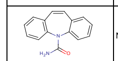
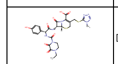
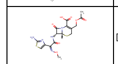
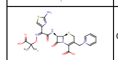
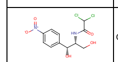
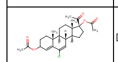
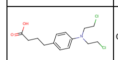
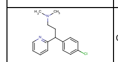
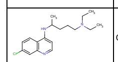
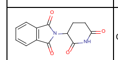
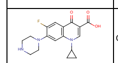
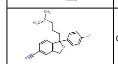
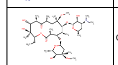
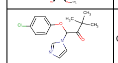
Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	COC(=O)C1=C(C)NC(C)=C(C1C1=CC=CC(=C1)[N+](O-])=O)C(=O)OCCCN1CCC(CC1)(C1=CC=CC=C1)C1=CC=CC=C1	3-[3-(4,4-diphenylpiperidin-1-yl)propyl] 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate	Nigulidpine	609.7	3	FDA Approved Drug Library	113317-61-6	CA-216	2mg/ml	DMSO	2841J
	Cl.Cl.FC1=CC=C(C=C1)C(N1CCN(C)C=C(C2=CC=CC=C2)CC1)C1=CC=C(F)C=C1	1-[bis(4-fluorophenyl)methyl]-4-[(2E)-3-phenylprop-2-en-1-yl]piperazine dihydrochloride	Flunarizine 2HCl	477.4	3	FDA Approved Drug Library	30484-77-6	CA-225	2mg/ml	DMSO	2841J
	NCC1(CC(O)=O)CCCCC1	2-[1-(aminomethyl)cyclohexyl]acetic acid	Gabapentin	171.2	3	FDA Approved Drug Library	60142-96-3	CA-234	2mg/ml	DMSO	2841J
	CCOC(=O)C1=C(C)NC(C)=C(C1C1=CC=CC(Cl)=C1Cl)C(=O)OC	3-ethyl 5-methyl 4-(2,3-dichlorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate	Felodipine	384.3	3	FDA Approved Drug Library	72509-76-3	CA-236	2mg/ml	DMSO	2841J
	COCCOC(=O)C1=C(C)NC(C)=C(C1C1=CC=CC(=C1)[N+](O-])=O)C(=O)OCIC=C1C1=CC=CC=C1	3-(2-methoxyethyl) 5-(2E)-3-phenylprop-2-en-1-yl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate	Cilnidipine	492.5	3	FDA Approved Drug Library	132203-70-4	CA-237	2mg/ml	DMSO	2841J
	Cl.CC(COC1=CC=CC=C1)N(CCCl)CC1=CC=CC=C1	benzyl(2-chloroethyl)(1-phenoxypropan-2-yl)amine hydrochloride	Phenoxybenzamine·HCl	340.0	3	FDA Approved Drug Library	63-92-3	CA-305	2mg/ml	DMSO	2841J
	Cl.Cl.CN1CCN(CCCN2C3=CC(=CC=C3SC3=C2C=CC=C3)C(F)(F)F)CC1	10-[3-(4-methylpiperazin-1-yl)propyl]-2-(trifluoromethyl)-10H-phenothiazine dihydrochloride	Trifluoperazine 2HCl	480.4	3	FDA Approved Drug Library	440-17-5	CA-310	2mg/ml	DMSO	2841J
	CCCCN1C2=C(N(CC(C)=O)C=N2)C(=O)N(CCCC)C1=O	1,3-dibutyl-7-(2-oxopropyl)-2,3,6,7-tetrahydro-1H-purine-2,6-dione	Denbufylline	320.4	3	FDA Approved Drug Library	57076-71-8	DL-218	2mg/ml	DMSO	2841J
	CCCCCCCCCCCCCCCOP([O-])(=O)OCC[N+](C)(C)C	hexadecyl 2-(trimethylazaniumyl)ethyl phosphate	Miltefosine	407.6	3	FDA Approved Drug Library	58066-85-6	DL-131	2mg/ml	DMSO	2841J
	CC(C)OC(=O)CCC/C=C/C[C@H]1[C@@H](O)C[C@@H](O)[C@@H]1CC[C@@H](O)CCC1=CC=CC=C1	propan-2-yl (5Z)-7-{(1R,2R,3R,5S)-3,5-dihydroxy-2-[(3R)-3-hydroxy-5-phenylpentyl]cyclopentyl}hept-5-enoate	Latanoprost	432.6	3	FDA Approved Drug Library	130209-82-4	DL-281	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@]3(O)C[C@H](C)C[C@@H](O)[C@]3(CO)[C@@]1([H])[C@H](O)C[C@]1(C)[C@H](CC[C@]21O)C1=CC(=O)OC1)O[C@@H]1O[C@@H](C)[C@H](O)[C@@H](O)[C@H]1O	4-[(1S,2R,3R,5S,7S,10R,11S,14R,15R,17R)-3,7,11,17-tetrahydroxy-2-(hydroxymethyl)-15-methyl-5-([(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy)tetracyclo[8.7.0.0^{1,7}.0^{11,15}]heptadecan-14-yl]-2,5-dihydrofuran-2-one	Ouabain	584.7	3	FDA Approved Drug Library	11018-89-6	CM-109	2mg/ml	DMSO	2841J
	C[C@H]1CCC[C@@H](C)N1NC(=O)C1=CC=C(C)C(=C1)S(N)(=O)=O	4-chloro-N-[(2R,6S)-2,6-dimethylpiperidin-1-yl]-3-sulfamoylbenzamide	Clopamide	345.8	3	FDA Approved Drug Library	636-54-4	CM-112	2mg/ml	DMSO	2841J
	COC(=O)N=C1O[N-][N+](=C/1)N1CCOCC1	5-[(ethoxycarbonyl)imino]-3-(morpholin-4-yl)-2,5-dihydro-1,2,3λ^{5}-oxadiazol-3-ylium-2-ide	Molsidomine	242.2	3	FDA Approved Drug Library	25717-80-0	CN-244	2mg/ml	DMSO	2841J
	COC1=CC=C(C=C1)C(=O)C1=C(C)N(CCN2CCOCC2)C2=C1C=CC=C2	3-[(4-methoxyphenyl)carbonyl]-2-methyl-1-[2-(morpholin-4-yl)ethyl]-1H-indole	Pravadoline	378.5	3	FDA Approved Drug Library	92623-83-1	CR-110	2mg/ml	DMSO	2841J
	COC1=CC=C(/C=C/C(=O)/NC2=C(C=CC=C2)C(O)=O)C=C1OC	2-[(2E)-3-(3,4-dimethoxyphenyl)prop-2-enamido]benzoic acid	Tranilast	327.3	3	FDA Approved Drug Library	53902-12-8	CT-110	2mg/ml	DMSO	2841J
	COC1=CC2=NC(=NC(N)=C2C=C1OC)N(C)CCCNC(=O)C1CCCO1	N-(3-[(4-amino-6,7-dimethoxyquinazolin-2-yl)(methyl)amino]propyl)oxolane-2-carboxamide	Alfuzosin	389.4	3	FDA Approved Drug Library	81403-80-7	DL-574	2mg/ml	DMSO	2841J
	[H][C@@]12CCCN1C(=O)[C@H](CC(C)C)N1C(=O)[C@@]N(C(=O)[C@H]3CN(C)C4CC5=C(Br)NC6=C5C(=CC=C6)C4=C3)(O[C@@]21O)C(C)C	(4R)-10-bromo-N-[(1S,2S,4R,7S)-2-hydroxy-7-(2-methylpropyl)-5,8-dioxo-4-(propan-2-yl)-3-oxa-6,9-diazatricyclo[7.3.0.0^{2,6}]dodecan-4-yl]-6-methyl-6,11-diazatetracyclo[7.6.1.0^{4,7}.0^{12,16}]hexadeca-1(15),2,9,12(16),13-pentaene-4-carboxamide	Bromocriptine	654.6	3	FDA Approved Drug Library	22260-51-1	D-102	2mg/ml	DMSO	2841J
	CN1CCN(CC1)C1=NC2=C(NC3=C1C=CC=C3)C=CC(Cl)=C2	6-chloro-10-(4-methylpiperazin-1-yl)-2,9-diazatricyclo[9.4.0.0^{3,8}]pentadeca-1(11),3(8),4,6,9,12,14-heptaene	Clozapine	326.8	3	FDA Approved Drug Library	5786-21-0	D-107	2mg/ml	DMSO	2841J
	CN1CCN(CC1)C1=NC2=C(SC3=C1C=C(Cl)C=C3)C=CC=C2	13-chloro-10-(4-methylpiperazin-1-yl)-2-thia-9-azatricyclo[9.4.0.0^{3,8}]pentadeca-1(11),3(8),4,6,9,12,14-heptaene	Clothiapine	343.9	3	FDA Approved Drug Library	2058-52-8	D-108	2mg/ml	DMSO	2841J
	COC1=CC(C)=C(/C=C/C(/C)=C/C=C/C(/C)=C/C(O)=O)C(C)=C1C	(2E,4E,6E,8E)-9-(4-methoxy-2,3,6-trimethylphenyl)-3,7-dimethylnona-2,4,6,8-tetraenoic acid	Acitretin	326.4	3	FDA Approved Drug Library	55079-83-9	DL-575	2mg/ml	DMSO	2841J
	CCN1CCC[C@H]1CNC(=O)C1=C(OC)C=CC(Br)=C1OC	3-bromo-N-[(2S)-1-ethylpyrrolidin-2-yl]methyl]-2,6-dimethoxybenzamide	Remoxipride	371.3	3	FDA Approved Drug Library	73220-03-8	D-111	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@H](C[C@H](C)CCCC(C)C)O)[C@@]1(C)CCC/C2=C/C=C1/C[C@@H](O)CC[C@H](O)CCC1=C	(1S,3Z)-3-[(2-[(1R,3aS,4E,7aR)-1-[(2R)-6-hydroxy-6-methylheptan-2-yl]-7a-methyl-octahydro-1H-inden-4-ylidene]ethylidene)-4-methylidenecyclohexan-1-ol	Calcifediol	400.6	3	FDA Approved Drug Library	19356-17-3	DM-100	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@H](C[C@H](C)CCCC(C)C)O)[C@@]1(C)CCC/C2=C/C=C1/C[C@@H](O)C[C@H](O)C1=C	(1R,3S,5Z)-5-(2-[(1R,3aS,4E,7aR)-1-[(2R)-6-hydroxy-6-methylheptan-2-yl]-7a-methyl-octahydro-1H-inden-4-ylidene]ethylidene)-4-methylidenecyclohexane-1,3-diol	Calcitriol	416.6	3	FDA Approved Drug Library	32222-06-3	DM-200	2mg/ml	DMSO	2841J
	CC(=O)N1CCN(CC1)C1=CC=C(OC[C@H]2CO[C@@](CN3C=CN=C3)(O2)C2=CC=C(Cl)C=C2Cl)C=C1	1-[4-(4-[[(2R,4S)-2-(2,4-dichlorophenyl)-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl)piperazin-1-yl]ethan-1-one	Ketoconazole	531.4	3	FDA Approved Drug Library	65277-42-1	EI-107	2mg/ml	DMSO	2841J
	O=C1NC2=C(C=CC=C2)N1CCCN1CCN(CC1)C(C1=CC=CC=C1)C1=CC=CC=C1	1-[3-[4-(diphenylmethyl)piperazin-1-yl]propyl]-2,3-dihydro-1H-1,3-benzodiazol-2-one	Oxatomide	426.6	3	FDA Approved Drug Library	60607-34-3	EI-114	2mg/ml	DMSO	2841J
	[Na+].[Na+].OC(COC1=CC=CC2=C1C(=O)C=C(O2)C([O-])=O)COC1=CC=CC2=C1C(=O)C=C(O2)C([O-])=O	disodium 5-[3-[(2-carboxylato-4-oxo-4H-chromen-5-yl)oxy]-2-hydroxypropoxy]-4-oxo-4H-chromene-2-carboxylate	Disodium Cromoglycate	512.3	3	FDA Approved Drug Library	15826-37-6	EI-121	2mg/ml	DMSO	2841J
	COC1=C(O)C=CC(CNC(=O)CCCC/C=C\C(C)C)=C1	(6E)-N-[(4-hydroxy-3-methoxyphenyl)methyl]-8-methylnon-6-enamide	Capsaicin	305.4	3	FDA Approved Drug Library	404-86-4	EI-125	2mg/ml	DMSO	2841J
	[H][C@@]12C[C@@H](C)[C@@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]1(F)[C@@]2([H])CCC2=CC(=O)C=C[C@]12C	(1R,2S,10S,11S,13R,14R,15S,17S)-1-fluoro-14,17-dihydroxy-14-(2-hydroxyacetyl)-2,13,15-trimethyltetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadeca-3,6-dien-5-one	Dexamethasone	392.5	3	FDA Approved Drug Library	50-02-2	EI-126	2mg/ml	DMSO	2841J
	OCCN(CCO)C1=NC(N2CCCCC2)=C2N=C(N=C(N3CCCCC3)C2=N1)N(CCO)CCO	2-({6-[bis(2-hydroxyethyl)amino]-4,8-bis(piperidin-1-yl)pyrimido[5,4-d][1,3]diazin-2-yl}(2-hydroxyethyl)amino)ethan-1-ol	Dipyridamole	504.6	3	FDA Approved Drug Library	58-32-2	EI-127	2mg/ml	DMSO	2841J
	CCC(=C)C(=O)C1=C(Cl)C(Cl)=C(OCC(O)=O)C=C1	2-[2,3-dichloro-4-(2-methylidenebutanoyl)phenoxy]acetic acid	Ethacrynic Acid	303.1	3	FDA Approved Drug Library	58-54-8	EI-128	2mg/ml	DMSO	2841J
	COC1=CC2=C(C=C1)N(C(=O)C1=CC=C(Cl)C=C1)C(=C2CC(O)=O	2-[1-[(4-chlorophenyl)carbonyl]-5-methoxy-2-methyl-1H-indol-3-yl]acetic acid	Indomethacin	357.8	3	FDA Approved Drug Library	53-86-1	EI-131	2mg/ml	DMSO	2841J
	COC1=CC2=CC=C(C=C2C=C1)[C@H](C)C(O)=O	(2S)-2-(6-methoxynaphthalen-2-yl)propanoic acid	Naproxen	230.3	3	FDA Approved Drug Library	22204-53-1	EI-133	2mg/ml	DMSO	2841J
	CCOC(=O)C(C)(C)OC1=CC=C(Cl)C=C1	ethyl 2-(4-chlorophenoxy)-2-methylpropanoate	Clofibrate	242.7	3	FDA Approved Drug Library	637-07-0	EI-160	2mg/ml	DMSO	2841J

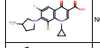
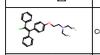
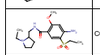
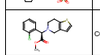
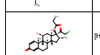
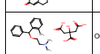
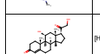
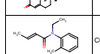
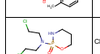
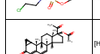
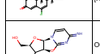
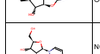
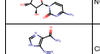
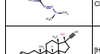
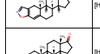
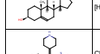
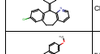
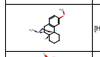
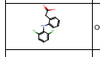
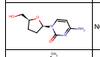
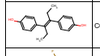
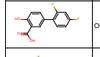
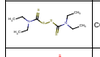
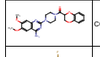
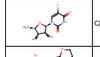
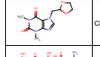
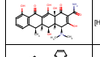
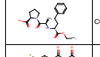
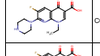
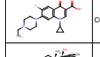
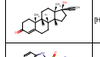
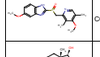
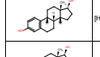
Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	CC(C)CC1=CC=C(C=C1)C(C)C(O)=O	2-[4-(2-methylpropyl)phenyl]propanoic acid	Ibuprofen	206.3	3	FDA Approved Drug Library	15687-27-1	EI-164	2mg/ml	DMSO	2841J
	NC(CO)C(=O)NNCC1=C(O)C(O)=C(O)C=C1	2-amino-3-hydroxy-N'-[(2,3,4-trihydroxyphenyl)methyl]propanehydrazide	Benserazide	257.2	3	FDA Approved Drug Library	322-35-0	EI-165	2mg/ml	DMSO	2841J
	NC(=N)N1CCC2=C(C1)C=CC=C2	1,2,3,4-tetrahydroisoquinoline-2-carboximidamide	Debrisoquin	175.2	3	FDA Approved Drug Library	581-88-4	EI-166	2mg/ml	DMSO	2841J
	CC(=O)NC1=CC=C(CC(O)=O)C=C1	2-(4-acetamidophenyl)acetic acid	Actarit	193.2	3	FDA Approved Drug Library	18699-02-0	DL-576	2mg/ml	DMSO	2841J
	CCCCNC1=C(OC2=CC=CC=C2)C(=CC(=C1)C(O)=O)S(N)(=O)=O	3-(butylamino)-4-phenoxy-5-sulfamoylbenzoic acid	Bumetanide	364.4	3	FDA Approved Drug Library	28395-03-1	EI-168	2mg/ml	DMSO	2841J
	NC[C@@H]1O[C@H](O[C@@H]2[C@@H](CO)O[C@@H](O[C@@H]3[C@@H](O)[C@H](N)C[C@H](N)[C@H]3O[C@H]3O[C@H](CN)[C@@H](O)[C@H](O)[C@H]3N)[C@@H]2O)[C@H](N)[C@@H](O)[C@@H]1O	(2S,3S,4R,5R,6R)-5-amino-2-(aminomethyl)-6-{[(2R,3S,4R,5S)-5-{[(1R,2R,3S,5R,6S)-3,5-diamino-2-{[(2R,3R,4R,5S,6R)-3-amino-6-(aminomethyl)-4,5-dihydroxyoxan-2-yl]oxy}-6-hydroxycyclohexyl]oxy}-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl]oxy}oxane-3,4-diol	Neomycin	614.6	3	FDA Approved Drug Library	1405-10-3	EI-180	2mg/ml	DMSO	2841J
	CCP(CC)(CC)=[Au]S[C@@H]1O[C@H](COC(C)=O)[C@@H](OC(C)=O)[C@H](OC(C)=O)[C@H]1OC(C)=O	[(2R,3R,4S,5R,6S)-3,4,5-tris(acetyloxy)-6-{[(triethylλ^5-phosphanylidene)aurio]sulfanyl}oxan-2-yl]methyl acetate	Auranofin	678.5	3	FDA Approved Drug Library	34031-32-8	EI-206	2mg/ml	DMSO	2841J
	C[C@H](CS)C(=O)N1CCC[C@H]1C(O)=O	(2S)-1-[(2S)-2-methyl-3-sulfanylpropanoyl]pyrrolidine-2-carboxylic acid	Captopril	217.3	3	FDA Approved Drug Library	62571-86-2	EI-213	2mg/ml	DMSO	2841J
	CC1=C(C)C(=O)C(CCCCC#CCCCC#CCO)=C(C)C1=O	2-(12-hydroxydodeca-5,10-diyn-1-yl)-3,5,6-trimethylcyclohexa-2,5-diene-1,4-dione	Docebenone	326.4	3	FDA Approved Drug Library	80809-81-0	EI-216	2mg/ml	DMSO	2841J
	N[C@H]1C[C@@H]1C1=CC=CC=C1	(1S,2R)-2-phenylcyclopropan-1-amine	Tranylcypromine	133.2	4	FDA Approved Drug Library	1986-47-6	EI-217	2mg/ml	DMSO	2841J
	CN1C(C(=O)NC2=NC=CC=C2)=C(O)C2=C(C=CC=C2)S1(=O)=O	4-hydroxy-2-methyl-1,1-dioxo-N-(pyridin-2-yl)-2H-1λ^6,2-benzothiazine-3-carboxamide	Piroxicam	331.3	4	FDA Approved Drug Library	36322-90-4	EI-219	2mg/ml	DMSO	2841J
	Cl.[H][C@]12CN(C[C@@]1([H])NCCC2)C1=C(F)C=C2C(=O)C(=CN(C3CC3)C2=C1OC)C(O)=O	7-[(4aS,7aS)-octahydro-1H-pyrrolo[3,4-b]pyridin-6-yl]-1-cyclopropyl-6-fluoro-8-methoxy-4-oxo-1,4-dihydroquinoline-3-carboxylic acid hydrochloride	Moxifloxacin·HCl	437.9	4	FDA Approved Drug Library	151096-09-2	DL-577	2mg/ml	DMSO	2841J
	CO[C@H]1C[C@H](O[C@H]2[C@H](C)[C@@H](O[C@@H]3O[C@H](C)C[C@@H]([C@H]3OC(C)=O)N(C)C)[C@@H](C)C[C@@]3(CO3)C(=O)[C@H](C)[C@@H](OC(C)=O)[C@@H](C)[C@@H](C)OC(=O)[C@@H]2C)O[C@@H](C)[C@@H]1OC(C)=O	(3R,5R,6S,7S,8R,11R,12S,13R,14S,15S)-14-{[(2S,3R,4S,6R)-3-(acetyloxy)-4-(dimethylamino)-6-methyloxan-2-yl]oxy}-12-{[(2R,4S,5S,6S)-5-(acetyloxy)-4-methoxy-6-methyloxan-2-yl]oxy}-5,7,8,11,13,15-hexamethyl-4,10-dioxo-1,9-dioxaspiro[2.13]hexadecan-6-yl acetate	Troleandomycin	814.0	4	FDA Approved Drug Library	2751-09-9	EI-249	2mg/ml	DMSO	2841J
	O.C[C@@](CC1=CC(O)=C(O)C=C1)(NN)C(O)=O	(2S)-3-(3,4-dihydroxyphenyl)-2-hydrazinyl-2-methylpropanoic acid hydrate	Carbidopa·H_2O	244.2	4	FDA Approved Drug Library	38821-49-7	EI-265	2mg/ml	DMSO	2841J
	CS(=O)(=O)NC1=C(OC2=CC=CC=C2)C=C(C=C1)[N+]([O-])=O	N-(4-nitro-2-phenoxyphenyl)methanesulfonamide	Nimesulide	308.3	4	FDA Approved Drug Library	51803-78-2	EI-287	2mg/ml	DMSO	2841J
	CC(C(O)=O)C1=CC(=CC=C1)C(=O)C1=CC=CC=C1	2-(3-benzoylphenyl)propanoic acid	Ketoprofen	254.3	4	FDA Approved Drug Library	22071-15-4	EI-288	2mg/ml	DMSO	2841J
	CN1C(C(=O)NC2=NC=C(C)S2)=C(O)C2=C(C=CC=C2)S1(=O)=O	4-hydroxy-2-methyl-N-(5-methyl-1,3-thiazol-2-yl)-1,1-dioxo-2H-1λ^6,2-benzothiazine-3-carboxamide	Meloxicam	351.4	4	FDA Approved Drug Library	71125-38-7	EI-292	2mg/ml	DMSO	2841J
	CN(C\C=C\C#CC(C)(C)C)CC1=C2C=CC=CC2=CC=C1	[(2E)-6,6-dimethylhept-2-en-4-yn-1-yl](methyl)(naphthalen-1-ylmethyl)amine	Terbinafine	291.4	4	FDA Approved Drug Library	91161-71-6	EI-318	2mg/ml	DMSO	2841J
	[Na+].[O-]C(=O)CCCC1=CC=CC=C1	sodium 4-phenylbutanoate	Sodium Phenylbutyrate	186.2	4	FDA Approved Drug Library	1716-12-7	EI-320	2mg/ml	DMSO	2841J
	C[N+](C)(C)[C@@H](CC1=CNC(S)=N1)C([O-])=O	(2S)-3-(2-sulfanyl-1H-imidazol-4-yl)-2-(trimethylazaniumyl)propanoate	Ergothioneine	229.3	4	FDA Approved Drug Library	497-30-3	FR-111	2mg/ml	DMSO	2841J
	NC1=C(Br)C=C(Br)C=C1CN[C@H]1CC[C@H](O)CC1	4-{[(2-amino-3,5-dibromophenyl)methyl]amino}cyclohexan-1-ol	Ambroxol	378.1	4	FDA Approved Drug Library	18683-91-5	FR-112	2mg/ml	DMSO	2841J
	COC1=C(OC)C(=O)C(CCCCCCCCCCO)=C(C)C1=O	2-(10-hydroxydecyl)-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione	Idebenone	338.4	4	FDA Approved Drug Library	58186-27-9	FR-114	2mg/ml	DMSO	2841J
	[H][C@]12[C@H](CCC=C1C=C[C@H](C)[C@@H]2CC[C@@H]1C[C@@H](O)CC(=O)O1)OC(=O)[C@@H](C)CC	(1S,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxooxan-2-yl]ethyl}-7-methyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl (2S)-2-methylbutanoate	Mevastatin	390.5	4	FDA Approved Drug Library	73573-88-3	G-233	2mg/ml	DMSO	2841J
	[H][C@]12[C@H](C[C@@H](C)C=C1C=C[C@H](C)[C@@H]2CC[C@@H]1C[C@@H](O)CC(=O)O1)OC(=O)C(C)(C)CC	(1S,3R,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxooxan-2-yl]ethyl}-3,7-dimethyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl 2,2-dimethylbutanoate	Simvastatin	418.6	4	FDA Approved Drug Library	79902-63-9	G-244	2mg/ml	DMSO	2841J
	CC1=C(NC(=O)C2=CC=CC(NC(=O)NC3=CC=CC(=C3)C(=O)NC3=C(C)C=CC(=C3)C(=O)NC3=CC=C(C4=C3C(=CC(=C4)S([O-])(=O)=O)S([O-])(=O)=O)S([O-])(=O)=O)=C2)C=C(C=C1)C(=O)NC1=CC=C(C2=C1C(=CC(=C2)S([O-])(=O)=O)S([O-])(=O)=O)S([O-])(=O)=O	8-[(4-methyl-3-{[3-({[3-({2-methyl-5-[(4,6,8-trisulfonatonaphthalen-1-yl)carbamoyl]phenyl}carbamoyl)phenyl]carbamoyl}amino)benzene]amido}benzene)amido]naphthalene-1,3,5-trisulfonate	Suramin	1291.2	4	FDA Approved Drug Library	129-46-4	G-430	2mg/ml	DMSO	2841J
	CC(C)C[C@H](NC(=O)[C@@H](COC(C)(C)C)NC(=O)[C@H](CC1=CC=C(O)C=C1)NC(=O)[C@H](CO)NC(=O)[C@H](CC1=CNC2=C1C=CC=C2)NC(=O)[C@H](CC1=CNC=N1)NC(=O)[C@@H]1CCC(=O)N1)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N1CCC[C@H]1C(=O)NNC(N)=O	(2S)-1-[(2S)-2-[(2S)-2-[(2R)-3-(tert-butoxy)-2-[(2S)-2-[(2S)-3-hydroxy-2-[(2S)-2-[(2S)-3-(1H-imidazol-4-yl)-2-{[(2S)-5-oxopyrrolidin-2-yl]formamido}propanamido]-3-(1H-indol-3-yl)propanamido]propanamido]-3-(4-hydroxyphenyl)propanamido]propanamido]-4-methylpentanamido]-5-carbamimidamidopentanoyl]-N-(carbamoylamino)pyrrolidine-2-carboxamide	Goserelin	1269.4	4	FDA Approved Drug Library	145781-92-6	DL-282	2mg/ml	DMSO	2841J
	COC1=C(O)C=CC=C1	2-methoxyphenol	Guaiacol	124.1	4	FDA Approved Drug Library	90-05-1	DL-283	2mg/ml	DMSO	2841J
	CC(/C=C/C1=C(C)CCCC1(C)C)=C\C=C\C(C)=C\C(O)=O	(2E,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraenoic acid	Retinoic Acid	300.4	4	FDA Approved Drug Library	302-79-4	GR-100	2mg/ml	DMSO	2841J
	CC1=C(C)C2=C(CCC(C)(COC3=CC=C(CC4SC(=O)NC4=O)C=C3)O2)C(C)=C1O	5-({4-[(6-hydroxy-2,5,7,8-tetramethyl-3,4-dihydro-2H-1-benzopyran-2-yl)methoxy]phenyl}methyl)-1,3-thiazolidine-2,4-dione	Troglitazone	441.5	4	FDA Approved Drug Library	97322-87-7	GR-210	2mg/ml	DMSO	2841J
	CC(C)(OC1=CC=C(CCNC(=O)C2=CC=C(Cl)C=C2)C=C1)C(O)=O	2-(4-{2-[(4-chlorophenyl)formamido]ethyl}phenoxy)-2-methylpropanoic acid	Bezafibrate	361.8	4	FDA Approved Drug Library	41859-67-0	GR-211	2mg/ml	DMSO	2841J
	OC1=CC=C(C=C1)C1=C(C(=O)C2=CC=C(OCCN3CCCCC3)C=C2)C2=C(S1)C=C(O)C=C2	2-(4-hydroxyphenyl)-3-({4-[2-(piperidin-1-yl)ethoxy]phenyl}carbonyl)-1-benzothiophen-6-ol	Raloxifene	473.6	4	FDA Approved Drug Library	82640-04-8	GR-243	2mg/ml	DMSO	2841J
	CC[C@@]1(O)C(=O)OCC2=C1C=C1N(CC3=CC4=C(C=CC=C4)N=C13)C2=O	(19S)-19-ethyl-19-hydroxy-17-oxa-3,13-diazapentacyclo[11.8.0.0^{2,11}.0^{4,9}.0^{15,20}]henicosa-1(21),2,4(9),5,7,10,15(20)-heptaene-14,18-dione	Camptothecin	348.4	4	FDA Approved Drug Library	7689-03-4	GR-301	2mg/ml	DMSO	2841J
	[H][C@]1(CC2=C(C(=O)[C@H]1O[C@H]1C[C@@H](O[C@H]3C[C@@H](O[C@H]4C[C@](C)(O)[C@H](O)[C@@H](C)O4)[C@H](O)[C@@H](C)O3)[C@H](O)[C@@H](C)O1)C(O)=C1C(C=C(O[C@H]3C[C@@H](O[C@H]4C[C@@H](O)[C@H](O)[C@@H](C)O4)[C@@H](O)[C@@H](C)O3)C(C)=C1O)=C2)[C@H](OC)C(=O)[C@@H](O)[C@@H](C)O	(2S,3S)-3-[(1S,3S,4R)-3,4-dihydroxy-1-methoxy-2-oxopentyl]-2-{[(2S,4R,5R,6R)-4-{[(2S,4R,5R,6R)-4-{[(2S,4S,5R,6R)-4,5-dihydroxy-4,6-dimethyloxan-2-yl]oxy}-5-hydroxy-6-methyloxan-2-yl]oxy}-5-hydroxy-6-methyloxan-2-yl]oxy}-6-{[(2S,4R,5S,6R)-4-{[(2S,4R,5S,6R)-4,5-dihydroxy-6-methyloxan-2-yl]oxy}-5-hydroxy-6-methyloxan-2-yl]oxy}-8,9-dihydroxy-7-methyl-1,2,3,4-tetrahydroanthracen-1-one	Plicamycin	1085.1	4	FDA Approved Drug Library	18378-89-7	GR-305	2mg/ml	DMSO	2841J

Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	CO[C@H]1\C=C\O[C@@]2(C)OC3=C(C2=O)C2=C(O)C(\C=N\N4CCN(C)CC4)=C(NC(=O)\C(C)=C/C=C/[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@@H]1C)C(O)=C2C(O)=C3C	(7S,9E,11S,12R,13S,14R,15R,16R,17S,18S,19E,21Z)-2,15,17,27,29-pentahydroxy-11-methoxy-3,7,12,14,16,18,22-heptamethyl-26-[(E)-N-(4-methylpiperazin-1-yl)carboximidoyl]-6,23-dioxo-8,30-dioxa-24-azatetracyclo[23.3.1.$1^{4,7}$.$0^{5,28}$]triaconta-1(29),2,4,9,19,21,25,27-octaen-13-yl acetate	Rifampicin	822.9	4	FDA Approved Drug Library	38776-75-9	GR-306	2mg/ml	DMSO	2841J
	[H][C@]12COC(=O)[C@]1([H])[C@H](C1=CC(OC)=C(O)C(OC)=C1)C1=C(C=C3OCOC3=C1)[C@H]2O[C@@H]1O[C@@H]2CO[C@@H](C)O[C@H]2[C@H](O)[C@H]1O	(10R,11R,15R,16S)-16-{[(2R,4aR,6R,7R,8R,8aS)-7,8-dihydroxy-2-methyl-hexahydro-2H-pyrano[3,2-d][1,3]dioxin-6-yl]oxy}-10-(4-hydroxy-3,5-dimethoxyphenyl)-4,6,13-trioxatetracyclo[7.7.0.$0^{3,7}$.$0^{11,15}$]hexadeca-1(9),2,7-trien-12-one	Etoposide	588.6	4	FDA Approved Drug Library	33419-42-0	GR-307	2mg/ml	DMSO	2841J
	[H][C@]12CN3C4=C([C@@H](COC(N)=O)[C@@]3(OC)[C@@]1([H])N2)C(=O)C(N)=C(C)C4=O	[(4S,6S,7R,8S)-11-amino-7-methoxy-12-methyl-10,13-dioxo-2,5-diazatetracyclo[7.4.0.$0^{2,7}$.$0^{4,6}$]trideca-1(9),11-dien-8-yl]methyl carbamate	Mitomycin C	334.3	4	FDA Approved Drug Library	50-07-7	GR-311	2mg/ml	DMSO	2841J
	COC1=CC=C(C[C@H](N)C(=O)N[C@@H]2[C@@H](CO)O[C@H]([C@@H]2O)N2C=NC3=C2N=CN=C3N(C)C)C=C1	(2S)-2-amino-N-[(2S,3S,4R,5R)-5-[6-(dimethylamino)-9H-purin-9-yl]-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl]-3-(4-methoxyphenyl)propanamide	Puromycin	471.5	4	FDA Approved Drug Library	58-58-2	GR-312	2mg/ml	DMSO	2841J
	CS(O)(=O)=O.CC(C)NC1=CC=CN=C1N1CCN(CC1)C(=O)C1=CC2=C(N1)C=CC(NS(C)(=O)=O)=C2	N-{2-[(4-{3-[(propan-2-yl)amino]pyridin-2-yl}piperazin-1-yl)carbonyl]-1H-indol-5-yl}methanesulfonamide; methanesulfonic acid	Delavirdine mesylate	552.7	4	FDA Approved Drug Library	147221-93-0	GR-314	2mg/ml	DMSO	2841J
	CC[C@@]1(O)C(=O)OCC2=C1C=C1N(CC3=CC4=C(C=CC=C4O)N=C13)C2=O	(19S)-19-ethyl-8,19-dihydroxy-17-oxa-3,13-diazapentacyclo[11.8.0.$0^{2,11}$.$0^{4,9}$.$0^{15,20}$]henicosa-1(21),2,4(9),5,7,10,15(20)-heptaene-14,18-dione	10-Hydroxycamptothecin	364.4	4	FDA Approved Drug Library	64439-81-2	GR-316	2mg/ml	DMSO	2841J
	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(C)=O)C(O)=C1C2=O	(8S,10S)-8-acetyl-10-{[(2R,4S,5S,6S)-4-amino-5-hydroxy-6-methyloxan-2-yl]oxy}-6,8,11-trihydroxy-1-methoxy-5,7,8,9,10,12-hexahydrotetracene-5,12-dione	Daunorubicin	527.5	4	FDA Approved Drug Library	23541-50-6	GR-318	2mg/ml	DMSO	2841J
	Cl.COC1=CC=CC2=C1C(=O)C1=C(C2=O)C(O)=C2C[C@](O)(C[C@H](O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C2=C1O)C(=O)CO	(8S,10S)-10-{[(2R,4S,5S,6S)-4-amino-5-hydroxy-6-methyloxan-2-yl]oxy}-6,8,11-trihydroxy-8-(2-hydroxyacetyl)-1-methoxy-5,7,8,9,10,12-hexahydrotetracene-5,12-dione hydrochloride	Doxorubicin·HCl	580.0	4	FDA Approved Drug Library	25316-40-9	GR-319	2mg/ml	DMSO	2841J
	Cl.Cl.OC(=O)COCCN1CCN(CC1)C(C1=CC=CC=C1)C1=CC=C(Cl)C=C1	2-(2-{4-[(4-chlorophenyl)(phenyl)methyl]piperazin-1-yl}ethoxy)acetic acid dihydrochloride	Cetirizine 2HCl	461.8	4	FDA Approved Drug Library	83881-52-1	DL-578	2mg/ml	DMSO	2841J
	CC1=CC=C(C=C1)S(O)(=O)=O.CC1=CC=C(C=C1)S(O)(=O)=O.CS(=O)(=O)CCNCC1=CC=C(O1)C1=CC2=C(C=C1)N=CN=C2NC1=CC(Cl)=C(OCC2=CC=CC(F)=C2)C=C1	bis(4-methylbenzene-1-sulfonic acid); N-{3-chloro-4-[(3-fluorophenyl)methoxy]phenyl}-6-(5-{[(2-methanesulfonylethyl)amino]methyl}furan-2-yl)quinazolin-4-amine	Lapatinib ditosylate	925.5	4	FDA Approved Drug Library	388082-78-8	DL-284	2mg/ml	DMSO	2841J
	COC(=O)C1=C(O)C=CC=C1	methyl 2-hydroxybenzoate	Methyl salicylate	152.1	4	FDA Approved Drug Library	119-36-8	DL-285	2mg/ml	DMSO	2841J
	CCC1=CC=C(CCOC2=CC=C(CC3SC(=O)NC3=O)C=C2)N=C1	5-({4-[2-(5-ethylpyridin-2-yl)ethoxy]phenyl}methyl)-1,3-thiazolidine-2,4-dione	Pioglitazone	356.4	4	FDA Approved Drug Library	112529-15-4	GR-240	2mg/ml	DMSO	2841J
	O=C(NC1=CC=CC2=C1OC(=CC2=O)C1=NN=NN1)C1=CC=C(OCCCCC2=CC=CC=C2)C=C1	N-[4-oxo-2-(1H-1,2,3,4-tetrazol-5-yl)-4H-chromen-8-yl]-4-(4-phenylbutoxy)benzamide	Pranlukast	481.5	4	FDA Approved Drug Library	103177-37-3	DL-287	2mg/ml	DMSO	2841J
	CCN(C)C(=O)OC1=CC(=CC=C1)[C@H](C)N(C)C	3-[(1S)-1-(dimethylamino)ethyl]phenyl N-ethyl-N-methylcarbamate	Rivastigmine	250.3	4	FDA Approved Drug Library	123441-03-2	DL-288	2mg/ml	DMSO	2841J
	CS(=O)(=O)C1=CC=C(C=C1)C1=C(C(=O)OC1)C1=CC=CC=C1	4-(4-methanesulfonylphenyl)-3-phenyl-2,5-dihydrofuran-2-one	Rofecoxib	314.4	4	FDA Approved Drug Library	162011-90-7	DL-289	2mg/ml	DMSO	2841J
			Blank		4	FDA Approved Drug Library			2mg/ml		2841J
	CC1=C(CC(O)=O)C2=C(C=CC(F)=C2)C\1=C\C1=CC=C(C=C1)S(C)=O	2-[(1E)-5-fluoro-1-[(4-methanesulfinylphenyl)methylidene]-2-methyl-1H-inden-3-yl]acetic acid	Sulindac	356.4	4	FDA Approved Drug Library	38194-50-2	ALX-430-105	2mg/ml	DMSO	2841J
	CCCC(CCC)C(O)=O	2-propylpentanoic acid	Valproic acid	144.2	4	FDA Approved Drug Library	99-66-1	DL-292	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@H]([C@H](C)\C=C\[C@@H](O)C3CC3)[C@@]1(C)CCC\C2=C/C=C1/C[C@@H](O)C[C@H](O)C1=C	(1R,3S,5Z)-5-{2-[(1R,3aS,4E,7aR)-1-[(2R,3E,5S)-5-cyclopropyl-5-hydroxypent-3-en-2-yl]-7a-methyl-octahydro-1H-inden-4-ylidene]ethylidene}-4-methylidenecyclohexane-1,3-diol	Calcipotriene	412.6	4	FDA Approved Drug Library	112965-21-6	DL-547	2mg/ml	DMSO	2841J
	COC1=CC(=CC=C1CC1=CN(C)C2=C1C=C(NC(=O)OC1CCCC1)C=C2)C(=O)NS(=O)(=O)C1=C(C)C=CC=C1	cyclopentyl N-{3-[(2-methoxy-4-{[(2-methylbenzene)sulfonyl]carbamoyl}phenyl)methyl]-1-methyl-1H-indol-5-yl}carbamate	Zafirlukast	575.7	4	FDA Approved Drug Library	107753-78-6	DL-294	2mg/ml	DMSO	2841J
	CC(N(O)C(N)=O)C1=CC2=CC=CC=C2S1	1-[1-(1-benzothiophen-2-yl)ethyl]-1-hydroxyurea	Zileuton	236.3	4	FDA Approved Drug Library	111406-87-2	DL-295	2mg/ml	DMSO	2841J
	NC(=N)C1=CC=C(OCCCCCOC2=CC=C(C=C2)C(N)=N)C=C1	4-{[5-(4-carbamimidoylphenoxy)pentyl]oxy}benzene-1-carboximidamide	Pentamidine	340.4	4	FDA Approved Drug Library	100-33-4	PR-118	2mg/ml	DMSO	2841J
	CC(C)C[C@@H](NC(=O)[C@H](CC1=CC=CC=C1)NC(=O)C1=NC=CN=C1)B(O)O	[(1S)-3-methyl-1-[(2S)-3-phenyl-2-(pyrazin-2-ylformamido)propanamido]butyl]boronic acid	Bortezomib	384.2	4	FDA Approved Drug Library	179324-69-7	DL-297	2mg/ml	DMSO	2841J
	CN(C)C(=O)OC1=CC(=CC(OC(=O)N(C)C)=C1)C(O)CNC(C)(C)C	3-[2-(tert-butylamino)-1-hydroxyethyl]-5-[(dimethylcarbamoyl)oxy]phenyl N,N-dimethylcarbamate	Bambuterol	367.4	4	FDA Approved Drug Library	81732-65-2	DL-161	2mg/ml	DMSO	2841J
	OC(=O)CC1=C(N=C(S1)C1=CC=CC=C1)C1=CC=C(Cl)C=C1	2-[4-(4-chlorophenyl)-2-phenyl-1,3-thiazol-5-yl]acetic acid	Fentiazac	329.8	4	FDA Approved Drug Library	18046-21-4	DL-186	2mg/ml	DMSO	2841J
	CCC1(NC(=O)N(C)C1=O)C1=CC=CC=C1	5-ethyl-3-methyl-5-phenylimidazolidine-2,4-dione	Mephenytoin	218.3	4	FDA Approved Drug Library	50-12-4	J-120	2mg/ml	DMSO	2841J
	CC1=NC2=CC=C(Cl)C=C2S(=O)(=O)N1	7-chloro-3-methyl-2H-1λ^{6},2,4-benzothiadiazine-1,1-dione	Diazoxide	230.7	4	FDA Approved Drug Library	364-98-7	KC-115	2mg/ml	DMSO	2841J
	COC1=CC=C(Cl)C=C1C(=O)NCCC1=CC=C(C=C1)S(=O)(=O)NC(=O)NC1CCCCC1	5-chloro-N-[2-(4-{[(cyclohexylcarbamoyl)amino]sulfonyl}phenyl)ethyl]-2-methoxybenzamide	Glyburide	494.0	4	FDA Approved Drug Library	10238-21-8	KC-120	2mg/ml	DMSO	2841J
	NC1=CC(=NC(=N)N1O)N1CCCCC1	6-amino-2-imino-4-(piperidin-1-yl)-1,2-dihydropyrimidin-1-ol	Minoxidil	209.2	4	FDA Approved Drug Library	38304-91-5	KC-125	2mg/ml	DMSO	2841J
	CC1=CC=C(C=C1)S(=O)(=O)NC(=O)NN1CCCCCC1	1-(azepan-1-yl)-3-[(4-methylbenzene)sulfonyl]urea	Tolazamide	311.4	4	FDA Approved Drug Library	1156-19-0	KC-135	2mg/ml	DMSO	2841J
	[O-][N+](=O)OCCNC(=O)C1=CN=CC=C1	2-(pyridin-3-ylformamido)ethyl nitrate	Nicorandil	211.2	4	FDA Approved Drug Library	65141-46-0	KC-152	2mg/ml	DMSO	2841J
	CC1=C(C=C2C(=C1)C(C)(C)CCC2(C)C)C(=C)C1=CC=C(C=C1)C(O)=O	4-[1-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)ethenyl]benzoic acid	Bexarotene	348.5	4	FDA Approved Drug Library	153559-49-0	DL-298	2mg/ml	DMSO	2841J
	NC[C@H]1CC[C@@H](CC1)C(O)=O	4-(aminomethyl)cyclohexane-1-carboxylic acid	Tranexamic acid	157.2	4	FDA Approved Drug Library	1197-18-8	DL-579	2mg/ml	DMSO	2841J

Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	CC1=CC=C(C=C1)C1=CC(=NN1C1=CC=C(C=C1)S(N)(=O)=O)C(F)(F)F	4-[5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzene-1-sulfonamide	Celecoxib	381.4	4	FDA Approved Drug Library	169590-42-5	DL-299	2mg/ml	DMSO	2841J
	CC[C@H](N1CCCC1=O)C(N)=O	(2S)-2-(2-oxopyrrolidin-1-yl)butanamide	Levetiracetam	170.2	4	FDA Approved Drug Library	102767-28-2	DL-172	2mg/ml	DMSO	2841J
	N#CC1=CC=C(C=C1)C(N1C=NC=N1)C1=CC=C(C=C1)C#N	4-[(4-cyanophenyl)(1H-1,2,4-triazol-1-yl)methyl]benzonitrile	Letrozole	285.3	4	FDA Approved Drug Library	112809-51-5	DL-300	2mg/ml	DMSO	2841J
	CO[C@H]1C[C@H](O)O[C@@H](C)[C@@H]1O.[H][C@](C)([*])[C@H]1O[C@@]2(C[C@]3([H])C[C@@]([H])(C\C=C(C)\[C@@H](O[C@@H]4C[C@@H](OC)[C@H](C)[C@@H](C)O4)[C@@H](C)\C=C\C=C4/CO[C@]5([H])[C@H](O)C(C)=C[C@@]([H])(C(=O)O3)[C@]45O)O2)C=C[C@@H]1C		Abamectin	860.1	4	FDA Approved Drug Library	71751-41-2	DL-301	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@H]([C@H](C)CCCC(C)C)[C@@]1(C)CCC\C2=C\C=C1/C[C@@H](O)C[C@H](O)C1=C	(1R,3S,5E)-5-{2-[(1R,3aS,4Z,7aR)-7a-methyl-1-[(2R)-6-methylheptan-2-yl]-octahydro-1H-inden-4-ylidene]ethylidene}-4-methylidenecyclohexane-1,3-diol	Alfacalcidol	400.6	4	FDA Approved Drug Library	41294-56-8	DL-222	2mg/ml	DMSO	2841J
	COC1=CC=C(C=C1)C1=CC(=S)SS1	5-(4-methoxyphenyl)-3H-1,2-dithiole-3-thione	Anethole-trithione	240.4	4	FDA Approved Drug Library	532-11-6	DL-151	2mg/ml	DMSO	2841J
	CC(C)(C#N)C1=CC(=CC(CN2C=NC=N2)=C1)C(C)(C)C#N	2-[3-(1-cyano-1-methylethyl)-5-(1H-1,2,4-triazol-1-ylmethyl)phenyl]-2-methylpropanenitrile	Anastrozole	293.4	4	FDA Approved Drug Library	120511-73-1	DL-144	2mg/ml	DMSO	2841J
	CC(O)(CS(=O)(=O)C1=CC=C(F)C=C1)C(=O)NC1=CC=C(C#N)C(=C1)C(F)(F)F	N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorobenzene)sulfonyl]-2-hydroxy-2-methylpropanamide	Bicalutamide	430.4	4	FDA Approved Drug Library	90357-06-5	DL-162	2mg/ml	DMSO	2841J
	OP(O)(=O)C(Cl)(Cl)P(O)(O)=O	[dichloro(phosphono)methyl]phosphonic acid	Clodronic acid	244.9	4	FDA Approved Drug Library	10596-23-3	DL-180	2mg/ml	DMSO	2841J
	CCC[C@@H]1C[C@H](N(C)C1)C(=O)N[C@H]([C@H](C)Cl)[C@H]1O[C@H](SC)[C@H](O)[C@@H](O)[C@H]1O	(2S,4R)-N-[(1S,2S)-2-chloro-1-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(methylsulfanyl)oxan-2-yl]propyl]-1-methyl-4-propylpyrrolidine-2-carboxamide	Clindamycin	425.0	4	FDA Approved Drug Library	24729-96-2	DL-102	2mg/ml	DMSO	2841J
	ONC(=O)CCCCCCC(=O)NC1=CC=CC=C1	N-hydroxy-N'-phenyloctanediamide	Vorinostat (SAHA)	264.3	4	FDA Approved Drug Library	149647-78-9	ALX-270-288	2mg/ml	DMSO	2841J
	OC[C@@H]1CC[C@@H](O1)N1C=NC2=C1N=CNC2=O	9-[(2R,5S)-5-(hydroxymethyl)oxolan-2-yl]-6,9-dihydro-1H-purin-6-one	Didanosine	236.2	4	FDA Approved Drug Library	69655-05-6	DL-302	2mg/ml	DMSO	2841J
	[H][C@@]1(C[C@]2([H])C[C@]3([H])C[C@@]([H])(C1)N2CC3=O)OC(=O)C1=CNC2=C1C=CC=C2	(3S,7S)-10-oxo-8-azatricyclo[5.3.1.$0^{3,8}$]undecan-5-yl 1H-indole-3-carboxylate	Dolasetron	324.4	4	FDA Approved Drug Library	115956-12-2	DL-199	2mg/ml	DMSO	2841J
	C[C@H](N[C@@H](CCC1=CC=CC=C1)C(O)=O)C(=O)N1CCC[C@H]1C(O)=O	(2S)-1-[(2S)-2-{[(1S)-1-carboxy-3-phenylpropyl]amino}propanoyl]pyrrolidine-2-carboxylic acid	Enalaprilat	348.4	4	FDA Approved Drug Library	76420-72-9	DL-192	2mg/ml	DMSO	2841J
	CC(C)N1C(\C=C\[C@@H](O)C[C@@H](O)CC(O)=O)=C(C2=C1C=CC=C2)C1=CC=C(F)C=C1	(3R,5S,6E)-7-[3-(4-fluorophenyl)-1-(propan-2-yl)-1H-indol-2-yl]-3,5-dihydroxyhept-6-enoic acid	Fluvastatin	411.5	4	FDA Approved Drug Library	93957-54-1	DL-108	2mg/ml	DMSO	2841J
	CCC(=O)OC(OP(=O)(CCCCC1=CC=CC=C1)CC(=O)N1C[C@@H](C[C@H]1C(O)=O)C1CCCCC1)C(C)C	(2S,4S)-4-cyclohexyl-1-(2-{[2-methyl-1-(propanoyloxy)propoxy](4-phenylbutyl)phosphoryl}acetyl)pyrrolidine-2-carboxylic acid	Fosinopril	563.7	4	FDA Approved Drug Library	98048-97-6	DL-155	2mg/ml	DMSO	2841J
	NC1=NC(=O)N(C=C1)[C@@H]1O[C@H](CO)[C@@H](O)C1(F)F	4-amino-1-[(2R,4R,5R)-3,3-difluoro-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,2-dihydropyrimidin-2-one	Gemcitabine	263.2	4	FDA Approved Drug Library	95058-81-4	DL-215	2mg/ml	DMSO	2841J
	[H][C@]12C[C@@]34[C@H]5C[C@@H](C(C)(C)C)[C@@]33[C@@H](O)C(=O)O[C@@]3([H])O[C@@]4(C(=O)O5)[C@@]1(O)[C@H](C)C(=O)O2	(1R,3R,6R,7S,8S,10R,11S,13S,16S,17R)-8-tert-butyl-6,17-dihydroxy-16-methyl-2,4,14,19-tetraoxahexacyclo[8.7.2.$0^{1,11}$.$0^{3,7}$.$0^{7,11}$.$0^{13,17}$]nonadecane-5,15,18-trione	Ginkgolide A	408.4	4	FDA Approved Drug Library	15291-75-5	DL-243	2mg/ml	DMSO	2841J
	[H][C@]12CCC[C@]([H])(C[C@@H](C1)NC(=O)C1=NN(C)C3=C1C=CC=C3)N2C	1-methyl-N-[(1R,3R,5S)-9-methyl-9-azabicyclo[3.3.1]nonan-3-yl]-1H-indazole-3-carboxamide	Granisetron	312.4	4	FDA Approved Drug Library	109889-09-0	DL-166	2mg/ml	DMSO	2841J
	N.N.O=C1CO[Pt]O1	1,3-dioxa-2-platinacyclopentan-4-one diamine	Nedaplatin	303.2	4	FDA Approved Drug Library	95734-82-0	DL-105	2mg/ml	DMSO	2841J
	O=C1O[Pt]OC1=O.[H][C@@]1(N)CCCC[C@@]1([H])N	(1R,2R)-cyclohexane-1,2-diamine; 1,3-dioxa-2-platinacyclopentane-4,5-dione	Oxaliplatin	397.3	4	FDA Approved Drug Library	61825-94-3	DL-303	2mg/ml	DMSO	2841J
	COC1=CC=C(\C=C\C)C=C1	1-methoxy-4-[(1E)-prop-1-en-1-yl]benzene	Anethole, trans-	148.2	4	FDA Approved Drug Library	104-46-1	DL-174	2mg/ml	DMSO	2841J
	COC(=O)N[C@H](C(=O)N[C@@H](CC1=CC=CC=C1)[C@@H](O)CN(CC1=CC=C(C=C1)C1=NC=CC=C1)NC(=O)[C@@H](NC(=O)OC)C(C)(C)C)C(C)(C)C	methyl N-[(1S)-1-{N'-[(2S,3S)-2-hydroxy-3-[(2S)-2-[(methoxycarbonyl)amino]-3,3-dimethylbutanamido]-4-phenylbutyl]-N'-{[4-(pyridin-2-yl)phenyl]methyl}hydrazinecarbonyl}-2,2-dimethylpropyl]carbamate	Atazanavir	704.9	4	FDA Approved Drug Library	198904-31-3	DL-546	2mg/ml	DMSO	2841J
	COC1=C(C)C2=C(C(=O)OC2)C(O)=C1C\C=C(/C)CCC(=O)OCCN1CCOCC1	2-(morpholin-4-yl)ethyl (4E)-6-(4-hydroxy-6-methoxy-7-methyl-3-oxo-1,3-dihydro-2-benzofuran-5-yl)-4-methylhex-4-enoate	Mycophenolate mofetil	433.5	5	FDA Approved Drug Library	128794-94-5	DL-545	2mg/ml	DMSO	2841J
	CC1=NC=C(C=C1)C1=NC=C(Cl)C=C1C1=CC=C(C=C1)S(C)(=O)=O	5-chloro-3-(4-methanesulfonylphenyl)-2-(6-methylpyridin-3-yl)pyridine	Etoricoxib	358.8	5	FDA Approved Drug Library	202409-33-4	DL-544	2mg/ml	DMSO	2841J
	NC1=NC(Cl)=NC2=C1N=CN2[C@@H]1O[C@H](CO)[C@@H](O)[C@@H]1F	(2R,3R,4S,5R)-5-(6-amino-2-chloro-9H-purin-9-yl)-4-fluoro-2-(hydroxymethyl)oxolan-3-ol	Clofarabine	303.7	5	FDA Approved Drug Library	123318-82-1	DL-103	2mg/ml	DMSO	2841J
	[H][C@@]12CC3=CNC4=C3C(=CC=C4)[C@@]1([H])C[C@H](CN2CC=C)C(=O)N(CCCN(C)C)C(=O)NCC	1-[3-(dimethylamino)propyl]-3-ethyl-1-{[(2R,4R,7R)-6-(prop-2-en-1-yl)-6,11-diazatetracyclo[7.6.1.$0^{2,7}$.$0^{12,16}$]hexadeca-1(15),9,12(16),13-tetraen-4-yl]carbonyl}urea	Cabergoline	451.6	5	FDA Approved Drug Library	81409-90-7	DL-219	2mg/ml	DMSO	2841J
	COC1=CC(=CC(OC)=C1OC)C(=O)OCCCN1CCCN(CCCOC(=O)C2=CC(OC)=C(OC)C(OC)=C2)CC1	3-(4-{3-[(3,4,5-trimethoxyphenyl)carbonyloxy]propyl}-1,4-diazepan-1-yl)propyl 3,4,5-trimethoxybenzoate	Dilazep	604.7	5	FDA Approved Drug Library	35898-87-4	DL-207	2mg/ml	DMSO	2841J
	CCCCCN(C)CCC(O)(P(O)(O)=O)P(O)(O)=O	{1-hydroxy-3-[methyl(pentyl)amino]-1-phosphonopropyl}phosphonic acid	Ibandronate	319.2	5	FDA Approved Drug Library	114084-78-5	DL-213	2mg/ml	DMSO	2841J
	[H][C@](C)(O)[C@@]1([H])C(=O)N2C(C(O)=O)=C(C[C@]12[H])SCCNC=N	(5R,6S)-6-[(1R)-1-hydroxyethyl]-3-[(2-methanimidamidoethyl)sulfanyl]-7-oxo-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid	Imipenem	299.3	5	FDA Approved Drug Library	64221-86-9	DL-202	2mg/ml	DMSO	2841J
	ClCCN(N=O)C(=O)NC1CCCCC1	3-(2-chloroethyl)-1-cyclohexyl-3-nitrosourea	Lomustine	233.7	5	FDA Approved Drug Library	13010-47-4	DL-156	2mg/ml	DMSO	2841J
	COC1=C(C=C(C=C1)C1=CC2=C(C=C1)C=C(C=C2)C(O)=O)C12CC3CC(CC(C3)C1)C2	6-[3-(adamantan-1-yl)-4-methoxyphenyl]naphthalene-2-carboxylic acid	Adapalene	412.5	5	FDA Approved Drug Library	106685-40-9	GR-111	2mg/ml	DMSO	2841J
	COC1=C(OC)C(OC)=C(CN2CCN(CC2)C(C2=CC=C(F)C=C2)C2=CC=C(F)C=C2)C=C1	1-[bis(4-fluorophenyl)methyl]-4-[(2,3,4-trimethoxyphenyl)methyl]piperazine	Lomerizine	468.5	5	FDA Approved Drug Library	101477-55-8	DL-244	2mg/ml	DMSO	2841J

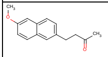
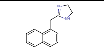
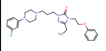
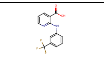
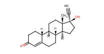
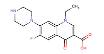
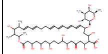
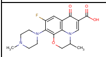
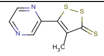
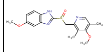
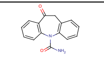
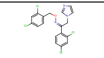
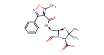
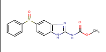
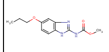
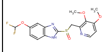
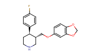
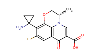
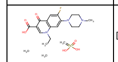
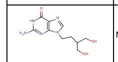
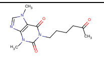
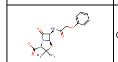
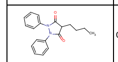
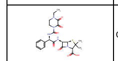
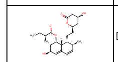
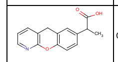
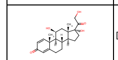
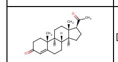
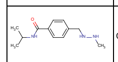
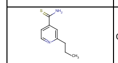
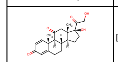
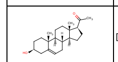
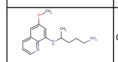
Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	Cl.CC(OC1=C(Cl)C=CC=C1Cl)C1=NCCN1	2-[1-(2,6-dichlorophenoxy)ethyl]-4,5-dihydro-1H-imidazole hydrochloride	Lofexidine·HCl	295.6	5	FDA Approved Drug Library	21498-08-8	DL-138	2mg/ml	DMSO	2841J
	[H][C@]12[C@@H](C)C(S[C@@H]3CN[C@@H](C3)C(=O)N(C)C)=C(N1C(=O)[C@]2([H])[C@@H](C)O)C(O)=O	(4R,5S,6S)-3-{[(3S,5S)-5-(dimethylcarbamoyl)pyrrolidin-3-yl]sulfanyl}-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid	Meropenem	383.5	5	FDA Approved Drug Library	96036-03-2	DL-167	2mg/ml	DMSO	2841J
	CN1C(=O)C=C(NCCN(CCO)CCCC2=CC=C(C=C2)[N+]([O-])=O)N(C)C1=O	6-({2-[(2-hydroxyethyl)[3-(4-nitrophenyl)propyl]amino]ethyl}amino)-1,3-dimethyl-1,2,3,4-tetrahydropyrimidine-2,4-dione	Nifekalant	405.4	5	FDA Approved Drug Library	130636-43-0	DL-205	2mg/ml	DMSO	2841J
	C[C@@H](O)[C@@H](CO)NC(=O)[C@@H]1CSSC[C@H](NC(=O)[C@H](N)CC2=CC=CC=C2)C(=O)N[C@@H](CC2=CC=CC=C2)C(=O)N[C@H](CC2=CNC3=C2C=CC=C3)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H]([C@@H](C)O)C(=O)N1	(4R,7S,10S,13R,16S,19R)-19-[(2R)-2-amino-3-phenylpropanamido]-10-(4-aminobutyl)-16-benzyl-N-[(2R,3R)-1,3-dihydroxybutan-2-yl]-7-[(1R)-1-hydroxyethyl]-13-(1H-indol-3-ylmethyl)-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaazacycloicosane-4-carboxamide	Octreotide	1019.2	5	FDA Approved Drug Library	79517-01-4	DL-309	2mg/ml	DMSO	2841J
			Blank		5	FDA Approved Drug Library			2mg/ml		2841J
	NCCC(O)(P(O)(O)=O)P(O)(O)=O	(3-amino-1-hydroxy-1-phosphonopropyl)phosphonic acid	Pamidronic acid	235.1	5	FDA Approved Drug Library	40391-99-9	DL-196	2mg/ml	DMSO	2841J
	CCCN[C@H]1CCC2=C(C1)SC(N)=N2	(6S)-6-N-propyl-4,5,6,7-tetrahydro-1,3-benzothiazole-2,6-diamine	Pramipexole	211.3	5	FDA Approved Drug Library	104632-26-0	DL-197	2mg/ml	DMSO	2841J
	CC(C)C[C@H](NC(=O)[C@@H](CC1=CNC2=C1C=CC=C2)NC(=O)[C@H](CC1=CC=C(O)C=C1)NC(=O)[C@H](CO)NC(=O)[C@H](CC1=CNC2=C1C=CC=C2)NC(=O)[C@H](CC1=CNC=N1)NC(=O)[C@@H]1CCC(=O)N1)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N1CCC[C@H]1C(=O)NCC(N)=O	(2S)-N-[(2S)-5-carbamimidamido-1-[(2S)-2-[(carbamoylmethyl)carbamoyl]pyrrolidin-1-yl]-1-oxopentan-2-yl]-2-[(2R)-2-[(2S)-2-[(2S)-3-hydroxy-2-[(2S)-2-[(2S)-3-(1H-imidazol-4-yl)-2-{[(2S)-5-oxopyrrolidin-2-yl]formamido}propanamido]-3-(1H-indol-3-yl)propanamido]propanamido]-3-(4-hydroxyphenyl)propanamido]-3-(1H-indol-3-yl)propanamido]-4-methylpentanamide	Triptorelin	1311.4	5	FDA Approved Drug Library	57773-63-4	DL-310	2mg/ml	DMSO	2841J
	CO[C@H]1\C=C\O[C@@]2(C)OC3=C(C2=O)C2=C(C(O)=C(NC(=O)\C(C)=C/C=C/[C@@H](C)[C@@H](O)[C@@H](C)[C@H](O)[C@H](C)[C@H]([C@H]1C)C(=O)OC)C=C2[O-])C(O)=C3C	(7S,9E,11R,12R,13R,14R,15R,16R,17R,18R,19E,21Z)-2,15,17,29-tetrahydroxy-11-methoxy-13-(methoxycarbonyl)-3,7,12,14,16,18,22-heptamethyl-6,23-dioxo-8,30-dioxa-24-azatetracyclo[23.3.1.1^{4,7}.0^{5,28}]triaconta-1(28),2,4,9,19,21,25(29),26-octaen-27-olate	RIFAMYCIN SV	696.8	5	FDA Approved Drug Library	6998-60-3	NP-526	2mg/ml	DMSO	2841J
	OC(CC1=CN=CC=C1)(P(O)(O)=O)P(O)(O)=O	[1-hydroxy-1-phosphono-2-(pyridin-3-yl)ethyl]phosphonic acid	Risedronic acid	283.1	5	FDA Approved Drug Library	105462-24-6	DL-198	2mg/ml	DMSO	2841J
	[Br-].[H][C@@]12C[C@@H]([C@H](OC(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CC[C@@]2([H])C[C@H](O)[C@H](C[C@]12C)N1CCOCC1)[N+]1(CC=C)CCCC1	1-[(1S,2S,4S,5S,7S,10R,11S,13S,14R,15S)-14-(acetyloxy)-5-hydroxy-2,15-dimethyl-4-(morpholin-4-yl)tetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadecan-13-yl]-1-(prop-2-en-1-yl)pyrrolidin-1-ium bromide	Rocuronium bromide	609.7	5	FDA Approved Drug Library	119302-91-9	DL-187	2mg/ml	DMSO	2841J
	CCCS(=O)C1=CC2=C(NC(NC(=O)OC)=N2)C=C1	methyl N-[5-(propane-1-sulfinyl)-1H-1,3-benzodiazol-2-yl]carbamate	Ricobendazole	281.3	5	FDA Approved Drug Library	54029-12-8	DL-148	2mg/ml	DMSO	2841J
	[H][C@@]12CC(=O)N1[C@@H](C(O)=O)C(C)(C)S2(=O)=O	(2S,5R)-3,3-dimethyl-4,4,7-trioxo-4λ^{6}-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid	Sulbactam	233.2	5	FDA Approved Drug Library	68373-14-8	DL-176	2mg/ml	DMSO	2841J
	CS(=O)(=O)C1=CC=C(C=C1)[C@@H](O)[C@@H](COC(=O)CN)NC(=O)C(Cl)Cl	(2R,3R)-2-(2,2-dichloroacetamido)-3-hydroxy-3-(4-methanesulfonylphenyl)propyl 2-aminoacetate	Thiamphenicol glycinate	413.3	5	FDA Approved Drug Library	2393-92-2	DL-143	2mg/ml	DMSO	2841J
	CC(C)(C)NCC(O)C1=CC=CC=C1Cl	2-(tert-butylamino)-1-(2-chlorophenyl)ethan-1-ol	Tulobuterol	227.7	5	FDA Approved Drug Library	41570-61-0	DL-175	2mg/ml	DMSO	2841J
	[H][C@@]12N3CC[C@]11[C@@H](N(C)C4=C1C=C(C(OC)=C4)[C@]1(C[C@@]4([H])CN(CC(CC)=C4)CC4=C1NC1=C4C=CC=C1)C(=O)OC)[C@](O)([C@H](OC(C)=O)[C@]2(CC)C=CC3)C(=O)OC	methyl (1R,9R,10S,11R,12R,19R)-11-(acetyloxy)-12-ethyl-4-[(12S,14R)-16-ethyl-12-(methoxycarbonyl)-1,10-diazatetracyclo[12.3.1.0^{3,11}.0^{4,9}]octadeca-3(11),4(9),5,7,15-pentaen-12-yl]-10-hydroxy-5-methoxy-8-methyl-8,16-diazapentacyclo[10.6.1.0^{1,9}.0^{2,7}.0^{16,19}]nonadeca-2(7),3,5,13-tetraene-10-carboxylate	Vinorelbine	778.9	5	FDA Approved Drug Library	71486-22-1	NP-461	2mg/ml	DMSO	2841J
	OS(O)(=O)=O.[H][C@@]12N3CC[C@@]11C4=C(C=C(OC)C(=C4)[C@]4(C[C@]5([H])C[N@@](C[C@](O)(CC)C5)CCC5=C4NC4=C5C=CC=C4)C(=O)OC)N(C)[C@@]1([H])[C@](O)([C@H](O)[C@]2(CC)C=CC3)C(N)=O	methyl (1S,13S,15S,17S)-13-[(1R,9R,10S,11R,12R,19R)-10-carbamoyl-12-ethyl-10,11-dihydroxy-5-methoxy-8-methyl-8,16-diazapentacyclo[10.6.1.0^{1,9}.0^{2,7}.0^{16,19}]nonadeca-2(7),3,5,13-tetraen-4-yl]-17-ethyl-17-hydroxy-1,11-diazatetracyclo[13.3.1.0^{4,12}.0^{5,10}]nonadeca-4(12),5(10),6,8-tetraene-13-carboxylate; sulfuric acid	Vindesine sulfate	852.0	5	FDA Approved Drug Library	59917-39-4	DL-220	2mg/ml	DMSO	2841J
	OC(=O)C1=C(O)C2=C(C=CC=C2)C=C1.OCC1=C(O)C=CC(=C1)C(O)CNCCCCCCOCCCCC1=CC=CC=C1	1-hydroxynaphthalene-2-carboxylic acid; 4-(1-hydroxy-2-{[6-(4-phenylbutoxy)hexyl]amino}ethyl)-2-(hydroxymethyl)phenol	Salmeterol xinafoate	603.7	5	FDA Approved Drug Library	94749-08-3	DL-210	2mg/ml	DMSO	2841J
	OS(O)(=O)=O.[H][C@@]12N3CC[C@@]11C4=C(C=C(OC)C(=C4)[C@]4(C[C@]5([H])C[N@@](C[C@](O)(CC)C5)CCC5=C4NC4=C5C=CC=C4)C(=O)OC)N(C=O)[C@@]1([H])[C@](O)([C@H](OC(C)=O)[C@]2(CC)C=CC3)C(=O)OC	methyl (1R,9R,10S,11R,12R,19R)-11-(acetyloxy)-12-ethyl-4-[(1S,13S,15S,17S)-17-ethyl-17-hydroxy-13-(methoxycarbonyl)-1,11-diazatetracyclo[13.3.1.0^{4,12}.0^{5,10}]nonadeca-4(12),5(10),6,8-tetraen-13-yl]-8-formyl-10-hydroxy-5-methoxy-8,16-diazapentacyclo[10.6.1.0^{1,9}.0^{2,7}.0^{16,19}]nonadeca-2(7),3,5,13-tetraene-10-carboxylate; sulfuric acid	Vincristine sulfate	923.0	5	FDA Approved Drug Library	2068-78-2	T-117	2mg/ml	DMSO	2841J
	COC1=CC2=C(C=C1)N(C(=O)C1=CC=C(Cl)C=C1)C(C)=C2CC(=O)OCC(O)=O	2-[(2-{1-[(4-chlorophenyl)carbonyl]-5-methoxy-2-methyl-1H-indol-3-yl}acetyl)oxy]acetic acid	Acemetacin	415.8	5	FDA Approved Drug Library	53164-05-9	DL-312	2mg/ml	DMSO	2841J
	CC(=O)OC1=C(C=CC=C1)C(O)=O	2-(acetyloxy)benzoic acid	Acetylsalicylic Acid	180.2	5	FDA Approved Drug Library	50-78-2	DL-313	2mg/ml	DMSO	2841J
	CC1=[N+]([O-])C=C(N=C1)C(O)=O	5-carboxy-2-methylpyrazin-1-ium-1-olate	Acipimox	154.1	5	FDA Approved Drug Library	51037-30-0	DL-314	2mg/ml	DMSO	2841J
	OC(=O)COC(=O)CC1=C(NC2=C(Cl)C=CC=C2Cl)C=CC=C1	2-[(2-{2-[(2,6-dichlorophenyl)amino]phenyl}acetyl)oxy]acetic acid	Aceclofenac	354.2	5	FDA Approved Drug Library	89796-99-6	DL-315	2mg/ml	DMSO	2841J
	NC1=NC2=C(N=CN2COCCO)C(=O)N1	2-amino-9-[(2-hydroxyethoxy)methyl]-6,9-dihydro-1H-purin-6-one	Acycloguanosine	225.2	5	FDA Approved Drug Library	59277-89-3	DL-316	2mg/ml	DMSO	2841J
	CC1=CN([C@H]2C[C@H](N=[N+]=[N-])[C@@H](CO)O2)C(=O)NC1=O	1-[(2R,4S,5S)-4-azido-5-(hydroxymethyl)oxolan-2-yl]-5-methyl-1,2,3,4-tetrahydropyrimidine-2,4-dione	3'-Azido-3'-deoxythymidine	267.2	5	FDA Approved Drug Library	30516-87-1	DL-317	2mg/ml	DMSO	2841J
	OC1=C2CN=NC2=NC=N1	3H-pyrazolo[3,4-d]pyrimidin-4-ol	Allopurinol	136.1	5	FDA Approved Drug Library	315-30-0	DL-318	2mg/ml	DMSO	2841J
	NCCCC(O)(P(O)(O)=O)P(O)([O-])=O	hydrogen (4-amino-1-hydroxy-1-phosphonobutyl)phosphonate	Alendronate	248.1	5	FDA Approved Drug Library	121268-17-5	PR-123	2mg/ml	DMSO	2841J
	CN(C)C1=NC(=NC(=N1)N(C)C)N(C)C	2-N,2-N,4-N,4-N,6-N,6-N-hexamethyl-1,3,5-triazine-2,4,6-triamine	Altretamine	210.3	5	FDA Approved Drug Library	645-05-6	DL-320	2mg/ml	DMSO	2841J
	CCCSC1=CC2=C(NC(NC(=O)OC)=N2)C=C1	methyl N-[5-(propylsulfanyl)-1H-1,3-benzodiazol-2-yl]carbamate	Albendazole	265.3	5	FDA Approved Drug Library	54965-21-8	DL321	2mg/ml	DMSO	2841J
	OC(=O)CCC(O)=O.CNS(=O)(=O)CC1=CC2=C(NC=C2CCN(C)C)C=C1	1-{3-[2-(dimethylamino)ethyl]-1H-indol-5-yl}-N-methylmethanesulfonamide; butanedioic acid	Sumatriptan Succinate	413.5	5	FDA Approved Drug Library	103628-48-4	DL-565	2mg/ml	DMSO	2841J
	NCCCNCCSP(O)(O)=O	({2-[(3-aminopropyl)amino]ethyl}sulfanyl)phosphonic acid	Amifostine	214.2	5	FDA Approved Drug Library	20537-88-6	GR-341	2mg/ml	DMSO	2841J
	CCC1(CCC(=O)NC1=O)C1=CC=C(N)C=C1	3-(4-aminophenyl)-3-ethylpiperidine-2,6-dione	DL-Aminoglutethimide	232.3	5	FDA Approved Drug Library	125-84-8	DL-324	2mg/ml	DMSO	2841J
	NC1=CC(O)=C(C=C1)C(O)=O	4-amino-2-hydroxybenzoic acid	4-Aminosalicylic acid	153.1	5	FDA Approved Drug Library	65-49-6	DL-325	2mg/ml	DMSO	2841J

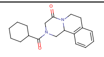
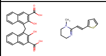
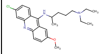
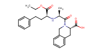
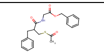
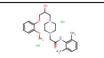
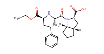
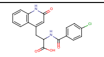
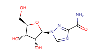
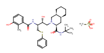
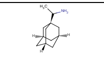
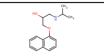
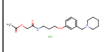
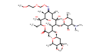
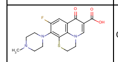
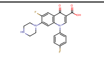
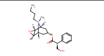
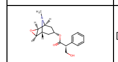
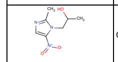
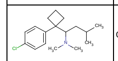
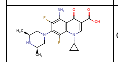
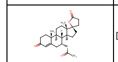
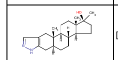
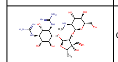
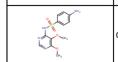
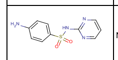
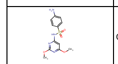
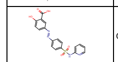
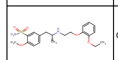
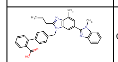
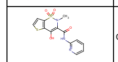
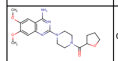
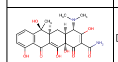
Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	NC1=CC(C(O)=O)=C(O)C=C1	5-amino-2-hydroxybenzoic acid	5-Aminosalicylic acid	153.1	5	FDA Approved Drug Library	89-57-6	DL-326	2mg/ml	DMSO	2841J
	CC1(C)S[C@@H]2[C@H](NC(=O)[C@H](N)C3=CC=CC=C3)C(=O)N2[C@H]1C(O)=O	(2S,5R,6R)-6-[(2R)-2-amino-2-phenylacetamido]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid	Ampicillin	349.4	5	FDA Approved Drug Library	7177-48-2	DL-327	2mg/ml	DMSO	2841J
	CCOC(=O)OC(C)OC1=C(N(C)S(=O)(=O)C2=C1C=CC=C2)C(=O)NC1=NC=CC=C1	ethyl 1-({2-methyl-1,1-dioxo-3-[(pyridin-2-yl)carbamoyl]-2H-1λ^{6},2-benzothiazin-4-yl}oxy)ethyl carbonate	Ampiroxicam	447.5	5	FDA Approved Drug Library	99464-64-9	DL-328	2mg/ml	DMSO	2841J
	[H][C@]12C[C@@H](N)[C@@H](O[C@@H]3[C@@H](N)C[C@@H](N)[C@H](O)[C@H]3O)O[C@]1([H])[C@H](O)[C@H](NC)[C@@H](O[C@H]1O[C@H](CO)[C@@H](N)[C@H](O)[C@H]1O)O2	(2R,3R,4S,5S,6S)-2-{[(2R,3S,4R,4aR,6S,7R,8aS)-7-amino-6-{[(1R,2R,3S,4R,6S)-4,6-diamino-2,3-dihydroxycyclohexyl]oxy}-4-hydroxy-3-(methylamino)-octahydropyrano[3,2-b]pyran-2-yl]oxy}-5-amino-6-(hydroxymethyl)oxane-3,4-diol	Apramycin	539.6	5	FDA Approved Drug Library	37321-09-8	DL-329	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@@H](C)[C@]3([H])CC[C@@]4(C)OO[C@@]13[C@]([H])(OC(=O)[C@@H]2C)O4	(1R,4S,5R,8S,9R,12S,13R)-1,5,9-trimethyl-11,14,15,16-tetraoxatetracyclo[10.3.1.0^{4,13}.0^{8,13}]hexadecan-10-one	Artemisinin	282.3	5	FDA Approved Drug Library	63968-64-9	NP-016	2mg/ml	DMSO	2841J
	CC(C)NCC(O)COC1=CC=C(CC(N)=O)C=C1	2-(4-{2-hydroxy-3-[(propan-2-yl)amino]propoxy}phenyl)acetamide	Atenolol	266.3	5	FDA Approved Drug Library	29122-68-7	AC-166	2mg/ml	DMSO	2841J
	OS(=O)(=O)C1=CC=CC=C1.OS(=O)(=O)C1=CC=CC=C1.COC1=CC2=C(C=C1OC)C(CC1=CC(OC)=C(OC)C=C1)[N+](C)(CCC(=O)OCCCCCOC(=O)CC[N+]1(C)CCC3=C(C=C(OC)C(OC)=C3)C1CC1=CC(OC)=C(OC)C=C1)CC2	1-[(3,4-dimethoxyphenyl)methyl]-2-[3-({5-[(3-{1-[(3,4-dimethoxyphenyl)methyl]-6,7-dimethoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-2-ium-2-yl}propanoyl)oxy]pentyl}oxy)-3-oxopropyl]-6,7-dimethoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-2-ium; bis(benzenesulfonic acid)	Atracurium besylate	1245.5	5	FDA Approved Drug Library	64228-81-5	DL-332	2mg/ml	DMSO	2841J
	FC1=CC=C(C=C1)C(=O)CCCN1CCN(CC1)C1=CC=CC=N1	1-(4-fluorophenyl)-4-[4-(pyridin-2-yl)piperazin-1-yl]butan-1-one	Azaperone	327.4	5	FDA Approved Drug Library	1649-18-9	DL-333	2mg/ml	DMSO	2841J
	[H][C@@]12N3CC[C@@]11C4=C(C=C(OC)C(=C4)[C@]4(C[C@]5([H])C[N@@](C[C@](O)(CC)C5)CCC5=C4NC4=C5C=CC=C4)C(=O)OC)N(C)[C@@]1([H])[C@](O)([C@H](OC(C)=O)[C@]2(CC)C=CC3)C(=O)OC	methyl (1R,9R,10S,11R,12R,19R)-11-(acetyloxy)-12-ethyl-4-[(1S,13S,15S,17S)-17-ethyl-17-hydroxy-13-(methoxycarbonyl)-1,11-diazatetracyclo[13.3.1.0^{4,12}.0^{5,10}]nonadeca-4(12),5(10),6,8-tetraen-13-yl]-10-hydroxy-5-methoxy-8-methyl-8,16-diazapentacyclo[10.6.1.0^{1,9}.0^{2,7}.0^{16,19}]nonadeca-2(7),3,5,13-tetraene-10-carboxylate	Vinblastine	811.0	5	FDA Approved Drug Library	143-67-9	T-116	2mg/ml	DMSO	2841J
	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	(2R,3S,4R,5R,8R,11R,12S,13S,14R)-11-{[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy}-2-ethyl-3,4,10-trihydroxy-13-{[(2R,4R,5S,6S)-5-hydroxy-4-methoxy-4,6-dimethyloxan-2-yl]oxy}-3,5,6,8,10,12,14-heptamethyl-1-oxa-6-azacyclopentadecan-15-one	Azithromycin	749.0	5	FDA Approved Drug Library	83905-01-5	DL-335	2mg/ml	DMSO	2841J
	C[C@H]1[C@H](NC(=O)C(=N/OC(C)(C)C(O)=O)\C2=CSC(N)=N2)C(=O)N1S(O)(=O)=O	2-{[(Z)-[(2-amino-1,3-thiazol-4-yl)({[(2S,3S)-2-methyl-4-oxo-1-sulfoazetidin-3-yl]carbamoyl})methylidene]amino]oxy}-2-methylpropanoic acid	Aztreonam	435.4	5	FDA Approved Drug Library	78110-38-0	DL-336	2mg/ml	DMSO	2841J
	[H][C@@]12C[C@H](C)[C@](OC(=O)CC)(C(=O)COC(=O)CC)[C@@]1(C)C[C@H](O)C1(F)[C@@]2([H])CCC2=CC(=O)C=C[C@]12C	2-[(2S,10S,11S,13S,14R,15S,17S)-1-fluoro-17-hydroxy-2,13,15-trimethyl-5-oxo-14-(propanoyloxy)tetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadeca-3,6-dien-14-yl]-2-oxoethyl propanoate	Betamethasone	504.6	5	FDA Approved Drug Library	378-44-9	DL-337	2mg/ml	DMSO	2841J
	C1=CN(C=N1)C(C1=CC=CC=C1)C1=CC=C(C=C1)C1=CC=CC=C1	1-[phenyl(4-phenylphenyl)methyl]-1H-imidazole	Bifonazole	310.4	5	FDA Approved Drug Library	60628-96-8	DL-338	2mg/ml	DMSO	2841J
	CC(=O)OC1=CC=C(C=C1)C(C1=CC=C(OC(C)=O)C=C1)C1=NC=CC=C1	4-{[4-(acetyloxy)phenyl](pyridin-2-yl)methyl}phenyl acetate	Bisacodyl	361.4	5	FDA Approved Drug Library	603-50-9	DL-339	2mg/ml	DMSO	2841J
	CN(CC1=C(N)C(Br)=CC(Br)=C1)C1CCCCC1	2,4-dibromo-6-{[cyclohexyl(methyl)amino]methyl}aniline	Bromhexine	376.1	5	FDA Approved Drug Library	611-75-6	DL-340	2mg/ml	DMSO	2841J
	O=C1CC2(CCCC2)CC(=O)N1CCCCN1CCN(CC1)C1=NC=CC=N1	8-{4-[4-(pyrimidin-2-yl)piperazin-1-yl]butyl}-8-azaspiro[4.5]decane-7,9-dione	Buspirone	385.5	5	FDA Approved Drug Library	33386-08-2	DL-341	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@@]3(CCC(=O)O3)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])C=CC2=CC(=O)CC[C@]12C	(1'S,2R,2'R,10'R,11'S,15'S)-2',15'-dimethylspiro[oxolane-2,14'-tetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadecane]-6',8'-diene-5,5'-dione	Canrenone	340.5	5	FDA Approved Drug Library	976-71-6	DL-342	2mg/ml	DMSO	2841J
	COC(=O)N\N=C\C1=[N+]([O-])C2=C(C=CC=C2)[N+]([O-])=C1	3-[(1E)-{[(methoxycarbonyl)amino]imino}methyl]quinoxaline-1,4-diium-1,4-bis(olate)	Carbadox	262.2	5	FDA Approved Drug Library	6804-07-5	DL-343	2mg/ml	DMSO	2841J
	O=C1O[Pt]OC(=O)C11CCC1	6,8-dioxa-7-platinaspiro[3.5]nonane-5,9-dione	Carboplatin	337.2	5	FDA Approved Drug Library	41575-94-4	DL-344	2mg/ml	DMSO	2841J
	NC(=O)N1C2=CC=CC=C2C=CC2=C1C=CC=C2	2-azatricyclo[9.4.0.0^{3,8}]pentadeca-1(11),3,5,7,9,12,14-heptaene-2-carboxamide	Carbamazepine	236.3	5	FDA Approved Drug Library	298-46-4	DL-345	2mg/ml	DMSO	2841J
	[H][C@]12SCC(CSC3=NN=NN3C)=C(N1C(=O)[C@H]2NC(=O)[C@H](NC(=O)N1CCN(CC)C(=O)C1=O)C1=CC=C(O)C=C1)C(O)=O	(6R,7R)-7-[(2R)-2-{[(4-ethyl-2,3-dioxopiperazin-1-yl)carbonyl]amino}-2-(4-hydroxyphenyl)acetamido]-3-{[(1-methyl-1H-1,2,3,4-tetrazol-5-yl)sulfanyl]methyl}-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid	Cefoperazone acid	645.7	5	FDA Approved Drug Library	62893-19-0	DL-346	2mg/ml	DMSO	2841J
	[H][C@]12SCC(COC(C)=O)=C(N1C(=O)[C@H]2NC(=O)C(=N/OC)\C1=CSC(N)=N1)C(O)=O	(6R,7R)-3-[(acetyloxy)methyl]-7-[(2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-(methoxyimino)acetamido]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid	Cefotaxime Acid	455.5	5	FDA Approved Drug Library	63527-52-6	DL-347	2mg/ml	DMSO	2841J
	CC(C)(O\N=C(C(=O)N[C@H]1[C@H]2SCC(C[N+]3=CC=CC=C3)=C(N2C1=O)C([O-])=O)\C1=CSC(N)=N1)C(O)=O	1-{[(6R,7R)-7-[(2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-[(1-carboxy-1-methylethoxy)imino]acetamido]-2-carboxylato-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl}pyridin-1-ium	Ceftazidime	546.6	5	FDA Approved Drug Library	72558-82-8	DL-348	2mg/ml	DMSO	2841J
	OC[C@@H](NC(=O)C(Cl)Cl)[C@H](O)C1=CC=C(C=C1)[N+]([O-])=O	2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide	Chloramphenicol	323.1	5	FDA Approved Drug Library	56-75-7	DL-349	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@](OC(C)=O)(C(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])C=C(Cl)C2=CC(CC[C@]12C)OC(C)=O	(1S,2R,10R,11S,14R,15S)-14-acetyl-5-(acetyloxy)-8-chloro-2,15-dimethyltetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadeca-6,8-dien-14-yl acetate	Chlormadinone Acetate	449.0	5	FDA Approved Drug Library	302-22-7	DL-350	2mg/ml	DMSO	2841J
	OC(=O)CCCC1=CC=C(C=C1)N(CCCl)CCCl	4-{4-[bis(2-chloroethyl)amino]phenyl}butanoic acid	Chlorambucil	304.2	5	FDA Approved Drug Library	305-03-3	DL-351	2mg/ml	DMSO	2841J
	CN(C)CCC(C1=CC=C(Cl)C=C1)C1=NC=CC=C1	[3-(4-chlorophenyl)-3-(pyridin-2-yl)propyl]dimethylamine	Chlorpheniramine	274.8	5	FDA Approved Drug Library	113-92-8	DL-352	2mg/ml	DMSO	2841J
	CCN(CC)CCCC(C)NC1=CC=NC2=C1C=CC(Cl)=C2	{4-[(7-chloroquinolin-4-yl)amino]pentyl}diethylamine	Chloroquine	319.9	5	FDA Approved Drug Library	50-63-5	DL-353	2mg/ml	DMSO	2841J
	O=C1N(C2CCC(=O)NC2=O)C(=O)C2=C1C=CC=C2	2-(2,6-dioxopiperidin-3-yl)-2,3-dihydro-1H-isoindole-1,3-dione	Thalidomide	258.2	5	FDA Approved Drug Library	50-35-1	T-115	2mg/ml	DMSO	2841J
	OC(=O)C1=CN(C2CC2)C2=C(C=C(F)C(=C2)N2CCNCC2)C1=O	1-cyclopropyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic acid	Ciprofloxacin	331.3	5	FDA Approved Drug Library	85721-33-1	DL-355	2mg/ml	DMSO	2841J
	CN(C)CCCC1(OCC2=C1C=CC(=C2)C#N)C1=CC=C(F)C=C1	1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-2-benzofuran-5-carbonitrile	Citalopram	324.4	5	FDA Approved Drug Library	59729-33-8	NS-112	2mg/ml	DMSO	2841J
	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@@](C)(C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O)OC	(3R,4S,5S,6R,7R,9R,11R,12R,13S,14R)-6-{[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy}-14-ethyl-12,13-dihydroxy-4-{[(2R,4R,5S,6S)-5-hydroxy-4-methoxy-4,6-dimethyloxan-2-yl]oxy}-7-methoxy-3,5,7,9,11,13-hexamethyl-1-oxacyclotetradecane-2,10-dione	Clarithromycin	748.0	5	FDA Approved Drug Library	81103-11-9	DL-357	2mg/ml	DMSO	2841J
	CC(C)(C)C(=O)C(OC1=CC=C(Cl)C=C1)N1C=CN=C1	1-(4-chlorophenoxy)-1-(1H-imidazol-1-yl)-3,3-dimethylbutan-2-one	Climbazole	292.8	5	FDA Approved Drug Library	38083-17-9	DL-358	2mg/ml	DMSO	2841J

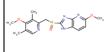
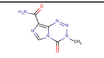
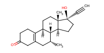
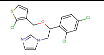
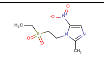
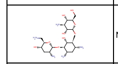
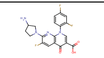
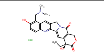
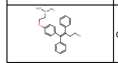
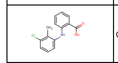
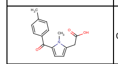
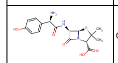
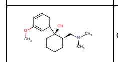
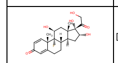
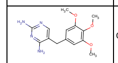
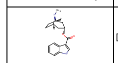
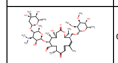
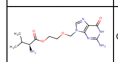
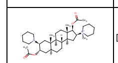
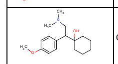
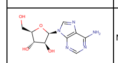
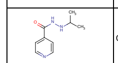
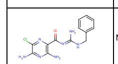
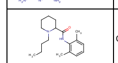
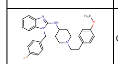
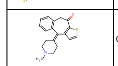
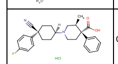
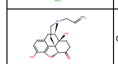
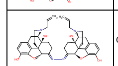
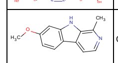
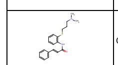
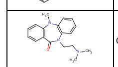
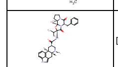
Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	NC1CCN(C1)C1=C(Cl)C2=C(C=C1F)C(=O)C(=CN2C1CC1)C(O)=O	7-(3-aminopyrrolidin-1-yl)-8-chloro-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid	Clinafloxacin	365.8	5	FDA Approved Drug Library	105956-99-8	DL-359	2mg/ml	DMSO	2841J
	CCN(CC)CCOC1=CC=C(C=C1)C(C1=CC=CC=C1)=C(Cl)C1=CC=CC=C1	(2-[4-[(E)-2-chloro-1,2-diphenylethenyl]phenoxy]ethyl)diethylamine	Clomiphene	406.0	5	FDA Approved Drug Library	50-41-9	DL-360	2mg/ml	DMSO	2841J
	CCN1CCCC1CNC(=O)C1=C(OC)C=C(N(C)(=C1)S(=O)(=O)CC	4-amino-5-(ethanesulfonyl)-N-[(1-ethylpyrrolidin-2-yl)methyl]-2-methoxybenzamide	Amisulpride	369.5	5	FDA Approved Drug Library	71675-85-9	DL-580	2mg/ml	DMSO	2841J
	COC(=O)[C@@H](N1CCC2=C(C1)C=CS2)C1=C(Cl)C=CC=C1	methyl (2S)-2-(2-chlorophenyl)-2-[4H,5H,6H,7H-thieno[3,2-c]pyridin-5-yl]acetate	Clopidogrel	321.8	5	FDA Approved Drug Library	135046-48-9	AC-1290	2mg/ml	DMSO	2841J
	[H][C@@]12C[C@H](C)[C@](OC(=O)CC)(C(=O)CCl)[C@@]1(C)[C@H](O)[C@@]1(F)[C@@]2([H])CCC2=CC(=O)C=C[C@]12C	(1R,2S,10S,11S,13S,14R,15S,17S)-14-(2-chloroacetyl)-1-fluoro-17-hydroxy-2,13,15-trimethyl-5-oxotetracyclo[8.7.0.0^{2},^{7}.0^{11},^{15}]heptadeca-3,6-dien-14-yl propanoate	Clobetasol Propionate	467.0	6	FDA Approved Drug Library	25122-46-7	DL-363	2mg/ml	DMSO	2841J
	OC(=O)CC(O)(CC(O)=O)C(O)=O.CN(C)CCOC(C1=CC=CC=C1)C1=C(C)C=CC=C1	2-hydroxypropane-1,2,3-tricarboxylic acid; dimethyl({2-[(2-methylphenyl)(phenyl)methoxy]ethyl})amine	Orphenadrine citrate	461.5	6	FDA Approved Drug Library	4682-36-4	AC-1386	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@H](C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]1([H])[C@@]2([H])CCC2=CC(=O)CC[C@]12C	(1S,2R,10S,11S,14S,15S,17S)-17-hydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7.0.0^{2},^{7}.0^{11},^{15}]heptadec-6-en-5-one	Corticosterone	346.5	6	FDA Approved Drug Library	50-22-6	DL-365	2mg/ml	DMSO	2841J
	CCN(C(=O)/C=C/C)C1=C(C)C=CC=C1	(2E)-N-ethyl-N-(2-methylphenyl)but-2-enamide	Crotamiton	203.3	6	FDA Approved Drug Library	483-63-6	DL-366	2mg/ml	DMSO	2841J
	ClCCN(CCCl)P1(=O)NCCCO1	2-[bis(2-chloroethyl)amino]-1,3,2λ^{5}-oxazaphosphinan-2-one	Cyclophosphamide	261.1	6	FDA Approved Drug Library	6055-19-2	DL-367	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@](OC(C)=O)(C(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])C=C(Cl)C2=CC(=O)[C@@H]3C[C@@H]3[C@]12C	(1S,2S,3S,5R,11R,12S,15R,16S)-15-acetyl-9-chloro-2,16-dimethyl-6-oxopentacyclo[9.7.0.0^{2},^{7}.0^{3},^{5}.0^{12},^{16}]octadeca-7,9-dien-15-yl acetate	Cyproterone Acetate	416.9	6	FDA Approved Drug Library	427-51-0	DL-368	2mg/ml	DMSO	2841J
	OC[C@H]1O[C@@H]2[C@@H](OC3=NC(=N)C=CN23)[C@@H]1O	(2R,4R,5R,6S)-4-(hydroxymethyl)-10-imino-3,7-dioxa-1,9-diazatricyclo[6.4.0.0^{2},^{6}]dodeca-8,11-dien-5-ol	Cyclocytidine	225.2	6	FDA Approved Drug Library	10212-25-6	DL-369	2mg/ml	DMSO	2841J
	NC1=NC(=O)N(C=C1)[C@@H]1O[C@H](CO)[C@@H](O)[C@@H]1O	4-amino-1-[(2R,3S,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,2-dihydropyrimidin-2-one	Cytarabine	243.2	6	FDA Approved Drug Library	147-94-4	DL-370	2mg/ml	DMSO	2841J
	CN(C)/N=N/C1=C(N=CN1)C(N)=O	5-[(1E)-dimethyltriaz-1-en-1-yl]-1H-imidazole-4-carboxamide	Dacarbazine	182.2	6	FDA Approved Drug Library	4342-03-4	DL-371	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@@](O)(C#C)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CCC2=CC3=C(C[C@]12C)C=NO3	(1S,2R,13R,14S,17R,18S)-17-ethynyl-2,18-dimethyl-7-oxa-6-azapentacyclo[11.7.0.0^{2},^{10}.0^{4},^{8}.0^{14},^{18}]icosa-4(8),5,9-trien-17-ol	Danazol	337.5	6	FDA Approved Drug Library	17230-88-5	DL-372	2mg/ml	DMSO	2841J
	[H][C@@]12CCC(=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CC=C2C[C@@H](O)CC[C@]12C	(1S,2R,5S,10R,11S,15S)-5-hydroxy-2,15-dimethyltetracyclo[8.7.0.0^{2},^{7}.0^{11},^{15}]heptadec-7-en-14-one	Dehydroepiandrosterone	288.4	6	FDA Approved Drug Library	53-43-0	DL-373	2mg/ml	DMSO	2841J
	ClC1=CC2=C(C=C1)C(=C1CCNCC1)C1=C(CC2)C=CC=N1	13-chloro-2-(piperidin-4-ylidene)-4-azatricyclo[9.4.0.0^{3},^{8}]pentadeca-1(11),3(8),4,6,12,14-hexaene	Desloratadine	310.8	6	FDA Approved Drug Library	100643-71-8	DL-154	2mg/ml	DMSO	2841J
	[H][C@]12CCC[C@]11CCN(C)[C@H]2CC2=C1C=C(OC)C=C2	(1S,9S,10S)-4-methoxy-17-methyl-17-azatetracyclo[7.5.3.0^{1},^{10}.0^{2},^{7}]heptadeca-2(7),3,5-triene	Dextromethorphan	271.4	6	FDA Approved Drug Library	125-69-9	DL-374	2mg/ml	DMSO	2841J
	OC(=O)CC1=CC=CC=C1NC1=C(Cl)C=CC=C1Cl	2-[2-[(2,6-dichlorophenyl)amino]phenyl]acetic acid	Diclofenac	296.1	6	FDA Approved Drug Library	15307-79-6	DL-375	2mg/ml	DMSO	2841J
	NC1=NC(=O)N(C=C1)[C@H]1OC[C@@H](CO)O1	4-amino-1-[(2R,5S)-5-(hydroxymethyl)oxolan-2-yl]-1,2-dihydropyrimidin-2-one	2′,3′ - Dideoxycytidine	211.2	6	FDA Approved Drug Library	7481-89-2	DL-376	2mg/ml	DMSO	2841J
	CC/C(C1=CC=C(O)C=C1)=C(/CC)C1=CC=C(O)C=C1	4-[(3E)-4-(4-hydroxyphenyl)hex-3-en-3-yl]phenol	Diethylstilbestrol	268.4	6	FDA Approved Drug Library	56-53-1	DL-377	2mg/ml	DMSO	2841J
	OC(=O)C1=C(O)C=CC(=C1)C1=C(F)C=C(F)C=C1	5-(2,4-difluorophenyl)-2-hydroxybenzoic acid	Diflunisal	250.2	6	FDA Approved Drug Library	22494-42-4	DL-378	2mg/ml	DMSO	2841J
	CCN(CC)C(=S)SSC(=S)N(CC)CC	N,N-diethyl[(diethylcarbamothioyl)disulfanyl]carbothioamide	Disulfiram	296.5	6	FDA Approved Drug Library	97-77-8	DL-379	2mg/ml	DMSO	2841J
	COC1=CC2=C(C=C1OC)C(N)=NC(=N2)N1CCN(CC1)C(=O)C1COC2=C(O1)C=CC=C2	2-[4-[(2,3-dihydro-1,4-benzodioxin-2-yl)carbonyl]piperazin-1-yl]-6,7-dimethoxyquinazolin-4-amine	Doxazosin	451.5	6	FDA Approved Drug Library	77883-43-3	DL-204	2mg/ml	DMSO	2841J
	C[C@H]1O[C@H](C[C@H](O)[C@@H]1O)N1C=C(F)C(=O)NC1=O	1-[(2R,3R,4S,5R)-3,4-dihydroxy-5-methyloxolan-2-yl]-5-fluoro-1,2,3,4-tetrahydropyrimidine-2,4-dione	Doxifluridine	246.2	6	FDA Approved Drug Library	3094-09-5	DL-380	2mg/ml	DMSO	2841J
	CN1C2=C(N(CC3OCCO3)C=N2)C(=O)N(C)C1=O	7-(1,3-dioxolan-2-ylmethyl)-1,3-dimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione	Doxofylline	266.3	6	FDA Approved Drug Library	69975-86-6	DL-181	2mg/ml	DMSO	2841J
	[H][C@@]12[C@@H](C)C3=C(C(O)=CC=C3)C(=O)C1=C(O)[C@]1(O)C(=O)C(C(N)=O)=C(O)[C@@H](N(C)C)[C@]1([H])[C@H]2O	(4S,4aR,5S,5aR,6R,12aS)-4-(dimethylamino)-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboxamide	Doxycycline	444.4	6	FDA Approved Drug Library	24390-14-5	DL-381	2mg/ml	DMSO	2841J
	CCOC(=O)[C@H](CCC1=CC=CC=C1)N[C@@H](C)C(=O)N1CCC[C@H]1C(O)=O	(2S)-1-[(2S)-2-[[(2S)-1-ethoxy-1-oxo-4-phenylbutan-2-yl]amino]propanoyl]pyrrolidine-2-carboxylic acid	Enalapril	376.4	6	FDA Approved Drug Library	75847-73-3	PI-152	2mg/ml	DMSO	2841J
	CCN1C=C(C(O)=O)C(=O)C2=C1N=C(N1CCNCC1)C(F)=C2	1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydro-1,8-naphthyridine-3-carboxylic acid	Enoxacin	320.3	6	FDA Approved Drug Library	74011-58-8	DL-383	2mg/ml	DMSO	2841J
	CCN1CCN(CC1)C1=C(C=C2C(=C1F)C(=O)C(=CN2C1CC1)C(O)=O	1-cyclopropyl-7-(4-ethylpiperazin-1-yl)-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid	Enrofloxacin	359.4	6	FDA Approved Drug Library	93106-60-6	DL-384	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@@](O)(C#C)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CCC2=CC(=O)CC[C@]12C	(1S,2R,10R,11S,14R,15S)-14-ethynyl-14-hydroxy-2,15-dimethyltetracyclo[8.7.0.0^{2},^{7}.0^{11},^{15}]heptadec-6-en-5-one	Ethisterone	312.4	6	FDA Approved Drug Library	434-03-7	DL-385	2mg/ml	DMSO	2841J
	COC1=CC2=C(NC(=N2)S(=O)CC2=C(C)C(OC)=C(C)C=N2)C=C1	5-methoxy-2-{[(4-methoxy-3,5-dimethylpyridin-2-yl)methane]sulfinyl}-1H-1,3-benzodiazole	Esomeprazole	345.4	6	FDA Approved Drug Library	119141-88-7	DL-386	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@H](O)[C@@]1(C)CC[C@]1([H])C3=C(CC[C@@]21[H])C=C(O)C=C3	(1S,10R,11S,14S,15S)-15-methyltetracyclo[8.7.0.0^{2},^{7}.0^{11},^{15}]heptadeca-2(7),3,5-triene-5,14-diol	Estradiol	272.4	6	FDA Approved Drug Library	50-28-2	BL-093	2mg/ml	DMSO	2841J
	[H][C@@]12C[C@@H](O)[C@H](O)[C@@]1(C)CC[C@]1([H])C3=C(CC[C@@]21[H])C=C(O)C=C3	(1S,10R,11S,13R,14R,15S)-15-methyltetracyclo[8.7.0.0^{2},^{7}.0^{11},^{15}]heptadeca-2(7),3,5-triene-5,13,14-triol	Estriol	288.4	6	FDA Approved Drug Library	50-27-1	DL-388	2mg/ml	DMSO	2841J

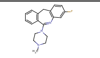
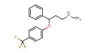
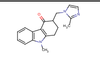
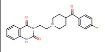
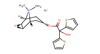
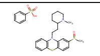
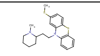
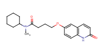
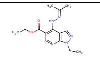
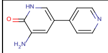
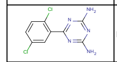
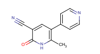
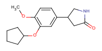
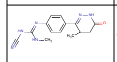
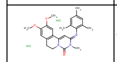
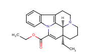
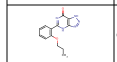
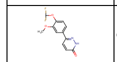
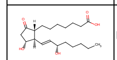
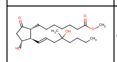
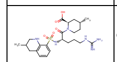
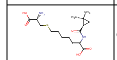
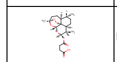
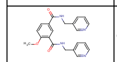
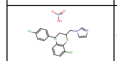
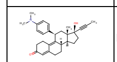
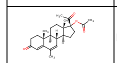
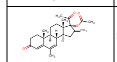
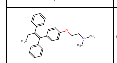
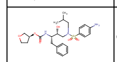
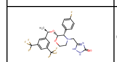
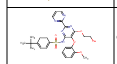
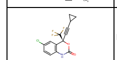
Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	[H][C@@]12CCC(=O)[C@@]1(C)CC[C@@]1([H])C3=C(CC[C@@]21[H])C=C(O)C=C3	(1S,10R,11S,15S)-5-hydroxy-15-methyltetracyclo[8.7.0.0^{1,7}.0^{11,15}]heptadeca-2(7),3,5-trien-14-one	Estrone	270.4	6	FDA Approved Drug Library	53-16-7	BL-090	2mg/ml	DMSO	2841J
	CC(O)(P(O)([O-])=O)P(O)([O-])=O	hydrogen (1-hydrogen phosphonato-1-hydroxyethyl)phosphonate	Etidronate	204.0	6	FDA Approved Drug Library	7414-83-7	DL-390	2mg/ml	DMSO	2841J
	CCOC(=O)/C=C(/C)/C=C/C=C(/C)/C=C/C1=C(C)CCC(C)(C)C1C	ethyl (2E,4E,6E,8E)-9-(4-methoxy-2,3,6-trimethylphenyl)-3,7-dimethylnona-2,4,6,8-tetraenoate	Etretinate	354.5	6	FDA Approved Drug Library	54350-48-0	DL-170	2mg/ml	DMSO	2841J
	NS(=O)(=O)C1=CC2=C(NC(NS2(=O)=O)C(Cl)Cl)C=C1Cl	6-chloro-3-(dichloromethyl)-1,1-dioxo-3,4-dihydro-2H-1λ^{6},2,4-benzothiadiazine-7-sulfonamide	Trichloromethiazide	380.7	6	FDA Approved Drug Library	133-67-5	DL-563	2mg/ml	DMSO	2841J
	CC(=O)OCC(CCN1C=NC2=C1N=C(N)NC2)COC(C)=O	2-[(acetyloxy)methyl]-4-(2-amino-9H-purin-9-yl)butyl acetate	Famciclovir	321.3	6	FDA Approved Drug Library	104227-87-4	DL-392	2mg/ml	DMSO	2841J
	COC(=O)NC1=NC2=C(N1)C=CC(SC1=CC=CC=C1)=C2	methyl N-[5-(phenylsulfanyl)-1H-1,3-benzodiazol-2-yl]carbamate	Fenbendazole	299.3	6	FDA Approved Drug Library	43210-67-9	DL-393	2mg/ml	DMSO	2841J
	OC(=O)CCC(=O)C1=CC=C(C=C1)C1=CC=CC=C1	4-oxo-4-(4-phenylphenyl)butanoic acid	Fenbufen	254.3	6	FDA Approved Drug Library	36330-85-5	DL-394	2mg/ml	DMSO	2841J
	Cl.OC1=CC=C(C=C1)C1CNCCC2=C1C=C(O)C(O)=C2Cl	6-chloro-1-(4-hydroxyphenyl)-2,3,4,5-tetrahydro-1H-3-benzazepine-7,8-diol hydrochloride	FenoldopamHCl	342.2	6	FDA Approved Drug Library	67227-56-9	DL-395	2mg/ml	DMSO	2841J
	CC(C(O)=O)C1=CC=CC(OC2=CC=CC=C2)=C1	2-(3-phenoxyphenyl)propanoic acid	Fenoprofen	242.3	6	FDA Approved Drug Library	31879-05-7	DL-396	2mg/ml	DMSO	2841J
	CC(C)OC(=O)C(C)(C)OC1=CC=C(C=C1)C(=O)C1=CC=C(Cl)C=C1	propan-2-yl 2-{4-[(4-chlorophenyl)carbonyl]phenoxy}-2-methylpropanoate	Fenofibrate	360.8	6	FDA Approved Drug Library	49562-28-9	DL-397	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@H](C(=O)N(C)(C)C)C[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CC[C@@]2([H])NC(=O)C=C[C@]12C	(1S,2R,7R,10S,11S,14S,15S)-N-tert-butyl-2,15-dimethyl-5-oxo-6-azatetracyclo[8.7.0.0^{1,7}.0^{11,15}]heptadec-3-ene-14-carboxamide	Finasteride	372.5	6	FDA Approved Drug Library	98319-26-7	DL-398	2mg/ml	DMSO	2841J
	FC1=CNC(=O)NC1=O	5-fluoro-1,2,3,4-tetrahydropyrimidine-2,4-dione	5-Fluorouracil	130.1	6	FDA Approved Drug Library	51-21-8	DL-399	2mg/ml	DMSO	2841J
	CC(C(O)=O)C1=CC=C(C(F)=C1)C1=CC=CC=C1	2-(3-fluoro-4-phenylphenyl)propanoic acid	Flurbiprofen	244.3	6	FDA Approved Drug Library	5104-49-4	DL-400	2mg/ml	DMSO	2841J
	CN1CCN(CC1)C1=C(F)C2=C(C=C1F)C(=O)C(=CN2CCF)C(O)=O	6,8-difluoro-1-(2-fluoroethyl)-7-(4-methylpiperazin-1-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylic acid	Fleroxacin	369.3	6	FDA Approved Drug Library	79660-72-3	DL-401	2mg/ml	DMSO	2841J
	Cl.CN(C)CCC=C1C2=CC=CC=C2CCC2=C1C=CC=C2	dimethyl(3-{tricyclo[9.4.0.0^{2,7}]pentadeca-1(11),3,5,7,12,14-hexaen-2-ylidene}propyl)amine hydrochloride	AmitriptylineHCl	313.9	6	FDA Approved Drug Library	549-18-8	DL-581	2mg/ml	DMSO	2841J
	OC[C@H]1O[C@H](C[C@@H]1O)N1C=C(F)C(=O)NC1=O	5-fluoro-1-[(2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,2,3,4-tetrahydropyrimidine-2,4-dione	Floxuridine	246.2	6	FDA Approved Drug Library	50-91-9	DL-403	2mg/ml	DMSO	2841J
	[H][C@@]12[C@H]3OC(C)(C)O[C@@]3(C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]1(F)[C@@]2([H])[C@H](F)C2=CC(=O)C=C[C@]12C	(1S,2S,4R,8S,9S,11S,12R,13S,19S)-12,19-difluoro-11-hydroxy-8-(2-hydroxyacetyl)-6,6,9,13-tetramethyl-5,7-dioxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{9,19}]icosa-14,17-dien-16-one	Fluocinolone acetonide	452.5	6	FDA Approved Drug Library	67-73-2	DL-404	2mg/ml	DMSO	2841J
	COC(=O)NC1=NC2=C(N1)C=CC(=C2)C(=O)C1=CC=C(F)C=C1	methyl N-[5-[(4-fluorophenyl)carbonyl]-1H-1,3-benzodiazol-2-yl]carbamate	Flubendazole	313.3	6	FDA Approved Drug Library	31430-15-6	DL-405	2mg/ml	DMSO	2841J
	CC(C)C(=O)NC1=CC=C(C(=C1)C(F)(F)F)[N+](=O)[O-]	2-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]propanamide	Flutamide	276.2	6	FDA Approved Drug Library	13311-84-7	DL-406	2mg/ml	DMSO	2841J
	OC(CN1C=NC=N1)(CN1C=NC=N1)C1=C(F)C=C(F)C=C1	2-(2,4-difluorophenyl)-1,3-bis(1H-1,2,4-triazol-1-yl)propan-2-ol	Fluconazole	306.3	6	FDA Approved Drug Library	86386-73-4	DL-407	2mg/ml	DMSO	2841J
	[H][C@@]12CCC(=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CCC2=C(O)C(=O)CC[C@]12C	(1S,2R,10R,11S,15S)-6-hydroxy-2,15-dimethyltetracyclo[8.7.0.0^{1,7}.0^{11,15}]heptadec-6-ene-5,14-dione	Formestane	302.4	6	FDA Approved Drug Library	566-48-3	DL-408	2mg/ml	DMSO	2841J
	FC1=CN(C2CCCO2)C(=O)NC1=O	5-fluoro-1-(oxolan-2-yl)-1,2,3,4-tetrahydropyrimidine-2,4-dione	Ftorafur	200.2	6	FDA Approved Drug Library	17902-23-7	DL-409	2mg/ml	DMSO	2841J
	NS(=O)(=O)C1=C(Cl)C=C(NCC2=CC=CO2)C(=C1)C(O)=O	4-chloro-2-[(furan-2-ylmethyl)amino]-5-sulfamoylbenzoic acid	Furosemide	330.7	6	FDA Approved Drug Library	54-31-9	DL-410	2mg/ml	DMSO	2841J
	NC1=NC2=C(N=CN2COC(CO)CO)C(=O)N1	2-amino-9-{[1,3-dihydroxypropan-2-yl]oxy}methyl-6,9-dihydro-1H-purin-6-one	Ganciclovir	255.2	6	FDA Approved Drug Library	82410-32-0	DL-411	2mg/ml	DMSO	2841J
	COC1=C(N2CCNC(C)C2)C(F)=CC2=C1N(C=C(C(O)=O)C2=O)C1CC1	1-cyclopropyl-6-fluoro-8-methoxy-7-(3-methylpiperazin-1-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylic acid	Gatifloxacin	375.4	6	FDA Approved Drug Library	112811-59-3	DL-412	2mg/ml	DMSO	2841J
	CN[C@H](C)C[C@@H]1CC[C@@H](N)[C@@H](O)[C@@H]2[C@@H](N)C[C@@H](N)[C@H](O)[C@H]3OC[C@](C)(O)[C@H](NC)[C@H]3O)[C@H]2O)O1	(2R,3R,4R,5R)-2-[[(1S,2S,3R,4S,6R)-4,6-diamino-3-[[(2R,3R,6S)-3-amino-6-[(1R)-1-(methylamino)ethyl]oxan-2-yl]oxy]-2-hydroxycyclohexyl]oxy]-5-methyl-4-(methylamino)oxane-3,5-diol	Gentamycin	477.6	6	FDA Approved Drug Library	1405-41-0	DL-413	2mg/ml	DMSO	2841J
	CC1=CC(OCCCC(C)(C)C(O)=O)=C(C)C=C1	5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoic acid	Gemfibrozil	250.3	6	FDA Approved Drug Library	25812-30-0	DL-414	2mg/ml	DMSO	2841J
	CC1=CC=C(C=C1)S(=O)(=O)NC(=O)NN1CC2CCCC2C1	1-[(4-methylbenzene)sulfonyl]-3-(octahydrocyclopenta[c]pyrrol-2-yl)urea	Glclazide	323.4	6	FDA Approved Drug Library	21187-98-4	DL-415	2mg/ml	DMSO	2841J
	CCC1=C(C)CN(C(=O)NCCC2=CC=C(C=C2)S(=O)(=O)NC(=O)N[C@H]2CC[C@H](C)CC2)C1=O	3-ethyl-4-methyl-N-{2-[4-({[(4-methylcyclohexyl)carbamoyl]amino}sulfonyl)phenyl]ethyl}-2-oxo-2,5-dihydro-1H-pyrrole-1-carboxamide	Glimepride	490.6	6	FDA Approved Drug Library	93479-97-1	DL-416	2mg/ml	DMSO	2841J
	COC1=C(OCC(O)CO)C=CC=C1	3-(2-methoxyphenoxy)propane-1,2-diol	Guaifenesin	198.2	6	FDA Approved Drug Library	93-14-1	DL-417	2mg/ml	DMSO	2841J
	CC[C@@H](C[C@@H](CC)C1=CC=C(O)C=C1)C1=CC=C(O)C=C1	4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]phenol	Hexestrol	270.4	6	FDA Approved Drug Library	84-16-2	DL-418	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]1([H])[C@@]2([H])CCC2=CC(=O)CC[C@]12C	(1S,2R,10S,11S,14R,15S,17S)-14,17-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7.0.0^{1,7}.0^{11,15}]heptadec-6-en-5-one	Hydrocortisone	362.5	6	FDA Approved Drug Library	50-23-7	DL-419	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@](O)(C(=O)COC(C)=O)[C@@]1(C)C[C@H](O)[C@@]1([H])[C@@]2([H])CCC2=CC(=O)CC[C@]12C	2-[(1S,2R,10S,11S,14R,15S,17S)-14,17-dihydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.0.0^{1,7}.0^{11,15}]heptadec-6-en-14-yl]-2-oxoethyl acetate	Hydrocortisone 21-acetate	404.5	6	FDA Approved Drug Library	50-03-3	DL-420	2mg/ml	DMSO	2841J

Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	[H][C@@]12CC[C@](O)(C(=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CCC2=CC(=O)CC[C@]12C	(1S,2R,10R,11S,14R,15S)-14-acetyl-14-hydroxy-2,15-dimethyltetracyclo[8.7.0.0^{1,7}.0^{7,11}.^{1,15}]heptadec-6-en-5-one	17- Hydroxyprogesterone	330.5	6	FDA Approved Drug Library	68-96-2	DL-421	2mg/ml	DMSO	2841J
	OC[C@H]1O[C@H][C@@H](I)N1C=C(I)C(=O)NC1=O	1-[(2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-5-iodo-1,2,3,4-tetrahydropyrimidine-2,4-dione	Idoxuridine	354.1	6	FDA Approved Drug Library	54-42-2	DL-422	2mg/ml	DMSO	2841J
	ClCCNP1(=O)OCCCN1CCl	3-(2-chloroethyl)-2-[(2-chloroethyl)amino]-1,3,2λ^{5}-oxazaphosphinan-2-one	Ifosfamide	261.1	6	FDA Approved Drug Library	3778-73-2	DL-423	2mg/ml	DMSO	2841J
	CC(C)CN1C=NC2=C(N)N=C3C=CC=CC3=C12	1-(2-methylpropyl)-1H-imidazo[4,5-c]quinolin-4-amine	Imiquimod	240.3	6	FDA Approved Drug Library	99011-02-6	ALX-420-039	2mg/ml	DMSO	2841J
	CC1CC2=C(C=CC=C2)N1NC(=O)C1=CC=C(Cl)C(=C1)S(N)(=O)=O	4-chloro-N-(2-methyl-2,3-dihydro-1H-indol-1-yl)-3-sulfamoylbenzamide	Indapamide	365.8	6	FDA Approved Drug Library	26807-65-8	DL-425	2mg/ml	DMSO	2841J
	COC1=CC=C(C=C1OC)C(=O)NCC1=CC=C(OCCN(C)C)C=C1	N-{[4-[2-(dimethylamino)ethoxy]phenyl]methyl}-3,4-dimethoxybenzamide	Itopride	358.4	6	FDA Approved Drug Library	122892-31-3	DL-426	2mg/ml	DMSO	2841J
	CCC(C)N1N=CN(C1=O)C1=CC=C(C=C1)N1CCN(CC1)C1=CC=C(OCC2COC(CN3C=NC=N3)(O2)C2=C(Cl)C=C(Cl)C=C2)C=C1	1-(butan-2-yl)-4-[4-[4-(4-[[2-(2,4-dichlorophenyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl)piperazin-1-yl]phenyl]-4,5-dihydro-1H-1,2,4-triazol-5-one	Itraconazole	705.6	6	FDA Approved Drug Library	84625-61-6	DL-427	2mg/ml	DMSO	2841J
	C[C@H](C(=O)C1=CC(=CC=C1)C(=O)C1=CC=CC=C1	(2S)-2-(3-benzoylphenyl)propanoic acid	(S)-(+)-Ketoprofen	254.3	6	FDA Approved Drug Library	22161-81-5	AO-1005	2mg/ml	DMSO	2841J
	C1CN2C[C@@H](N=C2S1)C1=CC=CC=C1	(6S)-6-phenyl-2H,3H,5H,6H-imidazo[2,1-b][1,3]thiazole	Levamisole	204.3	6	FDA Approved Drug Library	16595-80-5	DL-429	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@@](O)(C#C)[C@@]1(CC)CC[C@]1([H])[C@@]3([H])CCC(=O)C=C3CC[C@@]21[H]	(1S,2R,10R,11S,14R,15S)-15-ethyl-14-ethynyl-14-hydroxytetracyclo[8.7.0.0^{1,7}.0^{7,11}.^{1,15}]heptadec-6-en-5-one	Levonorgestrel	312.4	6	FDA Approved Drug Library	797-63-7	DL-430	2mg/ml	DMSO	2841J
	N[C@@H](CC1=CC(O)=C(O)C=C1)C(O)=O	(2S)-2-amino-3-(3,4-dihydroxyphenyl)propanoic acid	Levodopa	197.2	6	FDA Approved Drug Library	59-92-7	DL-431	2mg/ml	DMSO	2841J
	C[C@H]1COC2=C(N3CCN(C)CC3)C(F)=CC3=C2N1C=C(C(O)=O)C3=O	(2S)-7-fluoro-2-methyl-6-(4-methylpiperazin-1-yl)-10-oxo-4-oxa-1-azatricyclo[7.3.1.0^{5,}^{13}]trideca-5,7,9(13),11-tetraene-11-carboxylic acid	Levofloxacin	361.4	6	FDA Approved Drug Library	100986-85-4	DL-432	2mg/ml	DMSO	2841J
	CC1=C(C=NO1)C(=O)NC1=CC=C(C=C1)C(F)(F)F	5-methyl-N-[4-(trifluoromethyl)phenyl]-1,2-oxazole-4-carboxamide	Leflunomide	270.2	6	FDA Approved Drug Library	75706-12-6	DL-433	2mg/ml	DMSO	2841J
	NCCCC[C@H](N[C@@H](CCC1=CC=CC=C1)C(O)=O)C(=O)N1CCC[C@H]1C(O)=O	(2S)-1-[(2S)-6-amino-2-[[1S)-1-carboxy-3-phenylpropyl]amino]hexanoyl]pyrrolidine-2-carboxylic acid	Lisinopril	405.5	6	FDA Approved Drug Library	83915-83-7	DL-434	2mg/ml	DMSO	2841J
	CCN1C=C(C(O)=O)C(=O)C2=C1C(F)=C(N1CCNC(C)C1)C(F)=C2	1-ethyl-6,8-difluoro-7-(3-methylpiperazin-1-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylic acid	Lomefloxacin	351.3	6	FDA Approved Drug Library	98079-52-8	DL-435	2mg/ml	DMSO	2841J
	CCOC(=O)N1CCC(CC1)=C1C2=C(CCC3=C1N=CC=C3)C=C(Cl)C=C2	ethyl 4-[13-chloro-4-azatricyclo[9.4.0.0^{3,8}]pentadeca-1(11),3(8),4,6,12,14-hexaen-2-ylidene]piperidine-1-carboxylate	Loratadine	382.9	6	FDA Approved Drug Library	79794-75-5	DL-436	2mg/ml	DMSO	2841J
	CCCCCN(CCCCC)C(=O)C(CCC(O)=O)NC(=O)C1=CC(Cl)=C(Cl)C=C1	4-[(3,4-dichlorophenyl)formamido]-4-(dipentylcarbamoyl)butanoic acid	Lorglumide	459.4	6	FDA Approved Drug Library	97964-56-2	DL-437	2mg/ml	DMSO	2841J
	CCCCC1=NC(Cl)=C(CO)N1CC1=CC=C(C=C1)C1=C(C=CC=C1)C1=N[N-]N=N1[K]	[2-butyl-4-chloro-1-({4-[2-(1-potassio-1H-1,2,3,4-tetrazol-5-yl)phenyl]phenyl}methyl)-1H-imidazol-5-yl]methanol	Losartan potassium	461.0	6	FDA Approved Drug Library	124750-99-8	DL-438	2mg/ml	DMSO	2841J
	COC(=O)NC1=NC2=C(N1)C=CC(=C2)C(=O)C1=CC=CC=C1	methyl N-(5-benzoyl-1H-1,3-benzodiazol-2-yl)carbamate	Mebendazol	295.3	7	FDA Approved Drug Library	31431-39-7	DL-439	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@](OC(C)=O)(C(=O)CO)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])[C@H](C)C[C@H](C)C2=CC(=O)CC[C@]12C	(1S,2R,8S,10R,11S,14R,15S)-14-acetyl-2,8,15-trimethyl-5-oxotetracyclo[8.7.0.0^{1,7}.0^{7,11}.^{1,15}]heptadec-6-en-14-yl acetate	Medroxyprogesterone 17-Acetate	386.5	7	FDA Approved Drug Library	71-58-9	DL-440	2mg/ml	DMSO	2841J
	CC1=CC=CC(NC2=C(C=CC=C2)C(O)=O)=C1C	2-[(2,3-dimethylphenyl)amino]benzoic acid	Mefenamic acid	241.3	7	FDA Approved Drug Library	61-68-7	DL-441	2mg/ml	DMSO	2841J
	N[C@@H](CC1=CC=C(C=C1)N(CCCl)CCCl)C(O)=O	(2S)-2-amino-3-[4-[bis(2-chloroethyl)amino]phenyl]propanoic acid	Melphalan	305.2	7	FDA Approved Drug Library	148-82-3	DL-442	2mg/ml	DMSO	2841J
	C[C@](N)(CC1=CC(O)=C(O)C=C1)C(O)=O	(2S)-2-amino-3-(3,4-dihydroxyphenyl)-2-methylpropanoic acid	Methyldopa	211.2	7	FDA Approved Drug Library	555-30-6	DL-443	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]1([H])[C@@]2([H])[C@H](C)C[C@H](C)C2=CC(=O)C=C[C@]12C	(1S,2R,8S,10S,11S,14R,15S,17S)-14,17-dihydroxy-14-(2-hydroxyacetyl)-2,8,15-trimethyltetracyclo[8.7.0.0^{1,7}.0^{11,17}.^{1,15}]heptadeca-3,6-dien-5-one	Methylprednisolone	374.5	7	FDA Approved Drug Library	83-43-2	DL-444	2mg/ml	DMSO	2841J
	COCCC1=CC=C(OCC(O)CNC(C)C)C=C1	(2-hydroxy-3-[4-(2-methoxyethyl)phenoxy]propyl)(propan-2-yl)amine	Metoprolol	267.4	7	FDA Approved Drug Library	56392-17-7	DL-445	2mg/ml	DMSO	2841J
	CN1C=CNC1=S	1-methyl-2,3-dihydro-1H-imidazole-2-thione	Methimazole	114.2	7	FDA Approved Drug Library	60-56-0	DL-446	2mg/ml	DMSO	2841J
	CC1=NC=C(N1CCO)[N+](=O)[O-]=O	2-(2-methyl-5-nitro-1H-imidazol-1-yl)ethan-1-ol	Metronidazole	171.2	7	FDA Approved Drug Library	443-48-1	DL-447	2mg/ml	DMSO	2841J
	ClC1=CC=C(COC(CN2C=CN=C2)C2=C(Cl)C=C(Cl)C=C2)C(Cl)=C1	1-[2-(2,4-dichlorophenyl)-2-[(2,4-dichlorophenyl)methoxy]ethyl]-1H-imidazole	Miconazole	416.1	7	FDA Approved Drug Library	22916-47-8	DL-448	2mg/ml	DMSO	2841J
	[H][C@@]12CC3=C(C(O)=CC=C3N(C)C)C(=O)C1=C(O)[C@]1(O)C(=O)C(C(N)=O)=C(O)[C@@H](N(C)C)[C@]1([H])C2	(4S,4aS,5aR,12aS)-4,7-bis(dimethylamino)-3,10,12,12a-tetrahydroxy-1,11-dioxo-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboxamide	Minocycline	457.5	7	FDA Approved Drug Library	10118-90-8	DL-449	2mg/ml	DMSO	2841J
	OCCNCCNC1=CC=C(NCCNCCO)C2=C1C(=O)C1=C(C2=O)C(O)=CC=C1O	1,4-dihydroxy-5,8-bis([2-[(2-hydroxyethyl)amino]ethyl]amino)-9,10-dihydroanthracene-9,10-dione	Mitoxantrone	444.5	7	FDA Approved Drug Library	65271-80-9	DL-450	2mg/ml	DMSO	2841J
	[H][C@@]12C[C@H](O)[C@@]3(C)C(=O)[C@H](OC(=O)C4=C(C)[C@H](C)[C@@](O)([C@@H](OC(=O)C5=CC=CC=C5)[C@]3([H])[C@@]1(COC2)OC(C)=O)C4(C)C)OC(=O)[C@H](O)[C@@H](NC(=O)C1=CC=CC=C1)C1=CC=CC=C1	(1S,2S,3R,4S,7R,9S,10S,12R,15S)-4,12-bis(acetyloxy)-1,9-dihydroxy-15-[((2R,3S)-2-hydroxy-3-phenyl-3-(phenylformamido)propanoyl)oxy]-10,14,17,17-tetramethyl-11-oxo-6-oxatetracyclo[11.3.1.0^{1,10}.0^{3,7}]heptadec-13-en-2-yl benzoate	Taxol	853.9	7	FDA Approved Drug Library	33069-62-6	T-104	2mg/ml	DMSO	2841J
	CCCCC(CN1C=NC=N1)(C#N)C1=CC=C(Cl)C=C1	2-(4-chlorophenyl)-2-(1H-1,2,4-triazol-1-ylmethyl)hexanenitrile	Myclobutanil	288.8	7	FDA Approved Drug Library	88671-89-0	DL-452	2mg/ml	DMSO	2841J
	CC1CCC2=C(N3CCC(O)CC3)C(F)=CC3=C2N1C=C(C(O)=O)C3=O	7-fluoro-8-(4-hydroxypiperidin-1-yl)-12-methyl-4-oxo-1-azatricyclo[7.3.1.0^{5,}^{13}]trideca-2,5(13),6,8-tetraene-3-carboxylic acid	Nadifloxacin	360.4	7	FDA Approved Drug Library	124858-35-1	DL-453	2mg/ml	DMSO	2841J

Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	COC1=CC2=CC=C(CCC(C)=O)C=C2C=C1	4-(6-methoxynaphthalen-2-yl)butan-2-one	Nabumetone	228.3	7	FDA Approved Drug Library	42924-53-8	DL-454	2mg/ml	DMSO	2841J
	C(C1=NCCN1)C1=C2C=CC=CC2=CC=C1	2-(naphthalen-1-ylmethyl)-4,5-dihydro-1H-imidazole	Naphazoline	210.3	7	FDA Approved Drug Library	835-31-4	DL-455	2mg/ml	DMSO	2841J
	CCC1=NN(CCCN2CCN(CC2)C2=CC(Cl)=CC=C2)C(=O)N1CCOC1=CC=CC=C1	1-{3-[4-(3-chlorophenyl)piperazin-1-yl]propyl}-3-ethyl-4-(2-phenoxyethyl)-4,5-dihydro-1H-1,2,4-triazol-5-one	Nefazodone	470.0	7	FDA Approved Drug Library	83366-66-9	DL-456	2mg/ml	DMSO	2841J
	OC(=O)C1=CC=CN=C1NC1=CC(=CC=C1)C(F)(F)F	2-{[3-(trifluoromethyl)phenyl]amino}pyridine-3-carboxylic acid	Niflumic acid	282.2	7	FDA Approved Drug Library	4394-00-7	DL-457	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@@](O)(C#C)[C@@]1(C)CC[C@]1([H])[C@@]3([H])CCC(=O)C=C3CC[C@@]21[H]	(1S,2R,10R,11S,14R,15S)-14-ethynyl-14-hydroxy-15-methyltetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadec-6-en-5-one	Norethindrone	298.4	7	FDA Approved Drug Library	68-22-4	DL-458	2mg/ml	DMSO	2841J
	CCN1C=C(C(O)=O)C(=O)C2=CC(F)=C(C=C12)N1CCNCC1	1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic acid	Norfloxacin	319.3	7	FDA Approved Drug Library	70458-96-7	DL-459	2mg/ml	DMSO	2841J
	C[C@H]1O[C@@H](OC2CC(O)C(C(O)CC(=O)CC(O)C(O)CCC(O)CC(O)CC(O)CC(=O)OC(C)C(C)C(O)C(C)\C=C\C=C\CC\C=C\C=C\C=C\C=C\2)C(O)=O)[C@@H](O)[C@@H](N)[C@@H]1O	(21E,23E,25E,27E,31E,33E)-20-{[(2R,3S,4S,5S,6R)-4-amino-3,5-dihydroxy-6-methyloxan-2-yl]oxy}-4,6,8,11,12,16,18,36-octahydroxy-35,37,38-trimethyl-2,14-dioxo-1-oxacyclooctatriaconta-21,23,25,27,31,33-hexaene-17-carboxylic acid	Nystatin	926.1	7	FDA Approved Drug Library	1400-61-9	DL-460	2mg/ml	DMSO	2841J
	CC1COC2=C(N3CCN(C)CC3)C(F)=CC3=C2N1C=C(C(O)=O)C3=O	7-fluoro-2-methyl-6-(4-methylpiperazin-1-yl)-10-oxo-4-oxa-1-azatricyclo[7.3.1.0^{5,13}]trideca-5,7,9(13),11-tetraene-11-carboxylic acid	Ofloxacin	361.4	7	FDA Approved Drug Library	82419-36-1	DL-461	2mg/ml	DMSO	2841J
	CC1=C(SSC1=S)C1=CN=CC=N1	4-methyl-5-(pyrazin-2-yl)-3H-1,2-dithiole-3-thione	Oltipraz	226.3	7	FDA Approved Drug Library	64224-21-1	DL-106	2mg/ml	DMSO	2841J
	COC1=CC2=C(NC(=N2)S(=O)CC2=C(C)C(OC)=C(C)C=N2)C=C1	5-methoxy-2-{[(4-methoxy-3,5-dimethylpyridin-2-yl)methane]sulfinyl}-1H-1,3-benzodiazole	Omeprazole	345.4	7	FDA Approved Drug Library	73590-58-6	DL-462	2mg/ml	DMSO	2841J
	NC(=O)N1C2=C(CC(=O)C3=C1C=CC=C3)C=CC=C2	9-oxo-2-azatricyclo[9.4.0.0^{3,8}]pentadeca-1(11),3(8),4,6,12,14-hexaene-2-carboxamide	Oxcarbazepine	252.3	7	FDA Approved Drug Library	28721-07-5	DL-463	2mg/ml	DMSO	2841J
	ClC1=CC=C(CO\N=C(/CN2C=CN=C2)C2=C(Cl)C=C(Cl)C=C2)C(Cl)=C1	(Z)-[1-(2,4-dichlorophenyl)-2-(1H-imidazol-1-yl)ethylidene][(2,4-dichlorophenyl)methoxy]amine	Oxiconazole	429.1	7	FDA Approved Drug Library	64211-46-7	DL-464	2mg/ml	DMSO	2841J
	CC1=C(C(=O)N[C@H]2[C@H]3SC(C)(C)[C@@H](N3C2=O)C([O-])=O)C(=NO1)C1=CC=CC=C1	(2S,5R,6R)-3,3-dimethyl-6-(5-methyl-3-phenyl-1,2-oxazole-4-amido)-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylate	Oxacillin	400.4	7	FDA Approved Drug Library	7240-38-2	DL-465	2mg/ml	DMSO	2841J
	COC(=O)NC1=NC2=C(N1)C=CC(=C2)S(=O)C1=CC=CC=C1	methyl N-[5-(benzenesulfinyl)-1H-1,3-benzodiazol-2-yl]carbamate	Oxfendazole	315.3	7	FDA Approved Drug Library	53716-50-0	DL-466	2mg/ml	DMSO	2841J
	CCCOC1=CC2=C(NC(NC(=O)OC)=N2)C=C1	methyl N-(5-propoxy-1H-1,3-benzodiazol-2-yl)carbamate	Oxibendazole	249.3	7	FDA Approved Drug Library	20559-55-1	DL-467	2mg/ml	DMSO	2841J
	COC1=CC=NC(CS(=O)C2=NC3=C(N2)C=CC(OC(F)F)=C3)=C1OC	5-(difluoromethoxy)-2-{[(3,4-dimethoxypyridin-2-yl)methane]sulfinyl}-1H-1,3-benzodiazole	Pantoprazole	383.4	7	FDA Approved Drug Library	102625-70-7	DL-468	2mg/ml	DMSO	2841J
	FC1=CC=C(C=C1)[C@@H]1CCNC[C@H]1COC1=CC2=C(OCO2)C=C1	(3S,4R)-3-[(2H-1,3-benzodioxol-5-yloxy)methyl]-4-(4-fluorophenyl)piperidine	Paroxetine	329.4	7	FDA Approved Drug Library	110429-49-8	NS-710	2mg/ml	DMSO	2841J
	C[C@H]1COC2=C(C(F)=CC3=C2N1C=C(C(O)=O)C3=O)C1(N)CC1	(2S)-6-(1-aminocyclopropyl)-7-fluoro-2-methyl-10-oxo-4-oxa-1-azatricyclo[7.3.1.0^{5,13}]trideca-5,7,9(13),11-tetraene-11-carboxylic acid	Pazufloxacin	318.3	7	FDA Approved Drug Library	127045-41-4	DL-470	2mg/ml	DMSO	2841J
	[H]O[H].[H]O[H].OS(O)(=C)=O.CCN1C=C(C(O)=O)C(=O)C2=C1C=C(N1CCN(C)CC1)C(F)=C2	1-ethyl-6-fluoro-7-(4-methylpiperazin-1-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylic acid methanesulfurous acid dihydrate	Pefloxacine mesylate dihydrate	465.5	7	FDA Approved Drug Library	149676-40-4	DL-471	2mg/ml	DMSO	2841J
	NC1=NC2=C(N=CN2CCC(CO)CO)C(=O)N1	2-amino-9-[4-hydroxy-3-(hydroxymethyl)butyl]-6,9-dihydro-1H-purin-6-one	Penciclovir	253.3	7	FDA Approved Drug Library	39809-25-1	DL-472	2mg/ml	DMSO	2841J
	CN1C=NC2=C1C(=O)N(CCCCC(C)=O)C(=O)N2C	3,7-dimethyl-1-(5-oxohexyl)-2,3,6,7-tetrahydro-1H-purine-2,6-dione	Pentoxifylline	278.3	7	FDA Approved Drug Library	6493-05-6	DL-473	2mg/ml	DMSO	2841J
	CC1(C)S[C@@H]2[C@H](NC(=O)COC3=CC=CC=C3)C(=O)N2[C@H]1C([O-])=O	(2S,5R,6R)-3,3-dimethyl-7-oxo-6-(2-phenoxyacetamido)-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylate	Pencillin V	349.4	7	FDA Approved Drug Library	132-98-9	DL-474	2mg/ml	DMSO	2841J
	CCCCC1C(=O)N(N(C1=O)C1=CC=CC=C1)C1=CC=CC=C1	4-butyl-1,2-diphenylpyrazolidine-3,5-dione	Phenylbutazone	308.4	7	FDA Approved Drug Library	50-33-9	DL-475	2mg/ml	DMSO	2841J
	CCN1CCN(C(=O)N[C@@H](C(=O)N[C@H]2[C@H]3SC(C)(C)[C@@H](N3C2=O)C(O)=O)C2=CC=CC=C2)C(=O)C1=O	(2S,5R,6R)-6-[(2R)-2-{[(4-ethyl-2,3-dioxopiperazin-1-yl)carbonyl]amino}-2-phenylacetamido]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid	Piperacillin	517.6	7	FDA Approved Drug Library	61477-96-1	DL-476	2mg/ml	DMSO	2841J
	[H][C@]12[C@H](C[C@H](O)C=C1C=C[C@H](C)[C@@H]2CC[C@@H]1C[C@@H](O)CC(=O)O1)OC(=O)[C@@H](C)CC	(1S,3S,7S,8S,8aR)-3-hydroxy-8-{2-[(2R,4R)-4-hydroxy-6-oxooxan-2-yl]ethyl}-7-methyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl (2S)-2-methylbutanoate	Pravastatin Lactone	406.5	7	FDA Approved Drug Library	85956-22-5	DL-477	2mg/ml	DMSO	2841J
	CC(C(O)=O)C1=CC2=C(OC3=C(C2)C=CC=N3)C=C1	2-{5H-chromeno[2,3-b]pyridin-7-yl}propanoic acid	Pranoprofen	255.3	7	FDA Approved Drug Library	52549-17-4	DL-478	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]1([H])[C@@]2([H])CCC2=CC(=O)C=C[C@]12C	(1S,2R,10S,11S,14R,15S,17S)-14,17-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadeca-3,6-dien-5-one	Prednisolone	360.4	7	FDA Approved Drug Library	50-24-8	DL-479	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@H](C(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CCC2=CC(=O)CC[C@]12C	(1S,2R,10S,11S,14S,15S)-14-acetyl-2,15-dimethyltetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadec-6-en-5-one	Progesterone	314.5	7	FDA Approved Drug Library	57-83-0	DL-480	2mg/ml	DMSO	2841J
	CNNCC1=CC=C(C=C1)C(=O)NC(C)C	4-[(2-methylhydrazin-1-yl)methyl]-N-(propan-2-yl)benzamide	Procarbazine	221.3	7	FDA Approved Drug Library	366-70-1	DL-481	2mg/ml	DMSO	2841J
	CCCC1=CC(=CC=N1)C(N)=S	2-propylpyridine-4-carbothioamide	Prothionamide	180.3	7	FDA Approved Drug Library	14222-60-7	DL-482	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@](O)(C(=O)CO)[C@@]1(C)CC(=O)[C@@]1([H])[C@@]2([H])CCC2=CC(=O)C=C[C@]12C	(1S,2R,10S,11S,14R,15S)-14-hydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadeca-3,6-diene-5,17-dione	Prednisone	358.4	7	FDA Approved Drug Library	53-03-2	DL-483	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@H](C(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CC=C2C[C@@H](O)CC[C@]12C	1-[(1S,2R,5S,10S,11S,14S,15S)-5-hydroxy-2,15-dimethyltetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadec-7-en-14-yl]ethan-1-one	Pregnenolone	316.5	7	FDA Approved Drug Library	145-13-1	DL-484	2mg/ml	DMSO	2841J
	COC1=CC2=CC=CN=C2C(NC(C)CCCN)=C1	N-(5-aminopentan-2-yl)-6-methoxyquinolin-8-amine	Primaquine	259.3	7	FDA Approved Drug Library	63-45-6	DL-485	2mg/ml	DMSO	2841J

Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	O=C(C1CCCCC1)N1CC2N(CCC3=C2C=CC=C3)C(=O)C1	2-cyclohexanecarbonyl-1H,2H,3H,4H,6H,7H,11bH-piperazino[2,1-a]isoquinolin-4-one	Praziquantel	312.4	7	FDA Approved Drug Library	55268-74-1	DL-486	2mg/ml	DMSO	2841J
	CN1CCCN=C1\C=C\C1=CC=CS1.OC(=O)C1=C(O)C(CC2=C3C=CC=CC3=CC(C(O)=O)=C2O)=C2C=CC=CC2=C1	1-methyl-2-[(E)-2-(thiophen-2-yl)ethenyl]-1,4,5,6-tetrahydropyrimidine; 4-[(3-carboxy-2-hydroxynaphthalen-1-yl)methyl]-3-hydroxynaphthalene-2-carboxylic acid	Pyrantel Pamoate	594.7	7	FDA Approved Drug Library	22204-24-6	DL-487	2mg/ml	DMSO	2841J
	CCN(CC)CCCC(C)NC1=C2C=C(OC)C=CC2=NC2=CC(Cl)=CC=C12	{4-[(6-chloro-2-methoxyacridin-9-yl)amino]pentyl}diethylamine	Quinacrine	400.0	7	FDA Approved Drug Library	83-89-6	DL-488	2mg/ml	DMSO	2841J
	CCOC(=O)[C@H](CCC1=CC=CC=C1)N[C@@H](C)C(=O)N1CC2=CC=CC=C2C[C@H]1C(O)=O	(3S)-2-[(2S)-2-{[(2S)-1-ethoxy-1-oxo-4-phenylbutan-2-yl]amino}propanoyl]-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid	Quinapril	438.5	7	FDA Approved Drug Library	82586-55-8	DL-489	2mg/ml	DMSO	2841J
	CC(=O)SCC(CC1=CC=CC=C1)C(=O)NCC(=O)OCC1=CC=CC=C1	benzyl 2-{2-[(acetylsulfanyl)methyl]-3-phenylpropanamido}acetate	Racecadotril	385.5	7	FDA Approved Drug Library	81110-73-8	DL-159	2mg/ml	DMSO	2841J
	Cl.Cl.COC1=CC=CC=C1OCC(O)CN1CCN(CC(=O)NC2=C(C)C=CC=C2C)CC1	N-(2,6-dimethylphenyl)-2-{4-[2-hydroxy-3-(2-methoxyphenoxy)propyl]piperazin-1-yl}acetamide dihydrochloride	Ranolazine·2HCl	500.5	7	FDA Approved Drug Library	95635-56-6	DL-490	2mg/ml	DMSO	2841J
	[H][C@@]12CCC[C@]1([H])N([C@@H](C2)C(O)=O)C(=O)[C@H](C)N[C@@H](CCC1=CC=CC=C1)C(=O)OCC	(2S,3aS,6aS)-1-[(2S)-2-{[(2S)-1-ethoxy-1-oxo-4-phenylbutan-2-yl]amino}propanoyl]-octahydrocyclopenta[b]pyrrole-2-carboxylic acid	Ramipril	416.5	7	FDA Approved Drug Library	87333-19-5	DL-491	2mg/ml	DMSO	2841J
	OC(=O)C(CC1=CC(=O)NC2=C1C=CC=C2)NC(=O)C1=CC=C(Cl)C=C1	2-[(4-chlorophenyl)formamido]-3-(2-oxo-1,2-dihydroquinolin-4-yl)propanoic acid	Rebamipide	370.8	7	FDA Approved Drug Library	90098-04-7	DL-147	2mg/ml	DMSO	2841J
	NC(=O)C1=NN(C=N1)[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O	1-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1H-1,2,4-triazole-3-carboxamide	Ribavirin	244.2	7	FDA Approved Drug Library	36791-04-5	DL-492	2mg/ml	DMSO	2841J
	CS(O)(=O)=O.CC1=C(O)C=CC=C1C(=O)N[C@@H](CSC1=CC=CC=C1)[C@H](O)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C	(3S,4aS,8aS)-N-tert-butyl-2-[(2R,3R)-2-hydroxy-3-[(3-hydroxy-2-methylphenyl)formamido]-4-(phenylsulfanyl)butyl]-decahydroisoquinoline-3-carboxamide; methanesulfonic acid	Nelfinavir mesylate	663.9	7	FDA Approved Drug Library	159989-64-7	DL-566	2mg/ml	DMSO	2841J
	[H][C@]12C[C@]3([H])C[C@]([H])(C1)C[C@](C2)(C3)C(C)N	1-(adamantan-1-yl)ethan-1-amine	Rimantadine	179.3	7	FDA Approved Drug Library	1501-84-4	DL-494	2mg/ml	DMSO	2841J
	CC(C)NCC(O)COC1=CC=CC2=C1C=CC=C2	[2-hydroxy-3-(naphthalen-1-yloxy)propyl](propan-2-yl)amine	Propranolol	259.3	7	FDA Approved Drug Library	3506-09-0	ST-405	2mg/ml	DMSO	2841J
	Cl.CC(=O)OCC(=O)NCCCOC1=CC(CN2CCCCC2)=CC=C1	({3-[3-(piperidin-1-ylmethyl)phenoxy]propyl}carbamoyl)methyl acetate hydrochloride	Roxatidine acetate·HCl	384.9	7	FDA Approved Drug Library	93793-83-0	DL-496	2mg/ml	DMSO	2841J
	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@](C)(O)C[C@@H](C)\C(=N\OCOCCOC)[C@H](C)[C@@H](O)[C@]1(C)O	(3R,4S,5S,6R,7R,9R,10Z,11S,12R,13S,14R)-6-{[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy}-14-ethyl-7,12,13-trihydroxy-4-{[(2R,4R,5S,6S)-5-hydroxy-4-methoxy-4,6-dimethyloxan-2-yl]oxy}-3,5,7,9,11,13-hexamethyl-10-(2,4,7-trioxa-1-azaoctan-1-ylidene)-1-oxacyclotetradecan-2-one	Roxithromycin	837.0	7	FDA Approved Drug Library	80214-83-1	DL-497	2mg/ml	DMSO	2841J
	CN1CCN(CC1)C1=C2SCCN3C=C(C(O)=O)C(=O)C(C=C1F)=C23	7-fluoro-6-(4-methylpiperazin-1-yl)-10-oxo-4-thia-1-azatricyclo[7.3.1.0^{5,13}]trideca-5,7,9(13),11-tetraene-11-carboxylic acid	Rufloxacin	363.4	7	FDA Approved Drug Library	106017-08-7	DL-498	2mg/ml	DMSO	2841J
	OC(=O)C1=CN(C2=CC=C(F)C=C2)C2=C(C=C(F)C(=C2)N2CCNCC2)C1=O	6-fluoro-1-(4-fluorophenyl)-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic acid	Sarafloxacin	385.4	7	FDA Approved Drug Library	91296-87-6	DL-499	2mg/ml	DMSO	2841J
	[H][C@]12O[C@@]1([H])[C@]1([H])C[C@@H](C[C@@]2([H])[N+]1(C)CCCC)OC(=O)[C@H](CO)C1=CC=CC=C1	(1R,2R,4S,5S,7S)-9-butyl-7-{[(2S)-3-hydroxy-2-phenylpropanoyl]oxy}-9-methyl-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]nonan-9-ium	Scopolamine N-butyl	360.5	7	FDA Approved Drug Library	149-64-4	DL-500	2mg/ml	DMSO	2841J
	[H][C@]12O[C@@]1([H])[C@]1([H])C[C@@H](C[C@@]2([H])N1C)OC(=O)[C@H](CO)C1=CC=CC=C1	(1R,2R,4S,5S,7S)-9-methyl-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]nonan-7-yl (2S)-3-hydroxy-2-phenylpropanoate	Scopolamine	303.4	7	FDA Approved Drug Library	114-49-8	DL-501	2mg/ml	DMSO	2841J
	CC(O)CN1C(C)=NC=C1[N+]([O-])=O	1-(2-methyl-5-nitro-1H-imidazol-1-yl)propan-2-ol	Secnidazole	185.2	7	FDA Approved Drug Library	3366-95-8	DL-502	2mg/ml	DMSO	2841J
	CC(C)CC(N(C)C)C1(CCC1)C1=CC=C(Cl)C=C1	{1-[1-(4-chlorophenyl)cyclobutyl]-3-methylbutyl}dimethylamine	Sibutramine	279.8	7	FDA Approved Drug Library	125494-59-9	DL-503	2mg/ml	DMSO	2841J
	C[C@H]1CN(C[C@@H](C)N1)C1=C(F)C2=C(C(=O)C(=CN2C2CC2)C(O)=O)C(N)=C1F	5-amino-1-cyclopropyl-7-[(3R,5S)-3,5-dimethylpiperazin-1-yl]-6,8-difluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid	Sparfloxacin	392.4	7	FDA Approved Drug Library	110871-86-8	DL-149	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@@]3(CCC(=O)O3)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])[C@@H](CC2=CC(=O)CC[C@]12C)SC(C)=O	(1'S,2R,2'R,9'R,10'R,11'S,15'S)-9'-(acetylsulfanyl)-2',15'-dimethylspiro[oxolane-2,14'-tetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadecan]-6'-ene-5,5'-dione	Spironolactone	416.6	7	FDA Approved Drug Library	52-01-7	DL-504	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@](C)(O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CC[C@@]2([H])CC3=C(C[C@]12C)C=NN3	(1S,2S,10S,13R,14S,17S,18S)-2,17,18-trimethyl-6,7-diazapentacyclo[11.7.0.0^{2,10}.0^{4,8}.0^{14,18}]icosa-4(8),5-dien-17-ol	Stanozolol	328.5	7	FDA Approved Drug Library	10418-03-8	DL-505	2mg/ml	DMSO	2841J
	CN[C@H]1[C@H](O)[C@@H](O)[C@H](CO)O[C@H]1O[C@H]1[C@H](O[C@@H]2[C@@H](O)[C@H](O)[C@@H](NC(N)=N)[C@H](O)[C@H]2NC(N)=N)O[C@@H](C)[C@]1(O)C=O	1-[(1R,2S,3S,4R,5S,6S)-3-carbamimidamido-6-{[(2R,3R,4R,5S)-3-{[(2S,3S,4S,5R,6S)-4,5-dihydroxy-6-(hydroxymethyl)-3-(methylamino)oxan-2-yl]oxy}-4-formyl-4-hydroxy-5-methyloxolan-2-yl]oxy}-2,4,5-trihydroxycyclohexyl]guanidine	Streptomycin	581.6	7	FDA Approved Drug Library	3810-74-0	DL-506	2mg/ml	DMSO	2841J
	COC1=C(OC)C(NS(=O)(=O)C2=CC=C(N)C=C2)=NC=N1	4-amino-N-(5,6-dimethoxypyrimidin-4-yl)benzene-1-sulfonamide	Sulfadoxine	310.3	7	FDA Approved Drug Library	2447-57-6	DL-507	2mg/ml	DMSO	2841J
	NC1=CC=C(C=C1)S(=O)(=O)NC1=NC=CC=N1	4-amino-N-(pyrimidin-2-yl)benzene-1-sulfonamide	Sulfadiazine	250.3	7	FDA Approved Drug Library	68-35-9	DL-508	2mg/ml	DMSO	2841J
	COC1=NC(OC)=NC(NS(=O)(=O)C2=CC=C(N)C=C2)=C1	4-amino-N-(2,6-dimethoxypyrimidin-4-yl)benzene-1-sulfonamide	Sulfadimethoxine	310.3	7	FDA Approved Drug Library	122-11-2	DL-509	2mg/ml	DMSO	2841J
	OC(=O)C1=CC(=CC=C1O)\N=N\C1=CC=C(C=C1)S(=O)(=O)NC1=CC=CC=N1	2-hydroxy-5-[(E)-2-{4-[(pyridin-2-yl)sulfamoyl]phenyl}diazen-1-yl]benzoic acid	Sulfasalazine	398.4	7	FDA Approved Drug Library	599-79-1	DL-510	2mg/ml	DMSO	2841J
	CCOC1=C(OCCN[C@H](C)CC2=CC=C(OC)C(=C2)S(N)(=O)=O)C=CC=C1	5-[(2R)-2-{[2-(2-ethoxyphenoxy)ethyl]amino}propyl]-2-methoxybenzene-1-sulfonamide	Tamsulosin	408.5	7	FDA Approved Drug Library	106463-17-6	DL-160	2mg/ml	DMSO	2841J
	CCCC1=NC2=C(C=C(C=C2C)C2=NC3=C(C=CC=C3)N2C)N1CC1=CC=C(C=C1)C1=C(C=CC=C1)C(O)=O	2-(4-{[4-methyl-6-(1-methyl-1H-1,3-benzodiazol-2-yl)-2-propyl-1H-1,3-benzodiazol-1-yl]methyl}phenyl)benzoic acid	Telmisartan	514.6	7	FDA Approved Drug Library	144701-48-4	DL-511	2mg/ml	DMSO	2841J
	CN1C(C(=O)NC2=NC=CC=C2)=C(O)C2=C(C=CS2)S1(=O)=O	4-hydroxy-2-methyl-1,1-dioxo-N-(pyridin-2-yl)-2H-1λ^{6},5,2-thieno[2,3-e][1λ^{6},2]thiazine-3-carboxamide	Tenoxicam	337.4	7	FDA Approved Drug Library	59804-37-4	DL-512	2mg/ml	DMSO	2841J
	COC1=CC2=C(C=C1OC)C(N)=NC(=N2)N1CCN(CC1)C(=O)C1CCCO1	6,7-dimethoxy-2-{4-[(oxolan-2-yl)carbonyl]piperazin-1-yl}quinazolin-4-amine	Terazosin	387.4	7	FDA Approved Drug Library	63590-64-7	DL-513	2mg/ml	DMSO	2841J
	[H][C@@]12C[C@@]3([H])C(C(=O)C4=C(C=CC=C4O)[C@@]3(C)O)=C(O)[C@]1(O)C(=O)C(C(N)=O)=C(O)[C@H]2N(C)C	(4S,4aS,5aS,6S,12aS)-4-(dimethylamino)-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboxamide	Tetracycline	444.4	8	FDA Approved Drug Library	60-54-8	DL-514	2mg/ml	DMSO	2841J

Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	COC1=NC2=C(NC(=N2)S(=O)CC2=NC=C(C)C(OC)=C2C)C=C1	4-methoxy-2-({5-methoxy-1H-imidazo[4,5-b]pyridine-2-sulfinyl}methyl)-3,5-dimethylpyridine	Tenatoprazole	346.4	8	FDA Approved Drug Library	113712-98-4	DL-169	2mg/ml	DMSO	2841J
	CN1N=NC2=C(N=CN2C1=O)C(N)=O	3-methyl-4-oxo-3H,4H-imidazo[4,3-d][1,2,3,5]tetrazine-8-carboxamide	Temozolomide	194.2	8	FDA Approved Drug Library	85622-93-1	DL-190	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@@](O)(C#C)[C@@]1(C)CC[C@]1([H])C3=C(C[C@@H](C)[C@@]21[H])CC(=O)CC3	(1S,9R,10R,11S,14R,15S)-14-ethynyl-14-hydroxy-9,15-dimethyltetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadec-2(7)-en-5-one	Tibolone	312.4	8	FDA Approved Drug Library	5630-53-5	DL-206	2mg/ml	DMSO	2841J
	ClC1=C(COC(CN2C=CN=C2)C2=C(Cl)C=C(Cl)C=C2)C=CS1	1-{2-[(2-chlorothiophen-3-yl)methoxy]-2-(2,4-dichlorophenyl)ethyl}-1H-imidazole	Tioconazole	387.7	8	FDA Approved Drug Library	65899-73-2	DL-515	2mg/ml	DMSO	2841J
	CCS(=O)(=O)CCN1C(C)=NC=C1[N+]([O-])=O	1-[2-(ethanesulfonyl)ethyl]-2-methyl-5-nitro-1H-imidazole	Tinidazole	247.3	8	FDA Approved Drug Library	19387-91-8	DL-516	2mg/ml	DMSO	2841J
	NC[C@H]1O[C@H](O[C@@H]2[C@@H](N)C[C@@H](N)[C@H](O[C@H]3O[C@H](CO)[C@@H](O)[C@H](N)[C@H]3O)[C@H]2O)[C@H](N)C[C@@H]1O	(2S,3R,4S,5S,6R)-4-amino-2-{[(1S,2S,3R,4S,6R)-4,6-diamino-3-{[(2R,3R,5S,6R)-3-amino-6-(aminomethyl)-5-hydroxyoxan-2-yl]oxy}-2-hydroxycyclohexyl]oxy}-6-(hydroxymethyl)oxane-3,5-diol	Tobramycin (free base)	467.5	8	FDA Approved Drug Library	32986-56-4	DL-517	2mg/ml	DMSO	2841J
	NC1CCN(C1)C1=NC2=C(C=C1F)C(=O)C(=CN2C1=C(F)C=C(F)C=C1)C(O)=O	7-(3-aminopyrrolidin-1-yl)-1-(2,4-difluorophenyl)-6-fluoro-4-oxo-1,4-dihydro-1,8-naphthyridine-3-carboxylic acid	Tosufloxacin	404.3	8	FDA Approved Drug Library	100490-36-6	DL-188	2mg/ml	DMSO	2841J
	Cl.CC[C@@]1(O)C(=O)OCC2=C1C=C1N(CC3=CC4=C(C=CC(O)=C4CN(C)C)N=C13)C2=O	(19S)-8-[(dimethylamino)methyl]-19-ethyl-7,19-dihydroxy-17-oxa-3,13-diazapentacyclo[11.8.0.0^{2,11}.0^{4,9}.0^{15,20}]henicosa-1(21),2,4(9),5,7,10,15(20)-heptaene-14,18-dione hydrochloride	Topotecan·HCl	457.9	8	FDA Approved Drug Library	119413-54-6	DL-518	2mg/ml	DMSO	2841J
	CN(C)CCOC1=CC=C(C=C1)C(\C1=CC=CC=C1)=C(\CCCl)C1=CC=CC=C1	(2-{4-[(1Z)-4-chloro-1,2-diphenylbut-1-en-1-yl]phenoxy}ethyl)dimethylamine	Toremifene	406.0	8	FDA Approved Drug Library	89778-26-7	DL-519	2mg/ml	DMSO	2841J
	CC1=C(Cl)C=CC=C1NC1=C(C=CC=C1)C(O)=O	2-[(3-chloro-2-methylphenyl)amino]benzoic acid	Tolfenamic acid	261.7	8	FDA Approved Drug Library	13710-19-5	DL-520	2mg/ml	DMSO	2841J
	CN1C(CC(O)=O)=CC=C1C(=O)C1=CC=C(C)C=C1	2-{1-methyl-5-[(4-methylphenyl)carbonyl]-1H-pyrrol-2-yl}acetic acid	Tolmetin	257.3	8	FDA Approved Drug Library	64490-92-2	DL-521	2mg/ml	DMSO	2841J
	CC1(C)S[C@@H]2[C@H](NC(=O)[C@H](N)C3=CC=C(O)C=C3)C(=O)N2[C@H]1C(O)=O	(2S,5R,6R)-6-[(2R)-2-amino-2-(4-hydroxyphenyl)acetamido]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid	Amoxicillin	365.4	8	FDA Approved Drug Library	26787-78-0	DL-582	2mg/ml	DMSO	2841J
	COC1=CC(=CC=C1)[C@@]1(O)CCCC[C@@H]1CN(C)C	(1R,2R)-2-[(dimethylamino)methyl]-1-(3-methoxyphenyl)cyclohexan-1-ol	Tramadol	263.4	8	FDA Approved Drug Library	27203-92-5	DL-523	2mg/ml	DMSO	2841J
	[H][C@@]12C[C@@H](O)[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]1(F)[C@@]2([H])CCC2=CC(=O)C=C[C@]12C	(1R,2S,10S,11S,13R,14S,15S,17S)-1-fluoro-13,14,17-trihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadeca-3,6-dien-5-one	Triamcinolone	394.4	8	FDA Approved Drug Library	124-94-7	DL-524	2mg/ml	DMSO	2841J
	COC1=CC(CC2=CN=C(N)N=C2N)=CC(OC)=C1OC	5-[(3,4,5-trimethoxyphenyl)methyl]pyrimidine-2,4-diamine	Trimethoprim	290.3	8	FDA Approved Drug Library	738-70-5	DL-525	2mg/ml	DMSO	2841J
	[H][C@]12CC[C@]([H])(C[C@@H](C1)OC(=O)C1=CNC3=CC=CC=C13)N2C	(1R,3R,5S)-8-methyl-8-azabicyclo[3.2.1]octan-3-yl 1H-indole-3-carboxylate	Tropisetron	284.4	8	FDA Approved Drug Library	105826-92-4	DL-158	2mg/ml	DMSO	2841J
	CC[C@@H]1OC(=O)C[C@H](O)[C@@H](C)[C@@H](O[C@@H]2O[C@H](C)[C@@H](O[C@H]3C[C@@](C)(O)[C@@H](O)[C@H](C)O3)[C@@H]([C@H]2O)N(C)C)[C@H](C[C@@H](C)C(=O)\C=C\C(C)=C/[C@@H]1CO[C@H]1O[C@@H](C)[C@H](O)[C@H](OC)[C@@H]1OC)C=O	(4S,5R,6R,7S,9R,11E,13Z,15R,16S)-6-{[(2R,3R,4R,5S,6R)-5-{[(2S,4R,5S,6S)-4,5-dihydroxy-4,6-dimethyloxan-2-yl]oxy}-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy}-16-ethyl-4-hydroxy-15-({[(2S,3S,4S,5S,6S)-5-hydroxy-3,4-dimethoxy-6-methyloxan-2-yl]oxy}methyl)-5,9,13-trimethyl-2,10-dioxo-1-oxacyclohexadeca-11,13-diene-7-carbaldehyde	Tylosin	902.1	8	FDA Approved Drug Library	1405-54-5	DL-526	2mg/ml	DMSO	2841J
	CC(C)[C@H](N)C(=O)OCCOCN1C=NC2=C1N=C(N)NC2=O	2-[(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)methoxy]ethyl (2S)-2-amino-3-methylbutanoate	Valaciclovir	324.3	8	FDA Approved Drug Library	124832-27-5	DL-527	2mg/ml	DMSO	2841J
	[H][C@@]12C[C@@H]([C@H](OC(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CC[C@@]2([H])C[C@H](OC(C)=O)[C@H](C[C@]12C)N1CCCCC1)[N+]1(C)CCCCC1	1-[(1S,2S,4S,5S,7S,10R,11S,13S,14R,15S)-5,14-bis(acetyloxy)-2,15-dimethyl-4-(piperidin-1-yl)tetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadecan-13-yl]-1-methylpiperidin-1-ium	Vecuronium	557.8	8	FDA Approved Drug Library	50700-72-6	DL-528	2mg/ml	DMSO	2841J
	COC1=CC=C(C=C1)C(CN(C)C)C1(O)CCCCC1	1-[2-(dimethylamino)-1-(4-methoxyphenyl)ethyl]cyclohexan-1-ol	Venlafaxine	277.4	8	FDA Approved Drug Library	99300-78-4	DL-529	2mg/ml	DMSO	2841J
	NC1=NC=NC2=C1N=CN2[C@@H]1O[C@H](CO)[C@@H](O)[C@@H]1O	(2R,3S,4S,5R)-2-(6-amino-9H-purin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol	Vidarabine	267.2	8	FDA Approved Drug Library	5536-17-4	DL-530	2mg/ml	DMSO	2841J
	CC(C)NNC(=O)C1=CC=NC=C1	N'-(propan-2-yl)pyridine-4-carbohydrazide	Iproniazid	179.2	8	FDA Approved Drug Library	54-92-2	DL-531	2mg/ml	DMSO	2841J
	N\C(NCC1=CC=CC=C1)=N/C(=O)C1=C(N)N=C(N)C(Cl)=N1	3,5-diamino-N-[(1E)-amino(benzylamino)methylidene]-6-chloropyrazine-2-carboxamide	Benzamil	319.8	8	FDA Approved Drug Library	2898-76-2	NA-103	2mg/ml	DMSO	2841J
	CCCCN1CCCCC1C(=O)NC1=C(C)C=CC=C1C	1-butyl-N-(2,6-dimethylphenyl)piperidine-2-carboxamide	Bupivacaine	288.4	8	FDA Approved Drug Library	14252-80-3	NA-139	2mg/ml	DMSO	2841J
	COC1=CC=C(CCN2CCC(CC2)NC2=NC3=CC=CC=C3N2CC2=CC=C(F)C=C2)C=C1	1-[(4-fluorophenyl)methyl]-N-{1-[2-(4-methoxyphenyl)ethyl]piperidin-4-yl}-1H-1,3-benzodiazol-2-amine	Astemizole	458.6	8	FDA Approved Drug Library	68844-77-9	NH-101	2mg/ml	DMSO	2841J
	CN1CCC(CC1)=C1C2=C(SC=C2)C(=O)CC2=C1C=CC=C2	2-(1-methylpiperidin-4-ylidene)-6-thiatricyclo[8.4.0.0^{3,7}]tetradeca-1(10),3(7),4,11,13-pentaen-8-one	Ketotifen	309.4	8	FDA Approved Drug Library	34580-14-8	NH-106	2mg/ml	DMSO	2841J
	Cl.[H][C@@]1(CC[C@@](C#N)(CC1)C1=CC=C(F)C=C1)N1CC[C@@](C(O)=O)([C@H](C)C1)C1=CC=CC=C1	(3S,4R)-1-[4-cyano-4-(4-fluorophenyl)cyclohexyl]-3-methyl-4-phenylpiperidine-4-carboxylic acid hydrochloride	Levocabastine·HCl	457.0	8	FDA Approved Drug Library	79547-78-7	NH-107	2mg/ml	DMSO	2841J
	OC1=CC=C2C[C@H]3N(CC=C)CC[C@@]45[C@@H](OC1=C24)C(=O)CC[C@@]35O	(1S,5R,13R,17S)-10,17-dihydroxy-4-(prop-2-en-1-yl)-12-oxa-4-azapentacyclo[9.6.1.0^{1,13}.0^{5,17}.0^{7,18}]octadeca-7,9,11(18)-trien-14-one	Naloxone	327.4	8	FDA Approved Drug Library	357-08-4	NO-101	2mg/ml	DMSO	2841J
	OC1=C2O[C@@H]3[C@]45CCN(CC=C)[C@H](CC(C=C1)=C24)[C@]5(O)CC\C3=N/N=C1\CC[C@@]2(O)[C@H]3CC4=C5C(O[C@@H]1[C@@]25CCN3CC=C)=C(O)C=C4	(1S,5R,13R,14E,17S)-14-{2-[(1S,5R,13R,14E,17S)-10,17-dihydroxy-4-(prop-2-en-1-yl)-12-oxa-4-azapentacyclo[9.6.1.0^{1,13}.0^{5,17}.0^{7,18}]octadeca-7(18),8,10-trien-14-ylidene]hydrazin-1-ylidene}-4-(prop-2-en-1-yl)-12-oxa-4-azapentacyclo[9.6.1.0^{1,13}.0^{5,17}.0^{7,18}]octadeca-7(18),8,10-triene-10,17-diol	Naloxonazine	650.8	8	FDA Approved Drug Library	82824-01-9	NO-102	2mg/ml	DMSO	2841J
	COC1=CC2=C(C=C1)C1=CC=NC(C)=C1N2	7-methoxy-1-methyl-9H-pyrido[3,4-b]indole	Harmine	212.2	8	FDA Approved Drug Library	442-51-3	AC-1053	2mg/ml	DMSO	2841J
	CN(C)CCCSC1=C(NC(=O)\C=C\C2=CC=CC=C2)C=CC=C1	(2E)-N-(2-{[3-(dimethylamino)propyl]sulfanyl}phenyl)-3-phenylprop-2-enamide	Cinanserin	340.5	8	FDA Approved Drug Library	1166-34-3	NS-102	2mg/ml	DMSO	2841J
	CN(C)CCN1C2=C(C=CC=C2)N(C)C2=C(C=CC=C2)C1=O	9-[2-(dimethylamino)ethyl]-2-methyl-2,9-diazatricyclo[9.4.0.0^{3,8}]pentadeca-1(11),3(8),4,6,12,14-hexaen-10-one	Dibenzepine	295.4	8	FDA Approved Drug Library	315-80-0	NS-107	2mg/ml	DMSO	2841J
	[H][C@@]12CCCN1C(=O)[C@H](CC1=CC=CC=C1)N1C(=O)[C@](NC(=O)[C@H]3CN(C)[C@]4([H])CC5=CNC6=CC=CC(=C56)[C@@]4([H])C3)(O[C@@]21O)C(C)C	(2R,4R,7R)-N-[(1S,2S,4R,7S)-7-benzyl-2-hydroxy-5,8-dioxo-4-(propan-2-yl)-3-oxa-6,9-diazatricyclo[7.3.0.0^{2,6}]dodecan-4-yl]-6-methyl-6,11-diazatetracyclo[7.6.1.0^{2,7}.0^{12,16}]hexadeca-1(16),9,12,14-tetraene-4-carboxamide	Dihydroergocristine	611.7	8	FDA Approved Drug Library	24730-10-7	NS-108	2mg/ml	DMSO	2841J

Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	CN1CCN(CC1)C1=NC2=C(CC3=C1C=CC=C3)C=CC(F)=C2	6-fluoro-10-(4-methylpiperazin-1-yl)-9-azatricyclo$[9.4.0.0^{3,8}]$pentadeca-1(11),3(8),4,6,9,12,14-heptaene	Fluperlapine	309.4	8	FDA Approved Drug Library	67121-76-0	NS-109	2mg/ml	DMSO	2841J
	CNCCC(OC1=CC=C(C=C1)C(F)(F)F)C1=CC=CC=C1	methyl({3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl})amine	Fluoxetine	309.3	8	FDA Approved Drug Library	56296-78-7	NS-140	2mg/ml	DMSO	2841J
	CN1C2=C(C3=C1C=CC=C3)C(=O)C(CN1C=CN=C1C)CC2	9-methyl-3-[(2-methyl-1H-imidazol-1-yl)methyl]-2,3,4,9-tetrahydro-1H-carbazol-4-one	Ondansetron	293.4	8	FDA Approved Drug Library	99614-01-4	NS-145	2mg/ml	DMSO	2841J
	FC1=CC=C(C=C1)C(=O)C1CCN(CCN2C(=O)NC3=C(C=CC=C3)C2=O)CC1	3-(2-{4-[(4-fluorophenyl)carbonyl]piperidin-1-yl}ethyl)-1,2,3,4-tetrahydroquinazoline-2,4-dione	Ketanserin	395.4	8	FDA Approved Drug Library	74050-98-9	NS-515	2mg/ml	DMSO	2841J
	[Br-].[H][C@]12C[C@@H](C[C@]([H])([C@H]3O[C@@H]13)[N+]2(C)C)OC(=O)C(O)(C1=CC=CS1)C1=CC=CS1	(1R,2R,4S,5S,7S)-7-{[2-hydroxy-2,2-bis(thiophen-2-yl)acetyl]oxy}-9,9-dimethyl-3-oxa-9-azatricyclo$[3.3.1.0^{2,4}]$nonan-9-ium bromide	Tiotropium Bromide	472.4	8	FDA Approved Drug Library	136310-93-5	DL-562	2mg/ml	DMSO	2841J
	OS(=O)(=O)C1=CC=CC=C1.CN1CCCCC1CCN1C2=C(SC3=C1C=C(C=C3)S(C)=O)C=CC=C2	2-methanesulfinyl-10-[2-(1-methylpiperidin-2-yl)ethyl]-10H-phenothiazine; benzenesulfonic acid	Mesoridazine besylate	544.7	8	FDA Approved Drug Library	32672-69-8	NS-531	2mg/ml	DMSO	2841J
	CSC1=CC=C2SC3=C(C=CC=C3)N(CCC3CCCCN3C)C2=C1	10-[2-(1-methylpiperidin-2-yl)ethyl]-2-(methylsulfanyl)-10H-phenothiazine	Thioridazine	370.6	8	FDA Approved Drug Library	130-61-0	NS-835	2mg/ml	DMSO	2841J
	CN(C1CCCCC1)C(=O)CCCOC1=CC2=C(NC(=O)C=C2)C=C1	N-cyclohexyl-N-methyl-4-[(2-oxo-1,2-dihydroquinolin-6-yl)oxy]butanamide	Cilostamide	342.4	8	FDA Approved Drug Library	68550-75-4	PD-125	2mg/ml	DMSO	2841J
	CCOC(=O)C1=C(NN=C(C)C)C2=C(N=C1)N(CC)N=C2	ethyl 1-ethyl-4-[2-(propan-2-ylidene)hydrazin-1-yl]-1H-pyrazolo[3,4-b]pyridine-5-carboxylate	Etazolate	289.3	8	FDA Approved Drug Library	51022-77-6	PD-130	2mg/ml	DMSO	2841J
	NC1=CC(=CNC1=O)C1=CC=NC=C1	3-amino-5-(pyridin-4-yl)-1,2-dihydropyridin-2-one	amrinone	187.2	8	FDA Approved Drug Library	60719-84-8	DL-583	2mg/ml	DMSO	2841J
	NC1=NC(=NC(N)=N1)C1=C(Cl)C=CC(Cl)=C1	6-(2,5-dichlorophenyl)-1,3,5-triazine-2,4-diamine	Irsogladine	256.1	8	FDA Approved Drug Library	57381-26-7	PD-141	2mg/ml	DMSO	2841J
	CC1=C(C=C(C#N)C(=O)N1)C1=CC=NC=C1	6-methyl-2-oxo-5-(pyridin-4-yl)-1,2-dihydropyridine-3-carbonitrile	Milrinone	211.2	8	FDA Approved Drug Library	78415-72-2	PD-152	2mg/ml	DMSO	2841J
	COC1=C(OC2CCCC2)C=C(C=C1)C1CNC(=O)C1	4-[3-(cyclopentyloxy)-4-methoxyphenyl]pyrrolidin-2-one	Rolipram	275.3	8	FDA Approved Drug Library	61413-54-5	PD-175	2mg/ml	DMSO	2841J
	CN\C(NC#N)=N/C1=CC=C(C=C1)C1=NNC(=O)CC1C	(E)-1-cyano-3-methyl-2-[4-(4-methyl-6-oxo-1,4,5,6-tetrahydropyridazin-3-yl)phenyl]guanidine	Siguazodan	284.3	8	FDA Approved Drug Library	115344-47-3	PD-179	2mg/ml	DMSO	2841J
	Cl.Cl.COC1=CC2=C(C=C1OC)C1=C\C(N(C)C(=O)N1CC2)=N/C1=C(C)C=C(C)C=C1C	9,10-dimethoxy-3-methyl-2-[(2,4,6-trimethylphenyl)imino]-2H,3H,4H,6H,7H-pyrimido[4,3-a]isoquinolin-4-one dihydrochloride	Trequinsin·HCl	478.4	8	FDA Approved Drug Library	78416-81-6	PD-180	2mg/ml	DMSO	2841J
	[H][C@]12N3CCC[C@@]1(CC)C=C(N1C4=C(C=CC=C4)C(CC3)=C21)C(=O)OCC	ethyl (15S,19S)-15-ethyl-1,11-diazapentacyclo$[9.6.2.0^{2,7}.0^{8,18}.0^{15,19}]$nonadeca-2(7),3,5,8(18),16-pentaene-17-carboxylate	Vinpocetine	350.5	8	FDA Approved Drug Library	42971-09-5	PD-185	2mg/ml	DMSO	2841J
	CCCOC1=C(C=CC=C1)C1=NC(=O)C2=C(N1)N=NN2	5-(2-propoxyphenyl)-1H,4H,7H-[1,2,3]triazolo[4,5-d]pyrimidin-7-one	Zaprinast	271.3	8	FDA Approved Drug Library	37762-06-4	PD-190	2mg/ml	DMSO	2841J
	COC1=CC(=CC=C1OC(F)F)C1=NNC(=O)C=C1	6-[4-(difluoromethoxy)-3-methoxyphenyl]-2,3-dihydropyridazin-3-one	Zardaverine	268.2	8	FDA Approved Drug Library	101975-10-4	PD-195	2mg/ml	DMSO	2841J
	[H][C@]1(\C=C\[C@@H](O)CCCCC)[C@H](O)CC(=O)[C@]1([H])CCCCCCC(O)=O	7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoic acid	Alprostadil	354.5	8	FDA Approved Drug Library	745-65-3	PG-006	2mg/ml	DMSO	2841J
	CCCCC(C)(O)C\C=C\[C@H]1[C@H](O)CC(=O)[C@@H]1CCCCCCC(=O)OC	methyl 7-[(1R,2R,3R)-3-hydroxy-2-[(1E)-4-hydroxy-4-methyloct-1-en-1-yl]-5-oxocyclopentyl]heptanoate	Misoprostol	382.5	8	FDA Approved Drug Library	59122-46-2	PG-051	2mg/ml	DMSO	2841J
	C[C@@H]1CCN([C@H](C1)C(O)=O)C(=O)[C@H](CCCNC(N)=N)NS(=O)(=O)C1=CC=CC2=C1NCC(C)C2	(2R,4R)-1-[(2S)-5-carbamimidamido-2-(3-methyl-1,2,3,4-tetrahydroquinoline-8-sulfonamido)pentanoyl]-4-methylpiperidine-2-carboxylic acid	Argatroban	508.6	8	FDA Approved Drug Library	74863-84-6	PI-146	2mg/ml	DMSO	2841J
	CC1(C)C[C@H]1C(=O)N\C(C(O)=O)=C/CCCCSC[C@@H](N)C(O)=O	(2Z)-7-{[(2S)-2-amino-2-carboxyethyl]sulfanyl}-2-{[(1R)-2,2-dimethylcyclopropyl]formamido}hept-2-enoic acid	Cilastatin	358.5	8	FDA Approved Drug Library	82009-34-5	PI-153	2mg/ml	DMSO	2841J
	[H][C@@]1(C)CC[C@@]2([H])[C@@]([H])(C)[C@@]([H])(OC(=O)CCC(O)=O)O[C@]3([H])O[C@]4(C)CC[C@]1([H])[C@@]23OO4	4-oxo-4-{[(1S,4S,5R,8S,9R,10R,12R,13R)-1,5,9-trimethyl-11,14,15,16-tetraoxatetracyclo$[10.3.1.0^{4,13}.0^{8,13}]$hexadecan-10-yl]oxy}butanoic acid	Artesunate	384.4	8	FDA Approved Drug Library	88495-63-0	PR-117	2mg/ml	DMSO	2841J
	COC1=C(C=C(C=C1)C(=O)NCC1=CC=CN=C1)C(=O)NCC1=CC=CN=C1	4-methoxy-1-N,3-N-bis(pyridin-3-ylmethyl)benzene-1,3-dicarboxamide	Picotamide	376.4	8	FDA Approved Drug Library	32828-81-2	RA-104	2mg/ml	DMSO	2841J
	O[N+]([O-])=O.ClC1=CC=C(CCC(CN2C=CN=C2)SC2=C(Cl)C=CC=C2Cl)C=C1	1-[4-(4-chlorophenyl)-2-[(2,6-dichlorophenyl)sulfanyl]butyl]-1H-imidazole; oxoazinic acid	Butoconazole nitrate	474.8	8	FDA Approved Drug Library	64872-77-1	DL-584	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@@](O)(C#CC)[C@@]1(C)C[C@H](C1=CC=C(C=C1)N(C)C)C1=C3CCC(=O)C=C3CC[C@@]21[H]	(10S,11S,14S,15S,17R)-17-[4-(dimethylamino)phenyl]-14-hydroxy-15-methyl-14-(prop-1-yn-1-yl)tetracyclo$[8.7.0.0^{2,7}.0^{11,15}]$heptadeca-1,6-dien-5-one	Mifepristone	429.6	8	FDA Approved Drug Library	84371-65-3	S-510	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@](OC(C)=O)(C(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])C=C(C)C2=CC(=O)CC[C@]12C	(1S,2R,10R,11S,14R,15S)-14-acetyl-2,8,15-trimethyl-5-oxotetracyclo$[8.7.0.0^{2,7}.0^{11,15}]$heptadeca-6,8-dien-14-yl acetate	Megestrol Acetate	384.5	8	FDA Approved Drug Library	595-33-5	S-515	2mg/ml	DMSO	2841J
	[H][C@@]12CC(=C)[C@](OC(C)=O)(C(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])C=C(C)C2=CC(=O)CC[C@]12C	(1S,2R,10R,11S,14R,15S)-14-acetyl-2,8,15-trimethyl-13-methylidene-5-oxotetracyclo$[8.7.0.0^{2,7}.0^{11,15}]$heptadeca-6,8-dien-14-yl acetate	Melengestrol Acetate	396.5	8	FDA Approved Drug Library	2919-66-6	S-520	2mg/ml	DMSO	2841J
	CC\C(C1=CC=CC=C1)=C(/C1=CC=CC=C1)C1=CC=C(OCCN(C)C)C=C1	(2-{4-[(1Z)-1,2-diphenylbut-1-en-1-yl]phenoxy}ethyl)dimethylamine	Tamoxifen	371.5	8	FDA Approved Drug Library	54965-24-1	S-650	2mg/ml	DMSO	2841J
	CC(C)CN(C[C@@H](O)[C@H](CC1=CC=CC=C1)NC(=O)O[C@H]1CCOC1)S(=O)(=O)C1=CC=C(N)C=C1	(3S)-oxolan-3-yl N-[(2S,3R)-3-hydroxy-4-[N-(2-methylpropyl)(4-aminobenzene)sulfonamido]-1-phenylbutan-2-yl]carbamate	Amprenavir	505.6	8	FDA Approved Drug Library	161814-49-9	DL-532	2mg/ml	DMSO	2841J
	C[C@@H](O[C@H]1OCCN(CC2=NC(=O)NN2)[C@H]1C1=CC=C(F)C=C1)C1=CC(=CC(=C1)C(F)(F)F)C(F)(F)F	5-{[(2R,3S)-2-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]-3-(4-fluorophenyl)morpholin-4-yl]methyl}-2,3-dihydro-1H-1,2,4-triazol-3-one	Aprepitant	534.4	8	FDA Approved Drug Library	170729-80-3	DL-533	2mg/ml	DMSO	2841J
	COC1=CC=CC=C1OC1=C(OCCO)N=C(N=C1NS(=O)(=O)C1=CC=C(C=C1)C(C)(C)C)C1=NC=CC=N1	4-tert-butyl-N-[6-(2-hydroxyethoxy)-5-(2-methoxyphenoxy)-2-(pyrimidin-2-yl)pyrimidin-4-yl]benzene-1-sulfonamide	Bosentan	551.6	8	FDA Approved Drug Library	147536-97-8	DL-534	2mg/ml	DMSO	2841J
	FC(F)(F)[C@]1(OC(=O)NC2=C1C=C(Cl)C=C2)C#CC1CC1	(4S)-6-chloro-4-(2-cyclopropylethynyl)-4-(trifluoromethyl)-2,4-dihydro-1H-3,1-benzoxazin-2-one	Efavirenz	315.7	8	FDA Approved Drug Library	154598-52-4	DL-535	2mg/ml	DMSO	2841J

Structure	SMILES	IUPAC name	Name	MW	Plate number	Plate description	CAS	Catalog number	Concentration	Solvent	Plate part number
	[H][C@@]12CC[C@H](C[C@H](C)CCC(=O)NCCS(O)(=O)=O)[C@@]1(C)[C@@H](O)C[C@@]1([H])[C@@]2([H])[C@H](O)C[C@]2([H])[C@H](O)CC]C@@]12C	2-{(4R)-4-[(1S,2S,5R,7S,9R,10R,11S,14R,15R,16S)-5,9,16-trihydroxy-2,15-dimethyltetracyclo[8.7.0.0^{1,7}.0^{11,17}]heptadecan-14-yl]pentanamido}ethane-1-sulfonic acid	Taurocholic acid	515.7	8	FDA Approved Drug Library	81-24-3	DL-536	2mg/ml	DMSO	2841J
	CCCCN1C[C@H](O)[C@@H](O)[C@H](O)[C@H]1CO	(2R,3R,4R,5S)-1-butyl-2-(hydroxymethyl)piperidine-3,4,5-triol	Miglustat	219.3	8	FDA Approved Drug Library	72599-27-0	SL-230	2mg/ml	DMSO	2841J
	[H][C@@]12CC[C@H](O)[C@@]1(C)CC[C@]1([H])C3=C(C[C@@H](CCCCCCCCCS(=O)CCCC(F)(F)C)(F)(F)F)[C@@]21[H]C=C(O)C=C3	(1S,9R,10R,11S,14S,15S)-15-methyl-9-[9-[(4,4,5,5,5-pentafluoropentane)sulfinyl]nonyl]tetracyclo[8.7.0.0^{1,7}.0^{11,17}]heptadeca-2(7),3,5-triene-5,14-diol	Fulvestrant	606.8	8	FDA Approved Drug Library	129453-61-8	DL-104	2mg/ml	DMSO	2841J
	OC(=O)/C=C/C(O)=O.[H][C@@]12CC3=CN(C)C4=CC=CC(=C34)C1=C[C@H](CN2C)C(=O)N(C@@H](CC)CO	(2Z)-but-2-enedioic acid; (4R,7R)-N-[(2S)-1-hydroxybutan-2-yl]-6,11-dimethyl-6,11-diazatetracyclo[7.6.1.0^{1,7}.0^{2,4}]hexadeca-1(16),2,9,12,14-pentaene-4-carboxamide	Methysergide maleate	469.5	8	FDA Approved Drug Library	129-49-7	DL-538	2mg/ml	DMSO	2841J
	COC(=O)CCC1=CC=C(OCC(O)CNC(C)C)C=C1	methyl 3-(4-{2-hydroxy-3-[(propan-2-yl)amino]propoxy}phenyl)propanoate	Esmolol	295.4	8	FDA Approved Drug Library	81147-92-4	DL-107	2mg/ml	DMSO	2841J
	CC(C)(CO)[C@@H](O)C(=O)NCCC(O)=O	3-[(2R)-2,4-dihydroxy-3,3-dimethylbutanamido]propanoic acid	Pantothenic acid	219.2	8	FDA Approved Drug Library	79-83-4	DL-123	2mg/ml	DMSO	2841J
	CCCCCOC(=O)NC1=NC(=O)N(C=C1F)[C@@H]1O[C@H](C)[C@@H](O)[C@H]1O	pentyl N-{1-[(2R,3R,4S,5R)-3,4-dihydroxy-5-methyloxolan-2-yl]-5-fluoro-2-oxo-1,2-dihydropyrimidin-4-yl}carbamate	Capecitabine	359.4	8	FDA Approved Drug Library	154361-50-9	DL-585	2mg/ml	DMSO	2841J
	C[C@H](N)[C@H](O)C1=CC=CC=C1	(1R,2S)-2-amino-1-phenylpropan-1-ol	Phenylpropanolamine	151.2	8	FDA Approved Drug Library	14838-15-4	DL-225	2mg/ml	DMSO	2841J
	C[N+](C)(C)CCOC(=O)CCC(=O)OCC[N+](C)(C)C	trimethyl[2-({4-oxo-4-[2-(trimethylazaniumyl)ethoxy]butanoyl}oxy)ethyl]azanium	Succinylcholine	290.4	8	FDA Approved Drug Library	306-40-1	DL-234	2mg/ml	DMSO	2841J
	OC1(CCN(CCCC(=O)C2=CC=C(F)C=C2)CC1)C1=CC(=CC=C1)C(F)(F)F	1-(4-fluorophenyl)-4-{4-hydroxy-4-[3-(trifluoromethyl)phenyl]piperidin-1-yl}butan-1-one	Trifluperidol	409.4	8	FDA Approved Drug Library	749-13-3	DL-195	2mg/ml	DMSO	2841J
	N[C@@H](CC1=CC(I)=C(OC2=CC(I)=C(O)C(I)=C2)C(I)=C1)C(O)=O	(2S)-2-amino-3-{4-(4-hydroxy-3,5-diiodophenoxy)-3,5-diiodophenyl}propanoic acid	L-thyroxine	776.9	8	FDA Approved Drug Library	51-48-9	DL-540	2mg/ml	DMSO	2841J
	CN1CCC(CC1)=C1C2=CC=CC=C2C=CC2=C1C=CC=C2	1-methyl-4-[tricyclo[9.4.0.0^{3,8}]pentadeca-1(11),3,5,7,9,12,14-heptaen-2-ylidene]piperidine	Cyproheptadine	287.4	8	FDA Approved Drug Library	129-03-3	DL-136	2mg/ml	DMSO	2841J
	CN(C)CCCOC1=NN(CC2=CC=CC=C2)C2=C1C=CC=C2	{3-[(1-benzyl-1H-indazol-3-yl)oxy]propyl}dimethylamine	Benzydamine	309.4	8	FDA Approved Drug Library	642-72-8	DL-559	2mg/ml	DMSO	2841J