

Supplementary Table S1: List of Z' factor for library plates

Sl. No.	Plate ID	Vendor	Replicate A	Replicate B
1	2089	Biomol 4	0.698	0.485
2	2090	Biomol 4	0.517	0.517
3	3651	Selleck Chem	0.459	0.450
4	3652	Selleck Chem	0.882	0.526
5	3653	Selleck Chem	0.417	0.641
6	3654	Selleck Chem	0.525	0.343
7	3655	Selleck Chem	0.467	0.552
8	3656	Selleck Chem	0.645	0.539
9	3657	Selleck Chem	0.387	0.578
10	3720	Cayman Chemical	0.593	0.415
11	3721	Cayman Chemical	0.492	0.431
12	3722	Medchem Express	0.516	0.438
13	3723	Medchem Express	0.636	0.639
14	3724	Medchem Express	0.656	0.642
15	3725	Medchem Express	0.561	0.699
16	3726	Medchem Express	0.778	0.682
17	3727	Medchem Express	0.682	0.565
18	3728	Medchem Express	0.684	0.676
19	3729	Medchem Express	0.648	0.668
20	3730	Medchem Express	0.620	0.615

Supplementary Table S2: List of library and cherry-picked compounds from each plate

Sl. No.	Plate ID	Vendor	Cherry pick	No. of compounds
1	2089	Biomol 4	0	640
2	2090	Biomol 4	0	
3	3651	Selleck Chem	0	1902
4	3652	Selleck Chem	0	
5	3653	Selleck Chem	0	
6	3654	Selleck Chem	0	
5	3655	Selleck Chem	0	
6	3656	Selleck Chem	0	
7	3657	Selleck Chem	0	
8	3720	Cayman Chemical	3	1600
9	3721	Cayman Chemical	3	
10	3722	Medchem Express	0	
11	3723	Medchem Express	4	
12	3724	Medchem Express	2	
13	3725	Medchem Express	2	
14	3726	Medchem Express	7	
15	3727	Medchem Express	7	
16	3728	Medchem Express	9	
17	3729	Medchem Express	2	
18	3730	Medchem Express	11	
		Total	50	4142

Supplementary Table S3: List of IC₅₀ values for cherry picked compounds

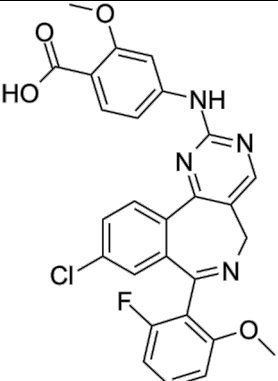
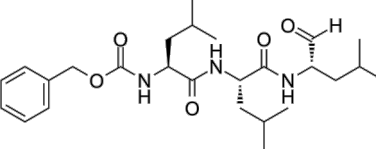
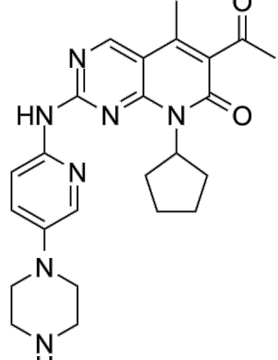
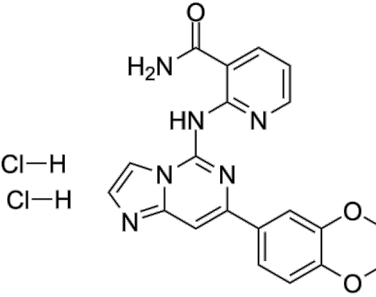
Compound name	IC₅₀ (μM)
Ascomycin	0.749
ONX 0914	ND
Ingenol-3-angelate	0.2787
NVP-BEP800	0.366
Radicicol	0.0000722
MI-773	0.8217
HY-10299	0.5974
MLN 8237	0.02419
MG-132	0.03263
KPT-330	ND
Palbociclib	0.1067
AZD8055	ND
Volasertib	1.192
Erlotinib	1.171
Cilengitide	1.166
OTSSP167	1.176
Flavopiridol	1.230
BAY 61-3606	1.229
Ruboxistaurin	1.214
Ispinesib	0.9359
Obatoclax	2.68
BI 2536	0.573
NVP-TAE 226	0.9528
SGI-1776	0.9178
LY2090314	0.7019
Quisinostat	0.8575
MEK162	1.212
PKC412	2.270
Amsacrine	0.6594
BNC105	0.9265
Tipifarnib	0.9954
Epoxomicin	0.5021
OSI-027	0.9978
RG7388	1.165
Duvelisib	0.6935
LEE011	2.222
PKI-587	1.211
CBL0137 HCl	1.193
AZD-7762	0.9865
MK 2206	4.17e-010
Nutlin (3a)	1.516
ARRY-520	1.086

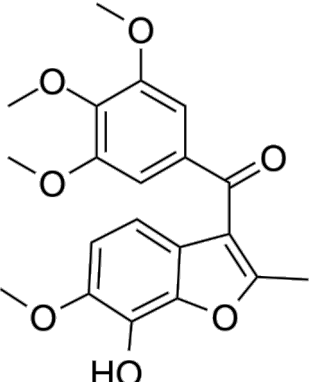
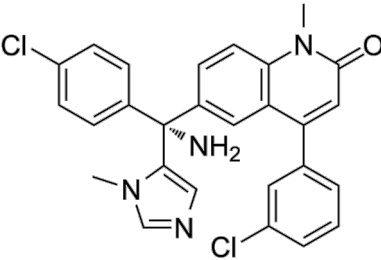
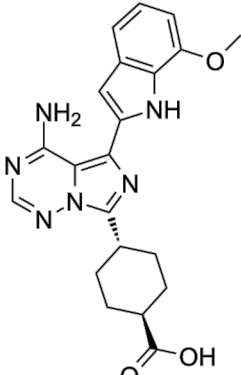
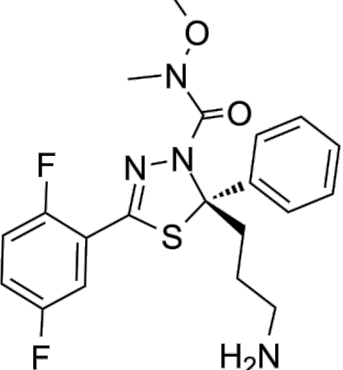
Zotarolimus	1.051
PF-431396	1.060
TAK-285	1.103
CH5132799	1.210
AZD-5438	373.4
LY2835219	1.461
Icotinib	1.129
Tozasertib	1.189

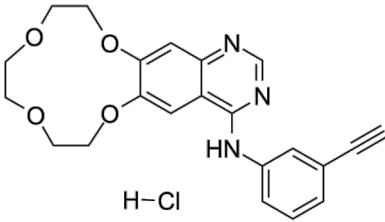
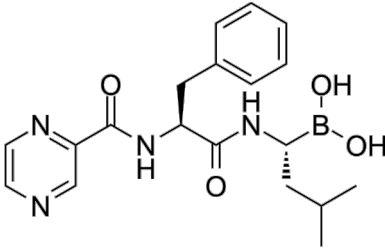
Supplementary Table S4: List of the top hits and their SMILES

Compound name	SMILES
MLN 8237	<chem>COc1cccc(c1C1=NCc2c(c3c1cc(Cl)cc3)nc(nc2)Nc1ccc(c(c1)OC)C(=O)O)F</chem>
MG-132	<chem>O=C[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)OCc1cccc1)CC(C)C)CC(C)C</chem>
Palbociclib	<chem>CC(=O)c1c(C)c2cnc(nc2n(c1=O)C1CCCC1)Nc1ccc(cn1)N1CCNCC1</chem>
BAY 61-3606 (dihydrochloride)	<chem>O=C(N)C1=CC=CN=C1NC2=NC(C3=CC=C(C(OC)=C3)OC)=CC4=NC=CN24.[H]Cl.[H]Cl</chem>
BNC105	<chem>COC1=CC(C(C2=C(C)OC3=C(O)C(OC)=CC=C23)=O)=CC(OC)=C1OC</chem>
Tipifarnib	<chem>O=C1N(C2=C(C(C3=CC=CC(Cl)=C3)=C1)C=C(C=C2)[C@@](N)(C4=CN=CN4C)C5=CC=C(C=C5)Cl)C</chem>
OSI-027	<chem>O=C([C@H]1CC[C@H](C2=NC(C(N3)=CC4=C3C(OC)=CC=C4)=C5C(N)=NC=NN52)CC1)O</chem>
ARRY-520	<chem>O=C1N(C2=C(C(C3=CC=CC(Cl)=C3)=C1)C=C(C=C2)[C@@](N)(C4=CN=CN4C)C5=CC=C(C=C5)Cl)C</chem>
Icotinib (Hydrochloride)	<chem>C#CC1=CC(NC2=C(C=C(OCCOCCOCCO3)C3=C4)C4=NC=N2)=CC=C1.[H]Cl</chem>
Bortezomib	<chem>B([C@H](CC(C)C)NC(=O)[C@H](CC1=CC=CC=C1)NC(=O)C2=NC=CN=C2)(O)O</chem>

Supplementary Table S5: Structures of the top hits

Compound name	Structures
MLN 8237	 <p>The structure of MLN 8237 is a complex molecule featuring a central benzimidazole core. It is substituted with a 4-methoxyphenyl group, a 4-chlorophenyl group, and a 2-fluorophenyl group. A carboxylic acid group is attached to the benzimidazole ring.</p>
MG-132	 <p>The structure of MG-132 is a cyclic peptide derivative. It consists of a six-membered ring with two amide bonds and two methyl groups. It is substituted with a benzyl group and a carboxylic acid group.</p>
Palbociclib	 <p>The structure of Palbociclib is a complex molecule featuring a central pyrimidine ring. It is substituted with a 4-piperidinophenyl group, a cyclopentyl group, and a carboxylic acid group.</p>
BAY 61-3606 (dihydrochloride)	 <p>The structure of BAY 61-3606 dihydrochloride is a complex molecule featuring a central pyrimidine ring. It is substituted with a 4-methoxyphenyl group, a carboxylic acid group, and a carboxylic acid group. The structure is shown as a dihydrochloride salt, with two Cl-H groups indicated.</p>

BNC105	 <p>Chemical structure of BNC105, a benzodioxole derivative. It features a benzodioxole core with a methoxy group at position 2, a hydroxyl group at position 3, and a 3,4,5-trimethoxybenzoyl group at position 4.</p>
Tipifarnib	 <p>Chemical structure of Tipifarnib, a farnesyl transferase inhibitor. It consists of a quinoline ring system with a carbonyl group at position 1, a 4-chlorophenyl group at position 2, a 4-chlorophenyl group at position 3, and a 4-amino-1-methyl-1H-imidazol-2-yl group at position 4.</p>
OSI-027	 <p>Chemical structure of OSI-027, a triazole derivative. It features a 1,2,4-triazole ring system with an amino group at position 3, a 4-methoxyphenyl group at position 4, and a cyclohexyl group at position 5. The cyclohexyl group is further substituted with a carboxylic acid group.</p>
ARRY-520	 <p>Chemical structure of ARRY-520, a thiazole derivative. It features a thiazole ring system with a 2,4-difluorophenyl group at position 2, a 4-aminophenyl group at position 3, and a 4-phenyl-1-methyl-1H-imidazol-2-yl group at position 4.</p>

Icotinib (Hydrochloride)	
Bortezomib	

Supplementary Table S6: List of compounds screened in primary screening

Vendor	Vendor Reagent ID	SMILES	Molecular Formula	Molecular Weight	Compound Name(s)
BIOMOL	DL-552	<chem>N1(CCCOCC1)C(=N)NC(=N)N.Cl</chem>	C6H14ClN5O	207.661	Moroxydine HCl
BIOMOL	AC-554	<chem>N(CCN(C)C1)(c2c(cccc2)Cc3c4ccccc3)C14</chem> <chem>[C@@H]1([C@@H]([C@H](C)C)NC(=O)[C@@H]2C[C@@H](CCC)CN2C)</chem> <chem>[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](SC)O1</chem>	C18H20N2	264.365	Mianserin hcl
BIOMOL	A-190	<chem>c([nH]cn1)(C(=O)N(C)C(=O)N2C)c12</chem>	C18H33ClN2O5S	424.983	Clindamycin HCl
BIOMOL	AC-615	<chem>[C@@]1([H])([C@H](O)[C@H](O)[C@H](O)C(=O)CCCCCCCCCCCCC</chem> <chem>C)[C@@H](SC)O1)C(C(C)C)NC(=O)[C@@]2([H])N(C)C[C@]([H])(CCC)C</chem>	C34H63ClN2O6S	663.392	Clindamycin PO4
BIOMOL	A-192	<chem>c1(nc(C)[nH]2)c2C(=O)N(C)C(=O)N1Cc3ccccc3</chem>	C12H12N4O3	260.249	Furafylline
BIOMOL	AC-626	<chem>[C@@H]1([C@H](O)[C@H](C)ClC=Cl)C(=O)N[C@@H](CC)C(=O)N(C)CC</chem> <chem>(=O)N(C)[C@@H](CC(C)C)C(=O)N[C@@H](C(C)C)C(=O)N(C)[C@@H](C</chem> <chem>C(C)C)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N(C)[C@@H](CC(C)C)</chem> <chem>C(=O)N(C)[C@@H](CC(C)C)C(=</chem>	C62H111N11O12	1202.611	Cyclosporin a
BIOMOL	DL-561	<chem>[C@@H]1(CC[C@@H](C(C)C)CC1)C(=O)N[C@@H](C(=O)O)Cc2ccccc2</chem>	C19H27NO3	317.423	nateglinide
BIOMOL	A-239	<chem>[C@@H]1([C@@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)O[C@H]2</chem> <chem>O[C@H](C)[C@@H](NC(=N)C(=O)O)C[C@@H]2N</chem>	C14H25N3O9	379.363	Kasugamycin
BIOMOL	AC-729	<chem>c1(C(O)CNC(C)C)ccc(O)c(O)c1</chem> <chem>[C@@H]1([C@H](O)[C@H](O)[C@@H](O)[C@@H](SC)O1)[C@@H]([C@</chem> <chem>H](O)C)NC(=O)[C@H]2N(C)C[C@H](CCC)C2</chem>	C11H17NO3	211.258	Isoproterenol HCl (rac)
BIOMOL	A-240	<chem>[N+](C)(C)(C)CCOC(=O)C</chem>	C18H34N2O6S	406.537	Lincomycin
BIOMOL	AC-734	<chem>c(c(C(=O)O)C)ccc1O)(nc(c2n3)c(O)cc(O)c2C=O)c13</chem>	C7H16NO2	146.207	Acetylcholine Cl
BIOMOL	A245	<chem>[C@@H]1(OC(=O)C(CO)c2ccccc2)C[C@@]3([H])N(C)[C@]([H])(CC3)C1</chem>	C15H10N2O6	314.25	Lomofungin
BIOMOL	AC-735	<chem>c(COC1=O)(c(C)c(O)C)c(ClC=C(Cl/C)CCC(=O)O)c2O)c12</chem>	C17H20O6	320.337	Mycophenolic acid
BIOMOL	A-249	<chem>C(CCCCCCCC[N+])(C)(C)C[N+](C)(C)C</chem>	C16H38N2	258.486	Decamethonium 2Br
BIOMOL	AC-737	<chem>c(c(C)c(O)[C@@H]1OC(C)C)[C@H](OC)[C@@H](OC(=O)N)[C@@H]1O)</chem> <chem>cc2)(OC(=O)C(NC(=O)O)c3ccc(O)c(ClC=C(Cl/C)c3)=C4O)c24</chem>	C31H36N2O11	612.624	Novobiocin Na
BIOMOL	A-256	<chem>C1(C)(NC)C(C)C[C@@]2([H])C[C@]1([H])CC2</chem>	C11H21N	167.291	Mecamylamine HCl
BIOMOL	AC-741	<chem>N(CCCC1)(C(=O)C(=O)[C@]2(O)O[C@@H](CC[C@H]2C)C[C@H](OC)C</chem> <chem>(\C)=ClC=ClC=Cl[C@@H](C)C[C@H](C)C(=O)[C@H](OC)[C@H](O))C</chem> <chem>(\C)=Cl[C@@H](C)C(=O)C[C@H]([C@H](C)C[C@@H]3CC[C@@H](O)</chem> <chem>[C@H](OC)C3)OC4=O)[C@@H]14</chem>	C51H79NO13	914.172	Rapamycin
BIOMOL	A-275	<chem>c1(O)C(=O)N(C)C)cccc([N+](C)(C)C)c1</chem>	C12H19N2O2	223.291	Neostigmine Br
BIOMOL	AC-743	<chem>c1(nsn2)c2ccc(Cl)c1NC3=NCCN3</chem>	C9H8ClN5S	253.711	Tizanidine HCl
BIOMOL	AR-103	<chem>[C@@H]1(C[C@@H]1N)c2ccccc2</chem>	C9H11N	133.19	Tranylcypromine
BIOMOL	DL-549	<chem>[C@@H](O)([C@@H](O)CNC)[C@H](O)[C@H](O)CO</chem>	C7H17NO5	195.214	Meglumine
BIOMOL	EI-217	<chem>c(cccc1)(C(O)=C(C(=O)Nc2ncccc2)N(C)S3(=O)=O)c13</chem>	C15H13N3O4S	331.346	Piroxicam
BIOMOL	EI-219	<chem>c1(cccc2)c2cccc1OC[C@@H](O)CNC(C)C</chem>	C16H21NO2	259.343	Propranolol HCl s(-)
BIOMOL	AR-107	<chem>c1(ccccc1)CC(C)N(C)CC#C</chem>	C13H17N	187.281	Deprenyl HCl r (-)
BIOMOL	EI-240	<chem>c1(c(O)C(O)CNCCOC2c2ccccc2O)C)ccc3)c3[nH]c4c1cccc4</chem> <chem>[C@@]12(C(=O)[C@H](C)[C@@H](OC(=O)C)[C@@H](C)[C@@H](C)O</chem> <chem>C(=O)[C@H](C)[C@@H](O)[C@@H]3O[C@@H](C)[C@H](OC(=O)C)[C</chem> <chem>@@H](OC)C3)[C@H](C)[C@@H](O)[C@@H]4O[C@H](C)C[C@H](N(C)C)</chem> <chem>[C@H]4O)C(=O)C)[C@@H](C)C1)OC2</chem>	C41H67NO15	813.968	Troleandomycin
BIOMOL	EI-249	<chem>c1(c2ccc(F)cc2)c(COC)c(Cl(C)C)nc(Cl(C)C)c1ClC=Cl[C@@H](O)C[C@@H](</chem> <chem>O)CC(O)=O</chem>	C26H34FNO5	459.55	Cerivastatin
BIOMOL	DL-223	<chem>[C@@](C)(NN)(C(=O)O)Cc1ccc(O)c(O)c1</chem>	C10H14N2O4	226.229	Carbidopa
BIOMOL	EI-265	<chem>c(cc(c1c2O)C(=O)c(c3C1=O)cccc3O)([C@@H](C(=O)OC)[C@@](O)(CC)</chem> <chem>C[C@@H]4O[C@@H]5O[C@@H](C)[C@@H](O)[C@@H]6O[C@@H](C)[</chem> <chem>C@@H](O)[C@H]7CCC(=O)[C@H](C)O7)[C@@H](O)C6)[C@@H](N(C)C)</chem> <chem>C5)c24</chem>	C42H53NO15	811.868	Aclarubicin
BIOMOL	AW8655	<chem>c1(Oc2ccccc2)cc([N+])([O-])=O)ccc1NS(=O)(=O)C</chem>	C13H12N2O5S	308.31	Nimesulide
BIOMOL	EI-287	<chem>n1(cnc2C(=O)O)CC2c2CN(C)C(=O)c3c1ccc(F)c3</chem>	C15H14FN3O3	303.288	Flumazenil
BIOMOL	B-100	<chem>c1(C(=O)c2ccccc2)cccc(C(C)C(=O)O)c1</chem>	C16H14O3	254.281	Ketoprofen
BIOMOL	EI-288	<chem>C1(\C=ClC(Cl)=ClC=ClC(\C)=ClC(=O)Nc2ccc(O)cc2)=C(C)CCCC1(C)C</chem>	C26H33NO2	391.546	Fenretinide
BIOMOL	GR-103	<chem>c(cccc1)(C(O)=C(C(=O)Nc2sc(C)cn2)N(C)S3(=O)=O)c13</chem>	C14H13N3O4S2	351.401	Meloxicam
BIOMOL	EI-292	<chem>c1(Nc2ccc(F)c(Cl)c2)ncnc3c1cc(OCCCN4CCOCC4)c(OC)c3</chem>	C22H24ClFN4O3	446.902	Gefitinib
BIOMOL	DL-269	<chem>c1(cccc2)c2cccc1CN(C)ClC=ClC#CC(C)(C)C</chem>	C21H25N	291.43	Terbinafine HCl
BIOMOL	EI-318	<chem>c1(C(=O)C(C)C)c(C(C)C)nn2c1ccccc2</chem>	C14H18N2O	230.306	Ibudilast
BIOMOL	DL-270	<chem>c1(ccccc1)CCCC([O-])=O.[Na+]</chem>	C10H11NaO2	186.183	Sodium phenylbutyrate
BIOMOL	EI-320				

BIOMOL	A-280	[C@]([H])([C@@H](NC)[C@@H](O)[C@@H](NC)[C@@H]1O)(O[C@@]([C@]2([H]O3)(O)C(=O)C[C@@H](C)O2)[C@@]13[H][C@@]1(CC2)([C@@H](C[C@@]([H])(C3=C4)[C@@]([H])([C@@]5([H])OC4)[C@]1([H])N6C(=O)C5)N2C3)c7c6cccc7	C14H24N2O7	332.35	Spectinomycin
BIOMOL	AC-745	N(Cc1cccc1)(CC(COCC(C)C)N2CCCC2)c3cccc3	C21H22N2O2	334.412	Strychnine HCl
BIOMOL	AC-104	c([C@@H]1[N+](C)(C)CC2(c2cc(OC)c3O)c3O c(ccc4C[C@H]5c(c6CCN5C)cc(c(OC)c6)Oc7cc(ccc7O)C1)cc4	C24H34N2O	366.54	Bepridil
BIOMOL	AC-746	c1(C(=O)c2cc(l)c(OCN(CC)CC)c(l)c2)c(CCCC)cc3c1cccc3	C37H41N2O6	609.731	Tubocurarine Cl (+)
BIOMOL	AC-105	c(c1ccc2)(c2CCc3c4cccc3)[C@@]4([H])CN([C@]15[H])CC[C@@](O)(C(C)(C)C)C5	C25H29I2NO3	645.312	Amiodarone
BIOMOL	AC-747	C1(C(C(=O)OC)=C(C)NC(C)=C1C(=O)OCCN(C)Cc2cccc2)c3cccc([N+](O-))=O)c3	C25H31NO	361.52	Butaclamol (+)
BIOMOL	AC-108	c(c1CCN2C)([C@@]2([H])Cc3c4c(O)c(O)c3)c4ccc1	C26H29N3O6	479.525	Nicardipine
BIOMOL	AC-748	N1(C2CCN(CCCC(c3ccc(F)cc3)c4ccc(F)cc4)CC2)C(=O)Nc5c1cccc5	C17H17NO2	267.322	Apomorphine r (-)
BIOMOL	AC-109	N1(CCCN(C)C)c2c(cccc2)Sc3c1cc(Cl)cc3	C28H29F2N3O	461.546	Pimozide
BIOMOL	AC-749	N1(CCCN(C)C)c2c(cccc2)Sc3c1cc(Cl)cc3	C17H19ClN2S	318.864	Chlorpromazine HCl
BIOMOL	AC-110	C(C(=O)N(C)C)(CCN1CCC(O)(c2ccc(Cl)cc2)CC1)(c3cccc3)c4cccc4	C29H33ClN2O2	477.038	Loperamide
BIOMOL	AC-751	N1(C2CCN(CCCN3C(=O)Nc4c3cccc4)CC2)C(=O)Nc5c1ccc(Cl)c5	C22H24ClN5O2	425.911	Domperidone
BIOMOL	AC-116	C12(CCN(CCCC(c3ccc(F)cc3)c4ccc(F)cc4)CC1)C(=O)Nc2c5cccc5	C29H31F2N3O	475.573	Fluspirilene
BIOMOL	AC-753	c1(cc(C(F)(F)F)cc2)c2Sc3c(cccc3)N1CCCN4CCN(CCO)CC4	C22H26F3N3OS	437.522	Fluphenazine 2HCl
BIOMOL	AC-117	c1(ccc(C)cc1)S(=O)(=O)NC(=O)NCCCC	C12H18N2O3S	270.348	Tolbutamide
BIOMOL	AC-755	c(c1[nH]c2)(c2C[C@]3([H])[C@]4([H])C[C@@H](CSC)CN3CCC)c4ccc1	C19H26N2S	314.488	Pergolide mesylate
BIOMOL	AC-118	C(=N(C#N)(N(C)C(C)C)C)Nc1ccncc1	C13H19N5	245.323	Pinacidil
BIOMOL	AC-757	c1(C(=O)NC[C@@H]2CCCN2CC)c(O)c(Cl)cc(Cl)c1OC	C15H20Cl2N2O3	347.237	Raclopride l-tartrate s(-)
BIOMOL	AC-120	c1(S(=O)(=O)NC(=O)NC2CCCC2)ccc(CCN(C(=O)c3ncc(Cl)nc3)cc1	C21H27N5O4S	445.535	Glipizide
BIOMOL	AC-758	c1(C2CCN(CCC3=C(C)N=C4N(CCCC4)C3=O)CC2)nc5c1ccc(F)c5	C23H27FN4O2	410.484	Risperidone
BIOMOL	DL-271	n1c(ccnc1Nc2c(C)ccc(NC(=O)c3ccc(CN4CCN(C)CC4)cc3)c2)c5ccncc5	C29H31N7O	493.603	Imatinib
BIOMOL	FR-111	[C@H](Cc1c[nH]c(S)n1)(C([O-])=O)[N+](C)C(C)c([C@@]([H])(O)[C@@H]1O[C@@H](C)[C@@H](O)[C@@H](N)C1)C[C@@](O)(C(=O)C)C2(c(O)c(c3c4O)C(=O)c(c5C3=O)cccc5)c24	C9H15N3O2S	229.299	Ergothioneine
BIOMOL	DL-548	c1(CN[C@@H]2CC[C@H](O)CC2)cc(Br)cc(Br)c1N	C26H27NO9	497.494	Idarubicin
BIOMOL	FR-112	c12c(ccc(n1))C=C1c3cccc([C@@H](CCc4cccc4C(C)C)O)SCC5(CC(O)=O)CC5)c3)ccc(Cl)c2	C13H18Br2N2O	378.103	Ambroxol
BIOMOL	DL-273	C(O)C(C(=O)C(CCCCCCCCCO)=C(C)C1=O)=C1OC	C35H36ClNO3S	586.183	Montelukast
BIOMOL	FR114	c1(ccccc1)C[C@@H](C)N(C)CC#C	C19H30O5	338.439	Idebenone
BIOMOL	EI-240	C1(=O)C[C@H](O)C[C@@H](CC[C@H]2[C@@H](C)C=CC([C@@]23[H])=CCC[C@@H]3OC([C@@H](C)CC)=O)O1	C13H17N	187.281	Selegiline
BIOMOL	G-233	n1nc(Cc2ccncc2)c(cccc3)c3c1Nc4ccc(Cl)cc4	C23H34O5	390.513	Mevastatin
BIOMOL	DL-275	[C@]1([H])([C@@H](CC[C@H]2OC(=O)C[C@H](O)C2)[C@@H](C)C=C3)[C@]1([H])(C)C[C@@H]1OC(=O)C(C)CC	C20H15ClN4	346.813	Vatalanib
BIOMOL	G-244	C3=C[C@H](C)C[C@@H]1OC(=O)C(C)CC	C25H38O5	418.566	Simvastatin
BIOMOL	CT-100	[C@@]12(OC1)C[C@@H](OC(=O)C=C1C=C1C=C1C(=O)O)[C@@H](OC)[C@@]2([H])[C@@]3(C)O[C@@H]3C1C=C(Cl)/C)C	C26H34O7	458.544	Fumagillone
BIOMOL	G-430	c(c(S([O-])(=O)=O)cc(S([O-])(=O)=O)c1)(c(NC(=O)c2ccc(C)c(NC(=O)c3cccc(NC(=O)Nc4cccc(C(=O)Nc5c(C)ccc(C(=O)Nc6ccc(S([O-])(=O)=O)c7c6c(S([O-])(=O)=O)cc(S([O-])(=O)=O)c7)c5)c4)c3)c2)ccc8S([O-])(=O)=O)c18	C51H34N6O23S6	1291.232	Suramin sodium
BIOMOL	DL-239	C1(CC)(O)c(c2C1)cccc2)C3=NCCN3	C13H16N2O	216.279	Efaroxan
BIOMOL	DL-282	c1(C[C@@H](C(=O)N[C@@H](CO)C(=O)N[C@@H](C(=O)N[C@@H](CO)C(C)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCCC(=N)N)C(=O)N2CC[C@H]2C(=O)NNC(=O)N)Cc3ccc(C)cc3)NC(=O)[C@@H](NC(=O)[C@@H]4NC(=O)CC4)Cc5nc[nH]c5)[nH]	C59H84N18O14	1269.41	Goserelin acetate
BIOMOL	PG-007	[C@@]1([H])([C@@H](C1C=C/C/CCCC(=O)O)C(=O)C[C@@H](O)[C@]1([H])C=C[C@@H](O)CCCCC	C20H32O5	352.465	Dinoprostone
BIOMOL	DL-283	c1(O)cccc1O	C7H8O2	124.137	Guaiacol
BIOMOL	DL-276	C(=N)(N(C)C)NC(=N)N	C4H11N5	129.164	Metformin
BIOMOL	GR-100	C1(\C=C1C1(C)=C1C=C1C(\C)=C1C(=O)O)=C(C)CCCC1(C)C	C20H28O2	300.435	Retinoic acid
BIOMOL	DL-277	c(c(Cl)c(Cl)cc1)(CN(C2=N3)CC(=O)N2)c13	C10H7Cl2N3O	256.088	Anagrelide
BIOMOL	GR-210	c(c(C)c(C)c(O)c1C(O)C(C)(COc2ccc(CC3SC(=O)NC3=O)cc2)CC4)c14	C24H27NO5S	441.54	Troglitazone
BIOMOL	AC-121	N(CC1=NCCN1)(c2ccc(C)cc2)c3cccc(O)c3	C17H19N3O	281.352	PhentolamineHCl
BIOMOL	AC-760	c1(C(=O)NC[C@@H]2CCCN2CC)cc(S(=O)(=O)N)ccc1OC	C15H23N3O4S	341.426	Sulpiride s (-)
BIOMOL	AC-122	c1(cc(OC)cc2)c2nccc1[C@@H](O)[C@]3([H])C[C@@]([H])(CCN34)[C@@H](C=C)C4	C20H24N2O2	324.417	Quinine
BIOMOL	AC-763	C(OCCN(C)C)(c1cccc1)c2cccc2	C17H21NO	255.355	Diphenhydramine HCl

BIOMOL	AC-123	c1(Nc2cccc(C(F)(F)F)c2)cccc1C(=O)O	C14H10F3NO2	281.23	Flufenamic acid
BIOMOL	AC-765	N1(CC(C)N(C)C)C)c2c(cccc2)Sc3c1cccc3	C17H20N2S	284.419	Promethazine HCl
BIOMOL	AC-124	c1(OCC(O)CNCCC)cccc1C(=O)CCc2cccc2	C21H27NO3	341.444	Propafenone
BIOMOL	AC-766	c1(CN(C)C)ccc(CSCCN(C)NC)=C/[N+](O-)=O]o1	C13H22N4O3S	314.404	Ranitidine HCl
BIOMOL	AC-125	C1(C(=O)NC(=O)N1)(c2cccc2)c3cccc3 [C@](CCN1CC2CC2)([C@@H]3c(c4C5)[nH]c(c46)cccc6)([C@]5O)[C@H]1 C7)c(c7ccc8O)c8O3	C15H12N2O2	252.268	Phenytoin
BIOMOL	AC-770	c1(ccc(N)cc1)C(=O)NCCN(CC)CC	C26H26N2O3	414.496	Naltindole HCl
BIOMOL	AC-127	C1(COc2c(cccc2)O)1C3=NCCN3	C13H21N3O	235.325	Procainamide
BIOMOL	AC-806	C1(COc2c(cccc2)O)1C3=NCCN3	C11H12N2O2	204.225	Idazoxan
BIOMOL	AC-128	c1(c(C)cccc1C)NC(=O)CN(CC)CC	C14H22N2O	234.337	Lidocaine
BIOMOL	AC-807	C12(CCN(CCCO(=O)c3ccc(F)cc3)CC1)C(=O)NCN2c4cccc4	C23H26FN3O2	395.47	Spiperone
BIOMOL	AC-130	c1(C(=O)NCC2NCNCC2)cc(OC(C(F)(F)F)ccc1OC(C(F)(F)F	C17H20F6N2O3	414.343	Flecainide
BIOMOL	AC-808	c1([C@@H](O)CN)ccc(O)c(O)c1	C8H11NO3	169.178	Epinephrine-(+)-tartrate
BIOMOL	AC-131	c1(nc(C)cc(N)nc1N)C(=O)NC(=N)Nc2cccc2	C12H12ClN7O	305.723	(-)
BIOMOL	AC-809	c1(c(C)cccc1C)NC(SCCC2)=N2	C12H16N2S	220.334	Phenamil
BIOMOL	AC-136	c1(ccccc1OCC2=NCCN2)C3CC3	C13H16N2O	220.334	Xylazine HCl
BIOMOL	AC-810	c1(ccc(O)c(O)c1)[C@@H](O)CN.[C@H](O)(C(=O)O)[C@@H](O)(C(=O)O	C12H17NO9	319.265	Cirazoline HCl
BIOMOL	DL-278	c1(NS(=O)=O)=O)C)ccc(CCN(C)CCOc2ccc(NS(=O)(=O)C)cc2)cc1	C19H27N3O5S2	441.565	Norepinephrine-(+)-tartrate I (-)
BIOMOL	GR-211	c1(ccc(Cl)cc1)C(=O)NCCc2ccc(OC(C)(C)C(=O)O)cc2	C19H20ClNO4	361.819	Dofetilide
BIOMOL	DL-279	c(c(Nc1cccc(C#C)c1)ncn2)(cc(OCOCOC)c(OCOCOC)c3)c23	C22H23N3O4	393.436	Bezafibrate
BIOMOL	GR243	c1(C(=O)c2ccc(OCN3CCCCC3)cc2)c4c(cc(O)c4)sc1c5ccc(O)cc5	C28H27NO4S	473.583	Erlotinib
BIOMOL	AC-227	[C@H]1[C@H](O)c2cccc2)CCC[C@H](CC(=O)c3cccc3)N1C	C22H27NO2	337.455	Raloxifene HCl
BIOMOL	GR-301	C([C@@](O)(CC)C(=O)O)C1(C(=N2C3=O)c4c(cc(c5n4)cccc5)C2)=C13	C20H16N2O4	348.352	Lobeline
BIOMOL	NS-520	c(cc(OC)cc1)(c(CNCC(=O)C)c[nH]2)c12	C13H16N2O2	232.278	Camptothecin
BIOMOL	GR-305	c(c(O)c(c1c2c(O)c(C)C(O)[C@@H]3O[C@H](C)[C@H](O)[C@H](O)[C@@H]4O[C@H](C)[C@@H](O)[C@H](O)(C4)C3)c1)C(=O)[C@@H](O)[C@@H]5O[C@H](C)[C@@H](O)[C@H](O)[C@@H]6O[C@H](C)[C@@H](O)[C@H](O)[C@@H]7O[C@H](C)[C@@H](O) [C@H]1(C)C=C/C(C)C(=O)O)[C@@H](O)C[C@H](O)[C@@H]1(C)C=C[C@@H](O)CCCCC	C52H76O24	1085.145	Melatonin
BIOMOL	PG-008	c(C(=O)[C@@]1(C)O)C=O[C@H](OC)[C@@H](C)[C@@H](OC(C)=O)C @H](C)[C@H](O)[C@H](C)[C@@H](O)[C@@H](C)C=C(C)C(=O)C N2)(c3O)1)c(O)c(1C=N1N4CCN(C)CC4)c2c5O)c5c(O)c3C	C20H34O5	354.481	Plicamycin
BIOMOL	GR-306	c1(ccnc2c2cccc1S(=O)(=O)N3CCNCCC3	C43H58N4O12	822.94	Dinoprost
BIOMOL	EI-233	[C@H]1(c2cc(OC)c(O)c(OC)c2)[C@]3([H])[C@]([H])(CO C3=O)[C@H](O)[C@H]4[C@H](O)[C@@H](O)[C@H]5[C@H]6[C@H](CO[C@H](C)O5)O4)c6c1cc(c7c6)OCO7	C14H17N3O2S	291.369	Rifampicin
BIOMOL	GR-307	c(C(O)CCC1)(c(N)c(c2n3)cccc2)c13	C29H32O13	588.557	Fasudil
BIOMOL	C-106	[C@@](O)(C)[C@]1([H])[C@@]([H])(N1)C2([C@H](CO(C)=O)N)C(=C34)C(=O)C)N=C(C)C3=O)N24	C13H14N2O	214.263	Etoposide
BIOMOL	GR-311	N1(CC#CCN2CCCC2)CCCC1=O	C15H18N4O5	334.327	Hydroxytacrine maleate
BIOMOL	C-109	n1([C@@H]2O[C@H](CO)[C@@H](NC(=O)[C@@H](N)Cc3ccc(OC)cc3)[C@H]2O)cnc4c1ncnc4N(C)C	C12H18N2O	206.284	Mitomycin c
BIOMOL	GR-312	c(cccc1)(nc(c2c3N)CCCC2)c13	C22H29N7O5	471.51	Oxotremorine sesquifumarate
BIOMOL	C-110	c1(ncccc1NC(C)C)N2CCN(C(=O)c3[nH]c(c4c3)ccc(NS(=O)(=O)C)c4)CC2	C13H14N2	198.264	Puromycin 2HCl
BIOMOL	GR-314	c1(OCC[N+](CC)(CC)CC)c(OC[CN+](CC)(CC)CC)cccc1OCC[N+](CC)(CC)CC	C22H28N6O3S	456.561	Tacrine HCl
BIOMOL	C-112	13	C30H60N3O3	510.816	Delavirdine mesylate
BIOMOL	GR-316	13	C20H16N2O5	364.351	Gallamine triethiodide
BIOMOL	AC-138	c1(CC2=NCCN2)c(C)cc(C(C)(C)C)c(O)c1C C1(N2CCN(CCOCCO)CC2)=Nc3c(cccc3)Sc4c1cccc4.C5(N6CCN(CCOCCO)CC6)=Nc7c(cccc7)Sc8c5cccc8.C(/(C(=O)O)C=Cl(C)=O)O	C16H24N2O	260.375	10-hydroxycamptothecin
BIOMOL	DL-557	C1(CCN(C)C)C(O)c2ccc(O)cc2)CC1)Cc3cccc3	C46H54N6O8S2	883.086	Oxymetazoline HCl
BIOMOL	AC-142	c1(OCC(O)CN(C)C)cccc1CC=C	C21H27NO2	325.445	Quetiapine fumarate
BIOMOL	AC-812	c1(cccc2)c2cccc1OCC(O)CN3CCN(c4cccc4OC)CC3	C15H23NO2	249.349	Ifenprodil
BIOMOL	AC-144	N1(CCCN(C)C)c2c(cccc2)CCc3c1cccc3	C24H28N2O3	392.491	Alprenolol HCl
BIOMOL	AC-813	N1(CCCN(C)C)c2c(cccc2)CCc3c1cccc3	C19H24N2	280.407	Naftopidil 2HCl
BIOMOL	AC-146	c(cc(OC)c(OC)c1)(c(N)nc(N2CCN(C(=O)c3cccc3)CC2)n4)c14	C19H21N5O4	383.401	Imipramine HCl
BIOMOL	AC-814	C1(N2CCNCC2)=Nc3c(cccc3)Oc4c1cc(Cl)cc4	C17H16ClN3O	313.781	Prazosin HCl
BIOMOL	AC-152	c1(c(Cl)cccc1Cl)NC2=NCCN2	C9H9Cl2N3	230.094	Amoxapine
BIOMOL	AC-152	c1(c(Cl)cccc1Cl)NC2=NCCN2	C9H9Cl2N3	230.094	Clonidine HCl

BIOMOL	AC-834	<chem>c(c1n(C)c2)(c2C[C@]3([H])[C@]4([H])C[C@H](NS(=O)(=O)N(C)C)CN3C)c4ccc1</chem>	C18H26N4O2S	362.49	Mesulergine HCl
BIOMOL	AC-153	<chem>c1(\C=N\N(C)=N)N)c(Cl)cccc1Cl</chem>	C8H8Cl2N4	231.082	Guanabenz acetate
BIOMOL	DL-558	<chem>c1(cccc(Cl)c1)C(=O)C(C)NC(C)(C)C</chem>	C13H18ClNO	239.741	Amfebutamone
BIOMOL	AC-154	<chem>C(NC(OCC1)=N1)(C2CC2)C3CC3</chem>	C10H16N2O	180.247	Rilmenidine hemifumarate
BIOMOL	AC-840	<chem>c1(C(=O)NCCN(CC)CC)cc(Cl)c(N)cc1OC</chem>	C14H22ClN3O2	299.796	Metoclopramide HCl
BIOMOL	AC-160	<chem>C12(CCN(C3COc4c(cccc4)O3)CC1)C(=O)NCCN2c5cccc5</chem>	C22H25N3O3	379.452	Spiroaxtrine
BIOMOL	AC-858	<chem>[C@]1([C@]2(O)[C@]([H])(C3)N(CC4CC4)CC1)([C@]5([H])c(c6C2)oc(c67)cccc7)c(c38)c(c(O)cc8)O5</chem>	C26H25NO4	415.481	Naltriben mesylate
BIOMOL	AC-161	<chem>c1([nH]c(c23)cccc2)c3CCN4[C@]1([H])C[C@]([H])([C@]5([H])C4)[C@]([H])(C(=O)O)C)[C@]([H])(O)CC5</chem>	C21H26N2O3	354.443	Yohimbine HCl
BIOMOL	DL-124	<chem>C(C(C1)(C)(\C=C\Cl(C)=ClC=Cl(C)\C=ClCO(C)=O)C)=C(C)CC1</chem>	C22H32O2	328.488	Vitamin a (acetate)
BIOMOL	AC-164	<chem>[C@](O)(O)[C@]([C](N(C)=O)[C@H]1CN(C)[C@]([H])(C2C1)Cc3c(c4[nH]c3)c2ccc4)C5=O)[C@]6([H])N(CCC6)C(=O)[C@]7C8cccc8)N57</chem>	C33H37N5O5	583.677	Dihydroergotamine mesylate
BIOMOL	AC-891	<chem>[C@]([CCCC1)(c2c(ccc(O)c2)C3)(CCN4C=ClC)[C@]1([H])[C@]([H])34</chem>	C19H25NO	283.408	Levallorphan tartrate
BIOMOL	C-115	<chem>[C@]([C]=C[C@H](O)C1)[C@H]1O2)(CCN(C)C3)c(c3ccc4OC)c24</chem>	C17H21NO3	287.354	Galanthamine HBr
BIOMOL	GR-318	<chem>c12c(c(O)c3c([C@]([H])(O)[C@H]4C[C@H](N)[C@H](O)[C@H](C)O4)C[C@](O)(O)(C(C)=O)C3)c1O)C(=O)c5c(c(O)C)ccc5)C2=O</chem>	C27H29NO10	527.52	Daunorubicin HCl
BIOMOL	CA-200	<chem>c1(nc(Cl)c(N)nc1N)C(=O)NC(=N)N</chem>	C6H8ClN7O	229.627	Amiloride
BIOMOL	GR-319	<chem>c(c(O)c1c(C(=O)c2c(cccc2OC)C1=O)c3O)(C[C@]([O])(C(=O)CO)C[C@]([H])4O[C@]([H])5O[C@]([H])(C)[C@]([H])(O)[C@]([H])(N)C5)c34</chem>	C27H29NO11	543.519	Doxorubicin HCl
BIOMOL	CA-202	<chem>C1(c2cccc2Cl)C(=O)OC(=O)C(=O)NC(COCCN)=C1C(=O)OCC</chem>	C20H25ClN2O5	408.876	Amlodipine
BIOMOL	GR336	<chem>c(c1c(C(C)(C)CCC1)cc2)(C(=O)C(=O)c3c4ccc3)c24</chem>	C19H18O3	294.344	Tanshinone iia
BIOMOL	CA-205	<chem>[C@]([H])1(c2ccc(O)C)cc2)Sc3c(cccc3N(CCN(C)C)C(=O)[C@]([H])1OC(=O)C</chem>	C22H26N2O4S	414.518	Diltiazem
BIOMOL	DL-284	<chem>c1(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)ncnc4c1cc(c5ccc(CNCCS(C(=O)=O)O)O5)cc4</chem>	C29H26ClFN4O4S	581.058	Lapatinib
BIOMOL	CA-210	<chem>C1(C(C(=O)OC)=C(C)NC(C)=C1C(=O)OC)c2cccc2[N+][([O-])=O</chem>	C17H18N2O6	346.335	Nifedipine
BIOMOL	DL-285	<chem>c1(C(=O)OC)cccc1O</chem>	C8H8O3	152.147	Methyl salicylate
BIOMOL	CA-211	<chem>C1(C(C(=O)OC(C)C)=C(C)NC(C)=C1C(=O)OCCOC)c2cccc([N+][([O-])=O)c2</chem>	C21H26N2O7	418.44	Nimodipine
BIOMOL	GR-240	<chem>C1(S(C(=O)NC1=O)Cc2ccc(OCc3ncc(CC)cc3)cc2</chem>	C19H20N2O3S	356.439	Pioglitazone
BIOMOL	CA-212	<chem>C1(c2cccc([N+][([O-])=O)c2)C(C(=O)OC)=C(C)NC(C)=C1C(=O)OCC</chem>	C18H20N2O6	360.361	Nitrendipine
BIOMOL	DL-287	<chem>5</chem>	C27H23N5O4	481.503	Pranlukast
BIOMOL	CA-215	<chem>C(C#N)(C(C)C)(CCCN(C)CCc1ccc(OC)c(O)c1)c2ccc(OC)c(O)c2</chem>	C27H38N2O4	454.602	Verapamil
BIOMOL	DL-288	<chem>c1(O(C(=O)N(C)C)CC)cccc([C@]([H])(N(C)C)C)c1</chem>	C14H22N2O2	250.337	Rivastigmine
BIOMOL	CA-216	<chem>C1(CCN(CCCOC(=O)C2=C(C)NC(C)=C(C(=O)OC)C2c3cccc([N+][([O-])=O)c3)CC1)(c4cccc4)c5cccc5</chem>	C36H39N3O6	609.711	Niguldipine HCl
BIOMOL	DL-289	<chem>C(c1ccc(S(=O)(=O)C)cc1)(COC2=O)=C2c3cccc3</chem>	C17H14O4S	314.356	Rofecoxib
BIOMOL	CA-225	<chem>C(c1ccc(F)cc1)(c2ccc(F)cc2)N3CCN(ClC=C1c4cccc4)CC3</chem>	C26H26F2N2	404.495	Flunarizine-2HCl
BIOMOL	DL-236	<chem>[C@](O)(O)[C@]([C](N(C)=O)[C@H]1CN(C)[C@]([H])(C2=C1)[H])Cc3c(c4[nH]c3)c2ccc4)C5=O)[C@]6([H])N(CCC6)C(=O)[C@]7C8cccc8)N57</chem>	C33H35N5O5	581.662	Ergotamine D-tartrate
BIOMOL	AC-165	<chem>[C@]1([OC])[C[C@]([H])(CO(C=O)c2cnc(Br)c2)CN3C)[C@]3([H])Cc4c(c5n(C)c4)c1ccc5</chem>	C24H26BrN3O3	484.386	Nicergoline
BIOMOL	AC-893	<chem>[C@]([CCN1CC2CCC2)([C@]([H])3[C@]([H])(O)CC4)([C@]4(O)[C@]([H])1C5)c(c5ccc6O)c6O3</chem>	C21H27NO4	357.443	Nalbuphine HCl
BIOMOL	DL-564	<chem>[C@H]1(CS[C@H](CO)O1)N2C=C(F)C(N)=NC2=O</chem>	C8H10FN3O3S	247.247	Emtricitabine
BIOMOL	AC-911	<chem>[N+](C)(C)(C)CCOC(=O)N</chem>	C6H15N2O2	147.195	Carbamylcholine Cl
BIOMOL	AC-169	<chem>c1(OCC(O)CNC(C)C)ccc(CCOCC2CC2)cc1</chem>	C18H29NO3	307.428	Betaxolol HCl
BIOMOL	AC-912	<chem>C(C(C)OC(=O)N)[N+](C)(C)C</chem>	C7H17N2O2	161.222	Carbamyl-beta-methylcholine Cl
BIOMOL	AC-171	<chem>c1(OCC(O)CNC(C)C)ccc(NC(=O)C)cc1</chem>	C14H22N2O3	266.336	Practolol
BIOMOL	AC-915	<chem>C(COC(=O)CCC)[N+](C)(C)C</chem>	C9H20NO2	174.261	Butyrylcholine Cl
BIOMOL	AC-172	<chem>c1(N2CCOCC2)nsnc1OC[C@]([H])(O)CNC(C)(C)C</chem>	C13H24N4O3S	316.42	Timolol maleate (s)
BIOMOL	AC-925	<chem>c1(N=C(N)/N)sc(CSCCC(=N)NS(=O)(=O)N)n1</chem>	C8H15N7O2S3	337.445	Famotidine
BIOMOL	AC-173	<chem>N1(CCOCC1)C(=O)NCCNCC(O)COc2ccc(O)cc2</chem>	C16H25N3O5	339.387	Xamoterol hemifumarate
BIOMOL	AC-928	<chem>C(O)(c1cccc1)(c2cccc2)C3CCN(CCCC(O)c4ccc(C(C)(C)C)cc4)CC3</chem>	C32H41NO2	471.673	Terfenadine
BIOMOL	AC-174	<chem>C(C)(C)(C)NCC(O)c1cc(Cl)c(N)c(Cl)c1</chem>	C12H18Cl2N2O	277.19	Clenbuterol
BIOMOL	AC-986	<chem>c1(ccncc1)C(=O)NN</chem>	C6H7N3O	137.139	Isoniazid
BIOMOL	AC-175	<chem>c1(C=CC(=O)N2)c2c(O)ccc1[C@]([H])(O)[C@H](CC)NC(C)C</chem>	C16H22N2O3	290.357	Procaterol hcl

BIOMOL	AC-993	c(ccs1)(CN(Cc2ccccc2Cl)CC3)c13	C14H14ClNS	263.786	Ticlopidine HCl
BIOMOL	AC-176	c1(C(O)CNC(C)(C)C)ccc(O)c(CO)c1	C13H21NO3	239.311	Salbutamol sulfate
BIOMOL	DL-246	c1(CC(C)CN2[C@@H](C)O[C@@H](C)C2)ccc(C(C)(C)CC)cc1	C21H35NO	317.509	Amorolfine
BIOMOL	AC-181	c(c(OCC(C)CNC(C)C)ccc1)(cc[nH]2)c12	C14H20N2O2	248.321	Pindolol
BIOMOL	DL-247	[C@@](C)(OCC[C@H]1CCCN1C)(c2ccccc2)c3ccc(Cl)cc3	C21H26ClNO	343.89	Clemastine fumarate
BIOMOL	CA-234	C1(CN)(CCCCC1)CC(O)=O	C9H17NO2	171.237	Gabapentin
BIOMOL	DL-291	c(ccc(F)c1)(\C(=Cl)c2ccc(S(=O)(=O)C)cc2)\C(C)=C3CC(=O)O)c13	C20H17FO3S	356.411	Sulindac
BIOMOL	CA-236	C1(C(C(=O)O)C)=C(C)NC(C)=C1C(=O)OCCc2ccccc(Cl)c2Cl	C18H19Cl2NO4	384.254	Felodipine
BIOMOL	DL-292	C(C(=O)O)(CCC)CCC C1(c2ccccc([N+])([O-]))=O)c2(C(=O)O)CCO=C(C)C(C)C(C)=C1C(=O)OCCc2ccccc3	C8H16O2	144.211	Valproic acid
BIOMOL	CA-237]=O)c2(C(=O)O)CCO=C(C)C(C)C(C)=C1C(=O)OCCc2ccccc3	C27H28N2O7	492.52	Cilnidipine
BIOMOL	DL-547	[C@@]([H])(\C(=Cl)C=C(Cl)C[C@@H](O)C[C@@H]1O)/C1=C(C)\CCC2)(CC[C@H]3[C@@H](C)C=C(Cl)[C@@H](O)C4CC4)[C@]23C	C27H40O3	412.605	Calcipotriene
BIOMOL	CA-305	c1(cccccc1)CN(CCC)C(C)COc2ccccc2 c1(cc(NC(=O)O)C2CCCC2)cc3c3n(C)cc1Cc4ccc(C(=O)NS(=O)(=O)c5ccccc5C)cc4OC	C18H22ClNO	303.826	Phenoxybenzamine HCl
BIOMOL	DL-294		C31H33N3O6S	575.675	Zafirlukast
BIOMOL	CA-310	c1(cc(C(F)(F)F)cc2)c2Sc3c(cccc3)N1CCCN4CCN(C)CC4	C21H24F3N3S	407.496	Trifluoperazine
BIOMOL	DL-295	c1(sc(c2c1)cccc2)C(C)N(O)C(=O)N	C11H12N2O2S	236.29	Zileuton
BIOMOL	DL-218	c(n(CC(=O)O)cn1)(C(=O)N(CCCC)C(=O)N2CCCC)c12	C16H24N4O3	320.387	Denbufylline
BIOMOL	PR-118	c1(C(=N)N)ccc(OCCCCCOc2ccc(C(=N)N)cc2)cc1	C19H24N4O2	340.419	Pentamidine
BIOMOL	DL-131	O(CCCCCCCCCCCCCCCC)P([O-])(=O)OCC[N+](C)(C)C	C21H46NO4P	407.568	Miltefosine
BIOMOL	DL-297	C(=O)([C@H](Cc1ccccc1)NC(=O)c2cncn2)N[C@H](CC(C)C)B(O)O [C@H]1(C)C=C/C(CCC(=O)O)C(C)C[C@@H](O)C[C@@H](O)C[C@@H]1C C[C@@H](O)CCc2ccccc2	C19H25BN4O4	384.237	Bortezomib
BIOMOL	DL-281		C26H40O5	432.593	Latanoprost
BIOMOL	DL-161	C(C)(C)(C)NCC(O)c1cc(O)C(=O)N(C)C)cc(O)C(=O)N(C)C)c1 [C@@]1(CO)([C@H](O)C[C@H](O)[C@@H]2O[C@@H](C)[C@H](O)C[C@@H](O)[C@H]2O)C3[C@@H](O)C[C@H]4([H])([C@@]1([C@H](O)C[C@@H]5C6=CC(=O)O)C6)[H]	C18H29N3O5	367.44	Bambuterol
BIOMOL	CM-109		C29H44O12	584.652	Ouabain
BIOMOL	DL-186	c1(c2ccc(Cl)cc2)nc(c3ccccc3)sc1CC(=O)O	C17H12ClNO2S	329.801	Fentiazac
BIOMOL	CM-112	c1(C(=O)NN2[C@H](C)CC[C@@H]2C)ccc(C)(S(=O)(=O)N)c1	C14H20ClN3O3S	345.845	Clopidamide
BIOMOL	J120	C1(CC)NC(=O)N(C)C1=O)c2ccccc2	C12H14N2O2	218.252	Mephénytoin
BIOMOL	AC-183	c1(C(O)CNC(C)C)ccc(N)c(C#N)c1	C12H17N3O	219.283	Cimaterol
BIOMOL	DL-248	O	C23H32N6O4S	488.603	Vardenafil
BIOMOL	AC-185	c1(CCNC(C)CCc2ccc(O)cc2)ccc(O)c(O)c1	C18H23NO3	301.38	Dobutamine HCl
BIOMOL	DL-249	N1(C(=O)O)[C@@H](CNC(=O)C)C1)c2ccc(N3CCOCC3)c(F)c2	C16H20FN3O4	337.346	Linezolid
BIOMOL	AC-189	c(cccc1)(cc(C)O)CNC(C)C)cc2c12 [C@]1(O)C(=O)C(CO2)[C@@]2([H])C[C@H](O)[C@@](C)([C@@]13[H])C(=O)[C@H](O)C(=C4C)C(C)C[C@@](O)(C[C@@H]4O)C(=O)[C@H](O)C[C@@H](NC(=O)O)C(C)C)c5ccccc5[C@@H]3O)C(=O)c6ccccc6	C15H19NO	229.317	Pronethalol HCl
BIOMOL	DL-250		C43H53NO14	807.879	Docetaxil
BIOMOL	AC-192	c1(ccc(NS(=O)(=O)C)cc1)C(O)CNC(C)C	C12H20N2O3S	272.364	Sotalol HCl
BIOMOL	DL-251	c(cc(C(C(=O)O)cc1)(c1O)C2)C=C/C(CCN(C)C)c(cccc3)c23	C21H23NO3	337.412	Olopatadine
BIOMOL	AR-111	[C@@](CCCNC)(CC1)(c2c3ccccc2)c(cccc4)c4[C@@]13[H] C1(c2ccccc([N+])([O-]))=O)c2(C(=O)O)C(=O)C(C)NC(C)=C1C(=O)OCCN3CCN(C(c4ccccc4)c5ccc5)CC3	C20H23N	277.403	Maprotiline HCl
BIOMOL	DL-258		C35H38N4O6	610.699	Manidipine
BIOMOL	AC-194	C(CNC)(O)c1ccccc1OC)c2ccccc2	C17H21NO2	271.354	Nisoxetine HCl
BIOMOL	DL-252	c1(cc(O)c(O)c([N+])([O-])=O)c1C(=O)c2ccc(C)cc2 C1(\C=C(Cl)C(\C)=ClC=Cl(C)C(\C)=ClC=C(Cl)C)/C)C=C(Cl)C=C(Cl)C2=C(C)C(=O)CCC2(C)C(=O)C(C)C(=O)CCC1(C)C	C14H11NO5	273.241	Tolcapone
BIOMOL	DL-553	[C@](CC)([C@](O)(C#C)CC1)(C=CC(=C(CCC2=O)C3=C2)[C@@]4([H])C3)[C@@]14[H]	C40H52O2	564.84	Canthaxanthin
BIOMOL	DL-253		C21H24O2	308.414	Gestrinone
BIOMOL	AC-214	[C@H]1(Cc2cncn2C)CO(C(=O)[C@H]1CC c1(C(=O)OCC(O)C(=O)O2)=C2C)c(C(C)C)O)nc(CCC)n1Cc3ccc(c4ccccc4c5nn[nH]5)cc3	C11H16N2O2	208.257	Pilocarpine HCl
BIOMOL	DL-254		C29H30N6O6	558.585	Olmesartan
BIOMOL	AC-218	[C@@]([H])(CC1)(C[C@H](OC(=O)C(CO)c2ccccc2)C3)[N+](C)(C)C)[C@@]13[H]	C20H30NO3	332.457	Ipratropium Br
BIOMOL	DL-255	C1(C(C(=O)O)C)=C(C)NC(C)=C1C(=O)OCC(C)C)c2ccccc2[N+])([O-])=O	C20H24N2O6	388.414	Nisoldipine
BIOMOL	AC-220	N1(C(=O)CN2CCN(C)CC2)c3c(ccccc3)C(=O)Nc4c1cccc4 C1(C(C(=O)O)CC)=C(C)NC(C)=C1C(=O)OCC)c2ccccc2)C=C(Cl)C(=O)O)C(C)C	C19H21N5O2	351.402	Pirenzepine 2HCl
BIOMOL	DL-256		C26H33NO6	455.543	Lacidipine
BIOMOL	CN-244	[N+](N-1)(=Cl)C(O)N=N(C(=O)OCC)N2CCOCC2	C9H14N4O4	242.232	Molsidomine

BIOMOL	KC-115	c(ccc(Cl)c1)(N=C(C)NS2(=O)=O)c12	C8H7ClN2O2S	230.671	Diazoxide
BIOMOL	CR110	c1(ccccc2)c2n(CCN3CCOCC3)c(C)c1C(=O)c4ccc(OC)cc4	C23H26N2O3	378.464	Pravastatin
BIOMOL	KC-120	c1(C(=O)NCCc2ccc(S(=O)(=O)NC(=O)NC3CCCC3)cc2)cc(Cl)ccc1OC	C23H28ClN3O5S	494.004	Glyburide
BIOMOL	CT110	c1(NC(=O))C=Cc2ccc(OC)c(OC)c2cccc1C(=O)O	C18H17NO5	327.331	Tranilast
BIOMOL	KC-125	C1(=NC(=N)N(O)C(N)=C1)N2CCCC2	C9H15N5O	209.248	Minoxidil
BIOMOL	CT115	c(c(O)ccc1O)(C(=O)C)[C@H](O)C1C=C(Cl)/C)=CC2=O)c12	C16H16O5	288.295	Shikonin
BIOMOL	KC-135	S(=O)(=O)(NC(=O)NN1CCCCC1)c2ccc(C)cc2 N(C(=O)[C@](C(C)C)(NC(=O)[C@H]1CN(C)C(C2=C1)Cc3c(c4[nH]c3Br)c2 ccc4)O5)[C@@H](CC(C)C)C(=O)N6[C@@]7([H])CCC6)[C@@]57O	C14H21N3O3S	311.4	Tolazamide
BIOMOL	D-102	c1(ncccc1)C(=O)NCCO[N+](=[O-])=O	C32H40BrN5O5	654.595	Bromocriptine mesylate
BIOMOL	KC-152	c1(ncccc1)C(=O)NCCO[N+](=[O-])=O	C8H9N3O4	211.175	Nicorandil
BIOMOL	D-107	C1(N2CCN(C)CC2)=Nc3c(ccc(Cl)c3)Nc4c1cccc4	C18H19ClN4	326.823	Clozapine
BIOMOL	DL-298	c(cc(C(=O)c1ccc(C(=O)O)cc1)c(C)c2)(C(C)(C)CCC(C)C)c23	C24H28O2	348.478	Bexarotene
BIOMOL	D-108	C1(N2CCN(C)CC2)=Nc3c(cccc3)Sc4c1cc(Cl)cc4	C18H18ClN3S	343.874	Clothiapine
BIOMOL	DL-221	c1(ccc(OC)cc1)C(=O)C(Cl)Br=C(Cl)=O	C11H9BrO4	285.091	Brometric acid
BIOMOL	D-109	[C@@]1([H])([H])(CCC)CCC1)(Cc(c2C3)c[nH]n2)[C@]13[H]	C13H21N3	219.326	Quinpirole HCl (-)
BIOMOL	DL-299	n1(c2ccc(S(=O)(=O)N)cc2)nc(C(F)F)cc1c3ccc(C)cc3	C17H14F3N3O2S	381.372	Celecoxib
BIOMOL	D-111	c1(C(=O)NC[C@@H]2CCCN2CC)c(O)ccc(Br)c1OC	C16H23BrN2O3	371.269	Remoxipride
BIOMOL	DL-172	N1(CCCC1=O)[C@@H](CC)C(=O)N [C@](C)([C@@H]([C@H](C)CCCC(O)(C)C)CC1)(CC2)[C@]1([H])C(Cl)C2= ClC=C(Cl)C[C@@H](O)CC3)/C3=C	C8H14N2O2	170.209	Levetiracetam
BIOMOL	DM100	C(n1ncnc1)(c2ccc(C#N)cc2)c3ccc(C#N)cc3	C27H44O2	400.637	Calcifediol
BIOMOL	DL-300	C(n1ncnc1)(c2ccc(C#N)cc2)c3ccc(C#N)cc3	C17H11N5	285.303	Letrozole
BIOMOL	AC-221	N1(C(=O)CN2CCN(C)CC2)c3c(cccc3)NC(=O)c4c1c(C)sc4	C19H22N4O2S	370.469	Telenzepine 2HCl
BIOMOL	DL-257	C1(N2CCN(C)CC2)=Nc3c(cccc3)Nc4c1cc(C)sc4	C17H20N4S	312.432	Olanzapine
BIOMOL	AC-222	C(CO)(C(=O)N(CC)Cc1cncnc1)c2cccc2 [C@]1([H])([C@@H](CC[C@H]2O(C(=O)C[C@H](O)C2)[C@@H](C)C=C3) C3=C[C@H](C)C[C@@H]1O(C(=O)[C@@H](C)CC [C@]1([H])([C@H](C)[C@@H]([N+](=O)C)CCCC2)[C@@H]3O(C(=O)C)[C@]3(C)CC[C@ @]4([H])([C@@]1([H])CC[C@]5([H])([C@]4(C)C[C@H]([N+](=O)C)CCCC6)[C@@H](O(C(=O)C)C5	C17H20N2O2	284.353	Tropicamide
BIOMOL	G-226	C3=C[C@H](C)C[C@@H]1O(C(=O)[C@@H](C)CC [C@]1([H])([C@H](C)[C@@H]([N+](=O)C)CCCC2)[C@@H]3O(C(=O)C)[C@]3(C)CC[C@ @]4([H])([C@@]1([H])CC[C@]5([H])([C@]4(C)C[C@H]([N+](=O)C)CCCC6)[C@@H](O(C(=O)C)C5	C24H36O5	404.54	Lovastatin
BIOMOL	AC-232	c1(nnc(N)nc1N)c2cccc(Cl)c2Cl	C35H60N2O4	572.862	Pancuronium Br
BIOMOL	NA-137	c1(nnc(N)nc1N)c2cccc(Cl)c2Cl [C@@](O)([C@@H]1C(=O)O[C@H]2C[C@H](O[C@@]3(CC[C@H](C)[C@ @]([H])([C@@H](C)CC)O3)C2)ClC=C(Cl)/C)[C@H]4O[C@@H]5O[C@@ H](C)[C@H](O)[C@@H]6O[C@@H](C)[C@H](O)[C@@H](O)C6)[C@@ H](O)C5)\Cl=C(Cl)C[C@@H]4C)CO7[C9H7Cl2N5	256.091	Lamotrigine
BIOMOL	AC-238	c1(ccc(O)cc1)C(O)CNC(C)CCc2ccc(O)cc2	C48H74O14	875.093	Ivermectin
BIOMOL	DL-260	c1(ccc(O)cc1)C(O)CNC(C)CCc2ccc(O)cc2	C18H23NO3	301.38	Ractopamine
BIOMOL	AC-241	[C@]1(C)(CCN2C)[C@@]2([H])N(C)c3c1cc(OC(=O)NC)cc3	C15H21N3O2	275.346	Physostigmine sulfate
BIOMOL	DL-261	c1(cc(S(=O)(=O)N2CCN(C)CC2)ccc1OCC)C(NC(=O)c3c4c(CCC)nn3C)=N4	C22H30N6O4S	474.576	Sildenafil
BIOMOL	DL-554	c1(ccncnc1)C(=O)NCCCC(=O)Nc2ccccc2	C16H18N4O2	298.34	Nialamide
BIOMOL	DL-262	[C@H]1(CC[C@H]([C@@H](c2ccc(Cl)cc2)CC1)C3=C(O)C(=O)c4c(cccc4)C3=O	C22H19ClO3	366.837	Atovaquone
BIOMOL	AC-250	c1(ccc(Cl)cc1)C2(O)CCN(CCCC(=O)c3ccc(F)cc3)CC2	C21H23ClFNO2	375.864	Haloperidol HCl
BIOMOL	DL-208	c(cccc1Cl)(c(COC(Cn2cnc2)c3ccc(Cl)cc3Cl)cs4)c14	C20H15Cl3N2O5	437.77	Sertaconazole
BIOMOL	AC-259	c(OCO1)(cc(CN2CCN(c3nccn3)CC2)cc4)c14 N(C)C([O-])=O=C(C[N+](=O)C)CCCC1CS2)(C(=O)[C@H]3NC(=O)C(=N/OC)\c4nc(N) sc4)[C@H]23	C16H18N4O2	298.34	Piribedil HCl
BIOMOL	DL-191	N(CCN(C)C)(Cc1ccc(OC)cc1)c2ncccc2	C19H24N6O5S2	480.561	Cefepime
BIOMOL	AC-277	N(CCN(C)C)(Cc1ccc(OC)cc1)c2ncccc2	C17H23N3O	285.384	Mepyramine maleate
BIOMOL	DL-178	c(NC(=O)CC1)(cc(OC)CCCN2CCN(c3cccc(Cl)c3Cl)CC2)cc4)c14	C23H27Cl2N3O2	448.385	Aripiprazole
BIOMOL	AC-279	C(=Cl)CN1CCCC1)/(c2ncccc2)\c3ccc(C)cc3	C19H22N2	278.391	Trans-triprolidine HCl
BIOMOL	DL-264	c1(c(C(=O)O)ccc2)c2nc(OC)n1Cc3ccc(c4ccccc4c5nn[nH]5)cc3 [C@@]1([H])([H])(C1C2)=ClC=C(Cl)C[C@@H](O)C[C@@H]3O)/C3=C)[C@@] (C)([C@@H]([C@H](C)CCCC(C)C)O)CC1)CC2	C24H20N6O3	440.454	Candesartan
BIOMOL	DM200	[C@H]1([C@H](C[C@H](O)O[C@H]1O(C)O)O(C)[C@]2(O3)C[C@@]([H])(OC(=O)[C@]([H])(C)=C(C)[C@H]4O)[C@](O)(\ClCO5)=ClC=C(Cl)[C@H](C) [C@H]([C@H](C(=Cl)C6)C)O[C@@H]([O][C@H]7C)C[C@H]([C@@H]7C)OC)[C@@]45[H])C[C@]36[H])=C	C27H44O3	416.636	Calcitriol
BIOMOL	DL-301	[C@]1(Cn2cnc2)(O[C@H](COc3ccc(N4CCN(C(=O)C)CC4)cc3)O1)c5ccc (Cl)cc5Cl	C47H71O14R	860.058	Abamectin
BIOMOL	EI-107	[C@](C)([C@@H]([C@H](C)CCCC(C)C)CC1)(CC2)[C@]1([H])C(Cl)C2=C/C =C(Cl)C[C@@H](O)C[C@@H]3O)/C3=C	C26H28Cl2N4O4	531.431	Ketoconazole
BIOMOL	DL-222	C(c1cccc1)(c2cccc2)N3CCN(CCCN4C(=O)Nc5c4cccc5)CC3	C27H44O2	400.637	Alfacalcidol
BIOMOL	EI-114	C(c1cccc1)(c2cccc2)N3CCN(CCCN4C(=O)Nc5c4cccc5)CC3	C27H30N4O	426.553	Oxatamide

BIOMOL	DL-151	<chem>C1(=CC(=S)SS1)c2ccc(OC)cc2</chem>	<chem>C10H8OS3</chem>	240.365	Anethole-trithione (anetholtrithion)
BIOMOL	EI-121	<chem>c(c(OCC(O)CO)c1cccc2c1C(=O)C=C(C([O-])=O)O2)ccc3(C(=O)C=C(C([O-])=O)O4)c34.[Na+].[Na+]</chem>	<chem>C23H14Na2O11</chem>	512.33	Disodium cromoglycate
BIOMOL	DL-144	<chem>c1(C(C)(C)C#N)cc(Cn2ncnc2)cc(C(C)(C)C#N)c1</chem>	<chem>C17H19N5</chem>	293.366	Anastrozole
BIOMOL	EI-125	<chem>c1(CNC(=O)CCCC(C=O)C(C)C)ccc(O)c(O)C1</chem>	<chem>C18H27NO3</chem>	305.412	Capsaicin
BIOMOL	DL-162	<chem>c1(C(F)(F)F)cc(NC(=O)C(O)(C)CS(=O)(=O)c2ccc(F)cc2)ccc1C#N</chem>	<chem>C18H14F4N2O4S</chem>	430.373	Bicalutamide
BIOMOL	EI-126	<chem>C(C(=O)C=C(C([C@@]12C)CC[C@@]3([H])(C@]1F)[C@@H](O)C[C@@]([C@]34[H])(C)[C@@]([O])(C(CO)=O)[C@H](C)C4)=C2</chem>	<chem>C22H29FO5</chem>	392.461	Dexamethasone
BIOMOL	DL-180	<chem>C(Cl)(Cl)(P(=O)(O)O)P(=O)(O)O</chem>	<chem>CH4Cl2O6P2</chem>	244.892	Clodronate disodium
BIOMOL	EI-127	<chem>c(c(N1CCCCC1)nc(N(CCO)CCO)n2)(nc(N(CCO)CCO)nc3N4CCCCC4)c23</chem>	<chem>C24H40N8O4</chem>	504.626	Dipyridamole
BIOMOL	DL-102	<chem>[C@H]([C@H](C)Cl)(NC(=O)[C@@H]1C[C@@H](CCC)CN1C)[C@@H]2[C@H](O)[C@H](O)[C@H](O)[C@H](SC)O2</chem>	<chem>C18H33ClN2O5S</chem>	424.983	Clindamycin palmitate
BIOMOL	EI-128	<chem>c1(C(=O)C(=C)CC)ccc(OCC(=O)O)c(Cl)c1Cl</chem>	<chem>C13H12Cl2O4</chem>	303.138	Ethacrynic acid
BIOMOL	DL-164	<chem>c1(cc(C)C)c(C(C#N)c2ccc(Cl)cc2)c(Cl)c1)N3N=CC(=O)NC3=O</chem>	<chem>C17H9Cl3N4O2</chem>	407.638	Diclazuril
BIOMOL	EI-131	<chem>c(ccc(O)C)c1(n(C(=O)c2ccc(Cl)cc2)c(C)C3CC(=O)O)c13</chem>	<chem>C19H16ClNO4</chem>	357.788	Indomethacin
BIOMOL	DL-302	<chem>n1([C@H]2CC[C@@H](CO)O2)cnc3c1N=CNC3=O</chem>	<chem>C10H12N4O3</chem>	236.227	Didanosine
BIOMOL	EI-133	<chem>c(cc([C@H](C)C(=O)O)cc1)(ccc(O)C)c12</chem>	<chem>C14H14O3</chem>	230.259	Naproxen
BIOMOL	DL-199	<chem>[C@]([H])([H])(C[C@@]([H])(O)C(=O)c1c[nH]c21cccc2)C3)(C4)N(CC5=O)[C@]3([H])C[C@@]45[H]</chem>	<chem>C19H20N2O3</chem>	324.374	Dolasetron
BIOMOL	AC-280	<chem>c1(CSCC1N=C1\NC)/NC#N)nc[nH]c1C</chem>	<chem>C10H16N6S</chem>	252.339	Cimetidine
BIOMOL	DL-101	<chem>c1(ccccc2c2cccc1CN(C)Cc3ccc(C(C)(C)C)cc3</chem>	<chem>C23H27N</chem>	317.467	Butenafine
BIOMOL	AC-282	<chem>c1(CSCCNC1\NC)=N.C#N)csc(NC(=N)N)n1</chem>	<chem>C10H16N8S2</chem>	312.418	Tiotidine
BIOMOL	DL-200	<chem>c(sc(S(=O)(=O)N)c1)(S(=O)(=O)[C@@H](C)C[C@@H]2NCC)c12</chem>	<chem>C10H16N2O4S3</chem>	324.44	Dorzolamide
BIOMOL	DL-555	<chem>c1c2c(ccc1)c(CS(=O)(=O)N)no2</chem>	<chem>C8H8N2O3S</chem>	212.226	Zonisamide
BIOMOL	DL-212	<chem>[C@]1(OCc(c12)cc(C#N)cc2)(CCCN(C)C)c3ccc(F)cc3</chem>	<chem>C20H21FN2O</chem>	324.392	Escitalopram
BIOMOL	DL-556	<chem>C(O)(Cn1cnc1)(P(=O)(O)O)P(=O)(O)O</chem>	<chem>C5H10N2O7P2</chem>	272.09	Zoledronic acid
BIOMOL	DL-209	<chem>n1(Cc2ccc(C(=O)O)cc2)c(CCCC)nc1C=C(C(=O)O)/Cc3sc3</chem>	<chem>C23H24N2O4S</chem>	424.513	Eprosartan
BIOMOL	AC-322	<chem>[C@](CCN1CC2CC2)([C@@H]3C(=O)CC4)([C@]4O)[C@H]1C5)c(c5ccc6O)c6O3</chem>	<chem>C20H23NO4</chem>	341.401	Naltrexone HCl
BIOMOL	DL-119	<chem>c1(CC([O-])=O)cccc1.[Na+]</chem>	<chem>C8H7NaO2</chem>	158.13	Sodium phenylacetate
BIOMOL	DL-560	<chem>[nH]1c(cc2)c(cc2[C@@H]3NC(=C)OC3)(CCN(C)C)c1.O</chem>	<chem>C17H25N3O2</chem>	303.399	zolmitriptan
BIOMOL	DL-551	<chem>c1(ccc(Cl)C(=O)O)cc1)Cn2cnc2</chem>	<chem>C13H12N2O2</chem>	228.247	Ozagrel
BIOMOL	AC-408	<chem>[C@]1(C)[C@]([H])([H])(C[C@@]2(C)C1)[C@]3(N)C2)C3</chem>	<chem>C12H21N</chem>	179.302	Memantine HCl
BIOMOL	DL-217	<chem>c1(C=C(C#N))C(=O)N(CC)CC)cc(O)c(O)c1n[([O-])=O)c1</chem>	<chem>C14H15N3O5</chem>	305.286	Entacapone
BIOMOL	AC-439	<chem>N1(CCCC1=O)C(=O)c2ccc(OC)cc2</chem>	<chem>C12H13NO3</chem>	219.237	Aniracetam
BIOMOL	AP-302	<chem>[C@@H](c1nc[nH]c1)(O)[C@H]2O[C@@H](CO)[C@@H](O)[C@H](O)[C@@H]2O[C@@H]3O[C@H](CO)[C@@H](O)[C@@H](OC(=O)N)[C@@H]3O)[C@H](C(=O)N)[C@H](C)[C@@H](O)[C@H](C)C(=O)N[C@H]([C@H](O)C)C(=O)NCCc4sc(c5ncc(C(=O)N)CC</chem>	<chem>C55H84N17O21S3</chem>	1415.552	Bleomycin sulfate
BIOMOL	AC-501	<chem>C(F)(F)F)Oc1ccc2c(sc(N)n2)c1</chem>	<chem>C8H5F3N2OS</chem>	234.198	Riluzole HCl
BIOMOL	AR-100	<chem>c(c(OCC(CNC(C)(C)C)OC(=O)c1cccc1)ccc2)(cc(C)[nH]3)c23</chem>	<chem>C23H28N2O3</chem>	380.48	Bopindolol malonate
BIOMOL	AC-508	<chem>c1(C(C)C)cccc(C(C)C)c1O</chem>	<chem>C12H18O</chem>	178.271	Propofol
BIOMOL	AR-102	<chem>c1(c(Cl)cccc1Cl)CC(=O)NC(=N)N.Cl</chem>	<chem>C9H10Cl3N3O</chem>	282.554	Guanfacine HCl
BIOMOL	EI-160	<chem>c1(ccc(Cl)cc1)OC(C)(C)C(=O)OCC</chem>	<chem>C12H15ClO3</chem>	242.699	Clofibrate
BIOMOL	DL-192	<chem>N1(C(=O)[C@H](C)N[C@H](C)O(=O)CCc2ccccc2)CCC[C@H]1C(=O)O</chem>	<chem>C18H24N2O5</chem>	348.394	Enalaprilat
BIOMOL	EI-164	<chem>c1(ccc(CC(C)C)cc1)C(C)C(=O)O</chem>	<chem>C13H18O2</chem>	206.281	Ibuprofen
BIOMOL	DL-108	<chem>c1(c2ccc(F)cc2)c(\C=C[C@@H](O)C[C@@H](O)CC(O)=O)n(C(C)C)c3c1cccc3</chem>	<chem>C24H26FNO4</chem>	411.466	Fluvastatin Na
BIOMOL	EI-165	<chem>c1(CNNC(=O)C(N)CO)ccc(O)c(O)c1O</chem>	<chem>C10H15N3O5</chem>	257.243	Benserazide HCl
BIOMOL	DL-155	<chem>[C@@H]1(C2CCCCC2)C[C@@H](C(=O)O)N(C(=O)CP(=O)(CCCCc3cccc3)OC(C(C)C)OC(=O)CC)C1</chem>	<chem>C30H46NO7P</chem>	563.663	Fosinopril
BIOMOL	EI-166	<chem>c(cccc1)(CN(C(=N)N)CC2)c12</chem>	<chem>C10H13N3</chem>	175.23	Debrisoquin sulfate
BIOMOL	DL-215	<chem>[C@H]1(O[C@H](CO)[C@@H](O)C1(F)F)N2C=CC(N)=NC2=O</chem>	<chem>C9H11F2N3O4</chem>	263.198	Gemcitabine HCl
BIOMOL	EI-167	<chem>C1(N2CCN(C)CC2)Cc3c(ccc3)Sc4c1cc(SC)cc4</chem>	<chem>C8H24N2S2</chem>	356.548	Methiothepin maleate
BIOMOL	DL-243	<chem>[C@]12(O3)[C@]([C@@H]4OC1=O)([C@@]([C@@H](O)C(=O)O5)([C@]35[H])(C@H](C(C)C)C4)C[C@@]6([H])(C@]2([C@H](C)C(=O)O6)</chem>	<chem>C20H24O9</chem>	408.399	Ginkgolide a
BIOMOL	EI-168	<chem>c1(Oc2cccc2)c(S(=O)(=O)N)cc(C(=O)O)cc1NCCCC</chem>	<chem>C17H20N2O5S</chem>	364.416	Bumetanide
BIOMOL	DL-166	<chem>c1(cccc2c2n(C)nc1C(=O)N[C@H]3C[C@]4([H])N(C)[C@@]([H])(CCC4)C3</chem>	<chem>C18H24N4O</chem>	312.409	Granisetron

BIOMOL	EI-180	[C@@H]1O[C@@H]2[C@H](N)[C@@H](O)[C@H](O)[C@@H](CN)O2[C@@H](N)C[C@@H](N)[C@H](O)[C@H]1O[C@@H]3O[C@H](CO)[C@@H](O)[C@@H]4[C@H](N)[C@@H](O)[C@H](O)[C@H](CN)O4[C@H]3	C23H46N6O13	614.644	Neomycin sulfate
BIOMOL	DL-105	C1(=O)O[Pt]OC1.N.N	C2H8N2O3Pt	303.175	Nedaplatin
BIOMOL	EI-206	[C@H]1(OC(=O)C)[C@H](OC(=O)C)[C@@H](COC(=O)C)O[C@@H](S[Au])=P(CC)(CC)CC[C@H]1OC(=O)C	C20H34AuO9PS	678.484	Auranofin
BIOMOL	DL-303	C1(=O)O[Pt]OC1=O.[C@]2([H])(N)CCCC[C@@]2([H])N	C8H14N2O4Pt	397.286	Oxaliplatin
BIOMOL	EI-213	N1(C(=O)[C@H](C)CS)CC[C@H]1C(=O)O	C9H15NO3S	217.285	Captopril
BIOMOL	DL-174	c1(\C=C\C)ccc(OC)cc1	C10H12O	148.202	Anethole, trans-
BIOMOL	EI-216	C(CCCCC#CCCC#CCO)(C(=O)C(C)=C(C)C1=O)=C1C	C21H26O3	326.429	Docenone
BIOMOL	DL-546	[C@@H](C(C)(C)C)(NC(OC)=O)C(=O)NN(Cc1ccc(c2ccccc2)cc1)C[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H](C(C)(C)C)NC(OC)=O	C38H52N6O7	704.855	Atazanavir
BIOMOL	DL-545	c(COC1=O)c(C(C)c(OC)c(C(C)=C(/)CCC(=O)OCCN2CCOCC2)c3O)c13	C23H31NO7	433.495	Mycophenolate mofetil
BIOMOL	DL-363	[C@]1(C(=O)CC)(OC(=O)CC)[C@@H](C)C[C@]2([H])[C@]1(C)C[C@H](O)[C@@]3(F)[C@@]2([H])CCC(=C4)[C@]3(C)C=CC4=O	C25H32ClFO5	466.97	Clobetasol propionate
BIOMOL	DL-544	c1(ccc(c2cc(Cl)ccc2c3ccc(C)nc3)cc1)S(C)(=O)=O	C18H15ClN2O2S	358.842	Etoricoxib
BIOMOL	DL-364	c1(cc(C)c(NC(=O)c2cc(l)cc(l)c2O)cc1C)(C#N)c3ccc(Cl)cc3	C22H14Cl2I2N2O2	663.074	Clozantel
BIOMOL	DL-103	c1(nc(Cl)nc2N)c2ncn1[C@H]3[C@@H](F)[C@H](O)[C@@H](CO)O3	C10H11ClFN5O3	303.677	Clofarabine
BIOMOL	DL-365	[C@]([H])([C@]1(C)C=CC(=O)CC1)CC2([C@@H](O)C[C@@]3(C)[C@@]4([H])CC[C@@H]3C(=O)CO)[C@@]24[H]	C21H30O4	346.461	Corticosterone
BIOMOL	DL-219	[C@@]1([H])(C[C@@H](C(=O)N(CCCN(C)C)C(=O)NCC)CN2CC=C)[C@@]2([H])Cc3c(c4[nH]c3)c1ccc4	C26H37N5O2	451.604	Cabergoline
BIOMOL	DL-366	c1(ccccc1C)N(CC)C(=O)C=C1C	C13H17NO	203.28	Crotamiton
BIOMOL	DL-207	c1(C(=O)OCCCN2CCCN(CCCOC(=O)c3cc(OC)c(OC)c(OC)c3)CC2)cc(OC)c(OC)c(OC)c1	C31H44N2O10	604.688	Dilazep
BIOMOL	DL-367	P1(=O)(OCCCN1)N(CCC)CCCl	C7H15Cl2N2O2P	261.086	Cyclophosphamide monohydrate
BIOMOL	DL-213	C(O)(P(=O)(O)O)(P(=O)(O)O)CCN(C)CCCC	C9H23NO7P2	319.229	Ibandronate
BIOMOL	DL-368	C1=C2[C@](C)([C@@H]3[C@@H](C3)C2=O)[C@]4([H])[C@]([H])([C@]([C@]5(C)CC4)([H])CC[C@@]5(C)C(=O)OC(=O)C=C1)C1	C24H29ClO4	416.938	Cyproterone acetate
BIOMOL	DL-202	N(C(C(=O)O)=C(SCCN=C)C1)(C(=O)[C@]2([H])[C@]([H])(O)C)[C@]12[H]	C12H17N3O4S	299.346	Imipenem
BIOMOL	DL-369	[C@H](O[C@H](CO)[C@H]1O)(N2C(=NC(=N)C=C2)O3)[C@H]13	C9H11N3O4	225.201	Cyclocytidine HCl
BIOMOL	DL-156	C1(CCCCC1)NC(=O)N(N=O)CCCl	C9H16ClN3O2	233.695	Lomustine
BIOMOL	DL-370	[C@@H]1([C@@H](O)[C@H](O)[C@@H](CO)O1)N2C=CC(N)=NC2=O	C9H13N3O5	243.217	Cytarabine
BIOMOL	DL-543	[C@]1([H])([C@]2([H])C[C@@H](O)[C@@H]1C=C[C@@H](O)C)CC#C(C)C(C(=O)C)CC(C(=O)O)C2	C22H32O4	360.487	Iloprost
BIOMOL	DL-371	c1(N=NN(C)C)[nH]cnc1C(=O)N	C6H10N6O	182.183	Dacarbazine
BIOMOL	DL-244	C(c1ccc(F)cc1)(c2ccc(F)cc2)N3CCN(Cc4ccc(OC)c(OC)c4OC)CC3	C27H30F2N2O3	468.536	Lomerizine HCl
BIOMOL	DL--372	[C@]([H])([C@]1(C)C=Cc(c2C1)onc2)CC3(CC[C@@]4(C)[C@@]5([H])C[C@@]4(O)C#C)[C@@]35[H]	C22H27NO2	337.455	Danazol
BIOMOL	DL-439	c(cc(C(=O)c1ccccc1)cc2)(nc(NC(=O)OC)[nH]3)c23	C16H13N3O3	295.293	Mebendazol
BIOMOL	DL-514	[C@@]([H])([C@@H](N(C)C)C(=O)C(C(=O)N)C1=O)[C[C@@]([H])(C2=C3O)[C@@]([O])(C)c(c4C2=O)cccc4O)[C@@]13O	C22H24N2O8	444.435	Tetracycline
BIOMOL	DL-440	c1(C(=O)N)cccc1	C6H6N2O	122.125	Medroxyprogesterone 17-acetate
BIOMOL	DL-169	c(nc(OC)cc1)(nc(S(=O)Cc2ncc(C)c(OC)c2C)[nH]3)c13	C16H18N4O3S	346.404	Tenatoprazole
BIOMOL	DL-441	c1(Nc2cccc(C)c2C)cccc1C(=O)O	C15H15NO2	241.285	Mefenamic acid
BIOMOL	DL-190	c(c(C(=O)N)nc1)(N=NN(C)C2=O)n12	C6H6N6O2	194.151	Temozolomide
BIOMOL	DL-442	c1(ccc(C[C@H](N)C(=O)O)cc1)N(CCC)CCCl	C13H18Cl2N2O2	305.2	Melphalan
BIOMOL	DL-206	[C@]1([H])([C@H](C)CC2=C3CCC(=O)C2)[C@]3([H])CC[C@@]4(C)[C@@]1([H])CC[C@@]4(O)C#C	C21H28O2	312.446	Tibolone
BIOMOL	DL-443	[C@@](N)(C)(Cc1ccc(O)c(O)c1)C(=O)O	C10H13NO4	211.215	Methyldopa
BIOMOL	DL-515	C(OC1ccsc1Cl)(Cn2cnc2)c3ccc(Cl)cc3Cl	C16H13Cl3N2OS	387.711	Tioconazole
BIOMOL	DL-444	[C@]1([H])(C[C@H](C)CC2=C3CCC(=O)C2)[C@]3([H])CC[C@@]4(C)[C@@]1([H])CC[C@@]4(O)C#C	C22H30O5	374.471	Methylprednisolone
BIOMOL	DL-516	S(=O)(=O)(CC)CCn1c(C)nc1[N+][O-]=O	C8H13N3O4S	247.272	Tinidazole
BIOMOL	DL-445	c1(OCC(O)CNC(C)C)ccc(COC)cc1	C15H25NO3	267.364	Metoprolol tartrate
BIOMOL	DL-517	[C@H]1O[C@@H]2[C@H](O)[C@@H](N)[C@H](O)[C@@H](CO)O2[C@@H](N)C[C@H](N)[C@@H](O)[C@@H]3[C@H](N)C[C@H](O)[C@@H](CN)O3[C@H]1O	C18H37N5O9	467.514	Tobramycin (free base)
BIOMOL	DL-446	C1(=S)NC=CN1C	C4H6N2S	114.169	Methimazole

BIOMOL	DL-188	c1(nc(N2CCC(N)C2)c(F)c3C(=O)C(C(=O)O)=CN1c4ccc(F)cc4F	C19H15F3N4O3	404.343	Tosufloxacin
BIOMOL	DL-447	n1(CCO)c(C)ncc1[N+][([O-])=O C([C@@](O)(CC)C(=O)O)C1)(C=C(N2C3=O)c4c(cc(c5n4)c(CN(C)C)c(O)cc5)C2)=C13	C6H9N3O3	171.154	Metronidazole
BIOMOL	DL-518		C23H23N3O5	421.446	Topotecan
BIOMOL	DL-448	c1(ccc(Cl)cc1Cl)C(OCc2ccc(Cl)cc2Cl)Cn3cncc3	C18H14Cl4N2O	416.129	Miconazole
BIOMOL	DL-519	C/(c1cccc1)\(c2ccc(OC CN(C)C)cc2)=C(/CCCl)\c3ccccc3	C26H28ClNO	405.96	Toremifene
BIOMOL	DL-138	c1(c(Cl)cccc1Cl)OC(C)C2=NCCN2	C11H12Cl2N2O	259.132	Lofexidine
BIOMOL	DL-373	[C@@]([H])([C@@]1([H])[C@@](C)(C(=O)CC1)CC2)(CC=C3[C@]4(C)COC[C@H](O)C3)[C@]24[H] N(C(C(=O)O)=C[S](C@H)1CN[C@H](C(=O)N(C)C)C1)[C@@H]2C)(C(=O)[C@]3([H])[C@H](O)C)[C@]23[H]	C19H28O2	288.424	Dehydroepiandrosterone
BIOMOL	DL-167	C(=C\C(CNCN1)/C1)/c2c(cccn2)CC3)c(ccc(Cl)c4)c34	C17H25N3O5S	383.463	Meropenem
BIOMOL	DL-154		C19H19ClN2	310.821	Desloratadine
BIOMOL	DL-205	C1(NCCN(CCO)CCCc2ccc([N+][([O-])=O)cc2)=CC(=O)N(C)C(=O)N1C	C19H27N5O5	405.448	Nifekalant HCl
BIOMOL	DL-374	[C@]1(CCN2C)(CCCC3)[C@]23([H])[C@H]2Cc4c1cc(O)C)cc4 c1(C[C@H]2C(=O)N[C@H](CCCN)C(=O)N[C@H]([C@H](O)C)C(=O)N[C@H](C(=O)N[C@H](CO)[C@H](O)C)CSSC[C@H](NC(=O)[C@H](N)Cc3ccccc3)C(=O)N[C@H]([Co4ccccc4])C(=O)N2)c[nH]c5c1cccc5	C18H25NO	271.397	Dextromethorphan HBr
BIOMOL	DL-309		C49H66N10O10S2	1019.239	Octreotide
BIOMOL	DL-375	c1(Nc2c(Cl)cccc2Cl)ccccc1CC(O)=O	C14H11Cl2NO2	296.149	Diclofenac, Na
BIOMOL	DL-194	[C@@H]1(O(C(C)CC)C)C=C(C(=O)OCC)C[C@H](N)[C@H]1NC(=O)C	C16H28N2O4	312.405	Osetamivir
BIOMOL	DL-376	[C@@H]1(CC[C@@H](CO)O1)N2C=CC(N)=NC2=O	C9H13N3O3	211.218	2',3'- dideoxycytidine
BIOMOL	DL-196	C(O)(CCN)(P(=O)(O)O)P(=O)(O)O	C3H11NO7P2	235.069	Pamidronic acid
BIOMOL	DL-377	C/(CC)\(c1ccc(O)cc1)=C(C(C)/c2ccc(O)cc2	C18H20O2	268.35	Diethylstilbestrol
BIOMOL	DL-197	c(nc(N)s1)(CC[C@H](NCCC)C2)c12	C10H17N3S	211.327	Pramipexole
BIOMOL	DL-378	c1(ccc(F)cc1F)c2ccc(O)c(C(=O)O)c2 c1(cccc2c2[nH]cc1C[C@H](C(=O)N[C@H](CC(C)C)C(=O)N[C@H](CCCN(C=N)N)C(=O)N3CCC[C@H]3C(=O)NCC(=O)N)NC(=O)[C@@H](NC(=O)[C@H](CO)NC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@H]4CCCC(=O)N4)Cc5nc[nH]c5)Cc6c[nH]c7c6	C13H8F2O3	250.198	Diflunisal
BIOMOL	DL-310		C64H82N18O13	1311.449	Triptorelin
BIOMOL	DL-379	N(CC)(CC)C(=S)SSC(=S)N(CC)CC c(c1o2)(C(=O)[C@@]2(C)O\C=C[C@H](O(C)[C@H](C)[C@H](C(=O)O)C)[C@H](C)[C@@H](O)[C@H](C)[C@H](O)[C@H](O)C=C\C(C(=O)C(=O)N3)c(c([O-])cc3c4O)c4C(O)c1C	C10H20N2S4	296.539	Disulfiram
BIOMOL	NP-526		C37H46NO12	696.761	Rifamycin sv
BIOMOL	DL-204	c(nc(N1CCN(C(=O)C2COc3c(cccc3)O2)CC1)nc4N)(cc(OC)c(O)C)c5)c45	C23H25N5O5	451.475	Doxazosin mesylate
BIOMOL	DL-198	C(O)(P(=O)(O)O)(P(=O)(O)O)Cc1cnccc1	C7H11NO7P2	283.112	Risedronic acid
BIOMOL	DL-380	[C@H]1(O[C@H](C)[C@@H](O)[C@H]1O)N2C=C(F)C(=O)NC2=O [C@]([H])([H])([C@H](N(C)C)C(O)=C(C(=O)N)C1=O)(C[C@@]([H])([H])(C2=C3O)Cc(c4C2=O)c(N(C)C)ccc4O)[C@@]13O	C9H11FN2O5	246.192	Doxifluridine
BIOMOL	DL-449		C23H27N3O7	457.476	Minocycline HCl
BIOMOL	DL-520	c1(Nc2cccc(Cl)c2C)ccccc1C(=O)O	C14H12ClNO2	261.704	Tofenamic acid
BIOMOL	DL-450	c(C(=O)c(c1C2=O)c(O)ccc1O)(c(NCCNCCO)ccc3NCCNCCO)c23	C22H28N4O6	444.481	Mitoxantrone 2HCl
BIOMOL	DL-521	c1(ccc(CC(O)=O)n1C)C(=O)c2ccc(C)cc2 [C@@]1([C@H](OC(=O)c2ccccc2)[C@@]3(O)C(C)C)C(=C(C)[C@@H](OC(=O)[C@H](O)[C@@H](NC(=O)c4ccccc4)c5ccccc5)C3)[C@H](OC(=O)C)c6=O)[C@@]6(C)[C@@H](O)[C@H](O)[C@H]([C@@]([C@]17O)C(C)=O)([H])O	C15H15NO3	257.285	Tolmetin Na
BIOMOL	T-104		C47H51NO14	853.906	Taxol
BIOMOL	DL-522	N1(C(=O)N)(C(=O)N)(C)C1=O)c2ccc(OC3ccc(SC(F)(F)F)cc3)c(C)c2	C18H14F3N3O4S	425.382	Toltrazuril
BIOMOL	DL-452	C(C#N)(CCCC)(Cn1ncnc1)c2ccc(Cl)cc2	C15H17ClN4	288.775	Myclobutanil
BIOMOL	DL-523	[C@]1(O)(CCCC[C@H]1CN(C)C)c2cccc(OC)c2	C16H25NO2	263.375	Tramadol HCl
BIOMOL	DL-453	c(N1C=C(C(=O)O)C2=O)(c2cc(F)c3N4CCCC(O)CC4)c3CCC1C [C@](F)([C@]1(C)C(=CC(=O)C=C1)CC2)([C@H](O)C[C@@]3(C)[C@@]4([H])C[C@H](O)[C@]3(O)C(=O)CO)[C@@]24[H]	C19H21FN2O4	360.379	Nadifloxacin
BIOMOL	DL-524		C21H27FO6	394.434	Triamcinolone
BIOMOL	DL-454	c(cc(CCC(=O)C)cc1)(ccc(OC)c2)c12	C15H16O2	228.286	Nabumetone
BIOMOL	DL-525	c1(cc(OC)c(O)C)c(OC)c1Cc2cnc(N)nc2N	C14H18N4O3	290.318	Trimethoprim
BIOMOL	DL-455	c1(cccc2)c2cccc1CC3=NCCN3	C14H14N2	210.274	Naphazoline HCl
BIOMOL	DL-158	3	C17H20N2O2	284.353	Tropisetron HCl
BIOMOL	DL-456	N1(CCOc2ccccc2)C(=O)N(CCCN3CCN(c4cccc(Cl)c4)CC3)N=C1CC [C@@H]1(O[C@H]2O[C@@H](C)[C@H](O)[C@@](O)(C)C2)[C@@H](C)O[C@@H](O[C@@H]3[C@H](C)[C@H](O)CC(=O)O)[C@@H](CC)[C@H](CO)[C@H]4O[C@@H](C)[C@H](O)[C@H](OC)[C@@H]4OC)C=C(\C)/C=C/C(=O)[C@@H](C)[C@H]3C(=O)[C@]	C25H32ClN5O2	470.007	Nefazodone
BIOMOL	DL-526		C45H75NO17	902.074	Tylosin tartrate
BIOMOL	DL-457	c1(Nc2cccc(C(F)(F)F)c2)ncccc1C(=O)O	C13H9F3N2O2	282.218	Niflumic acid
BIOMOL	DL-527	c(N=C(N)NC1=O)(n(COCCOC(=O)[C@H](N(C)C)C)cn2)c12	C13H20N6O4	324.336	Valaciclovir

BIOMOL	DL-458	[C@]([H])([C@@]1([H])[C@]2([H])([C@]2([H])C(=CC(=O)CC2)CC1)CC3)(CC[C@]4(O)C#C)[C@]34C	C20H26O2	298.419	Norethindrone
BIOMOL	DL-528	[C@](C)([C@@H](O)C(=O)C)[C@@H]([N+](C)CCCC1)C2)(CC[C@]3([H])[C@@]4([H])CC[C@]5([H])[C@]3(C)C[C@H](N6CCCC6)[C@@H](O)C(=O)C)C5)[C@@]24[H]	C34H57N2O4	557.827	Vecuronium Br
BIOMOL	DL-187	C1CCC[N+](C(=C=C)[C@H]2C[C@]([H])([C@@]3(C)[C@H]2O)C(=O)C)[C@@]4([H])[C@@]([H])([C@]5(C)[C@]([H])(C[C@H](O)[C@@H](N6CCOC6)C5)CC4)CC3	C32H53N2O4	529.774	Rocuronium bromide
BIOMOL	DL-181	c(n(CC1OCCO1)cnc2)(C(=O)N(C)C(=O)N3C)c23	C11H14N4O4	266.253	Doxofylline
BIOMOL	DL-148	c(cc(S(=O)CCC)cc1)(nc(NC(=O)O)C)[nH]2)c12	C12H15N3O3S	281.331	Ricobendazole
BIOMOL	DL-381	[C@]([H])([C@H](N(C)C)C(O)=C(C(=O)N)C1=O)[[C@@H](O)[C@@]([H])(C2=C3O)[C@@H](C)c(c4C2=O)cccc4O)[C@@]13O	C22H24N2O8	444.435	Doxycycline HCl
BIOMOL	DL-176	C1[C@]2([H])N([C@@H](C(O)=O)C(C)(C)S2(=O)=O)C1=O	C8H11NO5S	233.242	Sulbactam
BIOMOL	PI-152	N1(C(=O)[C@H](C)N[C@H](C(=O)O)CC)CCc2cccc2)CCC[C@H]1C(=O)O	C20H28N2O5	376.447	Enalapril
BIOMOL	DL-143	O	C14H18Cl2N2O6S	413.274	Thiamphenicol glycinate
BIOMOL	DL-383	c(nc(N1CCNCC1)c(F)c2)(N(CC)C=C(C(=O)O)C3=O)c23	C15H17FN4O3	320.319	Enoxacin
BIOMOL	DL-175	c1(ccccc1Cl)C(O)CNC(C)(C)C	C12H18ClNO	227.73	Tulobuterol
BIOMOL	DL-384	c1(cc(N2CCN(CC)CC2)c(F)c3)c3C(=O)C(C(=O)O)=CN1C4CC4	C19H22FN3O3	359.395	Enrofloxacin
BIOMOL	NP-461	[C@]([CC1])([C@@H]2[C@]([O])(C(=O)O)C[C@H]3O)C(=O)C)(c4c(cc(O)C)c([C@]5(C)O)C(=O)C[C@]([H])(CN6Cc7c5[nH]c(c78)cccc8)C=C(C)CC6)c4)N2C)[C@@]1(N1CC=C9)[[C@]39CC)[H]	C45H54N4O8	778.932	Vinorelbine
BIOMOL	DL-385	[C@]1([H])(CC[C@]2(O)C#C)[C@]2(C)CC[C@]3([H])[C@@]1([H])CC(C(=C)[C@]3(C)CCC4=O	C21H28O2	312.446	Ethisterone
BIOMOL	DL-220	[C@]([CC1)(c2c(cc(O)C)[[C@@]3(C(=O)O)C(C)[C@]4([H])CN(C[C@]([O])(C)C4)CCc5c3[nH]c(c56)cccc6)c2)N7C)([C@]7([H])[C@@]([O])(C(=O)N)[C@@H]8O)[C@@]([H])(N1CC=C9)[C@]89CC	C43H55N5O7	753.926	Vindesine
BIOMOL	DL-386	c(cc(O)cc1)(nc(S(=O)Cc2ncc(C)C(O)C)c2C)[nH]3)c13	C17H19N3O3S	345.416	Esomeprazole potassium
BIOMOL	DL-210	c1(C(O)CNCCCCCO)CCCC2cccc2)ccc(O)c(CO)c1	C25H37NO4	415.566	Salmeterol
BIOMOL	BL-093	[C@]1([H])(CC[C@H]2O)[C@]2(C)CC[C@]3([H])[C@@]1([H])CCc4c3ccc(O)c4	C18H24O2	272.382	Estradiol
BIOMOL	T-117	c1([nH]c(c23)cccc2)c3CCN(C[C@]([CC](O)C4)[C@]4(C)[C@]1(C(=O)O)C)c5c(O)c6cc([C@@]7([C@@]8([H])N6C=O)[C@]([N9CC7]([H])[C@]([C=CC9)CC)[C@@H](O)C(C)=O)[C@]8(O)C(O)C(=O)c5)[H]	C46H56N4O10	824.958	Vincristine sulfate
BIOMOL	DL-388	[C@]1([H])(C[C@H](O)[C@@H]2O)[C@]2(C)CC[C@]3([H])[C@@]1([H])CCc4c3ccc(O)c4	C18H24O3	288.381	Estriol
BIOMOL	DL-312	c(ccc(O)C)c1)(n(C(=O)c2ccc(Cl)cc2)c(C)c3CC(=O)O)CC(=O)O)c13	C21H18ClNO6	415.824	Acemetacin
BIOMOL	BL-090	[C@]1([H])(CCC2=O)[C@]2(C)CC[C@]3([H])[C@@]1([H])CCc4c3ccc(O)c4	C18H22O2	270.366	Estrone
BIOMOL	DL-459	c(cc(N1CCNCC1)c(F)c2)(N(CC)C=C(C(=O)O)C3=O)c23	C16H18FN3O3	319.331	Norfloracin
BIOMOL	DL-529	C1(O)(CCCCC1)C(CN(C)C)c2ccc(O)cc2	C17H27NO2	277.402	Venlafaxine HCl
BIOMOL	DL-460	[C@H]1(O)[C@H](C)[C@@H](O)[C@H](N)[C@@H]1O)O)C2)C=C)C1C=C)			

BIOMOL	NO-102	[C@](CCN1CC=C)([C@H]2[C@H](N1C=CC3)[C@H](O4)[C@H](CCN5CC=C)([C@]3O)[C@H]5C6)c(c4c(O)cc7)c67)CC8)[C@]8(O)[C@H]1C9)c(c9ccc%10O)c%10O2	C38H42N4O6	650.763	Naloxonazine 2HCl
BIOMOL	DL-313	c1(C(=O)O)cccc1OC(=O)C	C9H8O4	180.157	Acetylsalicylic acid
BIOMOL	DL-390	C(O)(C)P([O-])(=O)OP([O-])(=O)O	C2H6O7P2	204.012	Etidronate 2Na
BIOMOL	DL-314	c1(C(=O)O)nc(c(C)[n+])([O-])c1	C6H6N2O3	154.123	Acipimox
BIOMOL	DL-170	c1(\C=C1C1C(=C1C=C1C1C(=C1C(=O)OCC)c(C)cc(OC)c(C)c1C	C23H30O3	354.482	Etretinate
BIOMOL	DL-315	c1(Nc2c(C1)cccc2Cl)cccc1CC(=O)OCC(=O)O	C16H13Cl2NO4	354.185	Aceclofenac
BIOMOL	DL-563	c(cc(S(=O)(=O)N)c(C)C1)(S(=O)(=O)NC(C1Cl)Cl)N2)c12	C8H8Cl3N3O4S2	380.656	Trichloromethiazide
BIOMOL	DL-316	c(N=C(N)NC1=O)(n(COCCO)cn2)c12	C8H11N5O3	225.205	Acycloguanosine
BIOMOL	DL-392	c1(nc(N)nc2)c2nen1CCC(COC(=O)C)COC(=O)C	C14H19N5O4	321.332	Famciclovir
BIOMOL	DL-317	[C@H]1(O[C@H](CO)[C@@H](N=[N+]=[N-])C1N2C=C(C)C(=O)NC2=O	C10H13N5O4	267.241	3'-azido-3'-deoxythymidine
BIOMOL	DL-393	c(cc(Sc1ccccc1)cc2)(nc(NC(=O)O)C)[nH]3)c23	C15H13N3O2S	299.348	Fenbendazole
BIOMOL	DL-318	n1c(O)c2c(N=NC2)nc1	C5H4N4O	136.111	Allopurinol
BIOMOL	DL-394	c1(ccc(C(=O)CCC(=O)O)cc1)c2ccccc2	C16H14O3	254.281	Fenbufen
BIOMOL	PR-123	C(O)(CCCN)(P([O-])(=O)OP(=O)(O)O	C4H12NO7P2	248.088	Alendronate
BIOMOL	DL-395	c12c(C(c3ccc(O)cc3)CNCC1)cc(O)c(O)c2Cl	C16H16ClNO3	305.756	Fenoldopam mesylate
BIOMOL	DL-320	c1(N(C)C)nc(N(C)C)nc(N(C)C)n1	C9H18N6	210.279	Altretamine
BIOMOL	DL-396	c1(Oc2ccccc2)cccc(C(C)C(=O)O)c1	C15H14O3	242.27	Fenoprofen
BIOMOL	DL321	c(ccc(SCCC)c1)([nH]c(NC(=O)O)C)n2)c12	C12H15N3O2S	265.331	Albendazole
BIOMOL	DL-397	c1(ccc(OC(C)(C)C(=O)O)C(C)cc1)C(=O)c2ccc(Cl)cc2	C20H21ClO4	360.831	Fenofibrate
BIOMOL	DL-565	C(C(=O)O)CC(=O)O . c(cc(CS(=O)(=O)NC)cc1)(c(CCN(C)C)c[nH]2)c12	C18H27N3O6S	413.488	Sumatriptan Succinate
BIOMOL	DL-398	[C@]1([H])(CC[C@H]2C(=O)NC(C)(C)C)[C@]2(C)CC[C@H]3([H])[C@	C23H36N2O2	372.544	Finasteride
BIOMOL	DL-468	c(ccc(OC(F)F)c1)([nH]c(S(=O)Cc2nccc(OC)c2OC)n3)c13	C16H15F2N3O4S	383.37	Pantoprazole
BIOMOL	AC-1053	c1(ccnc2C)c2[nH]c3c1ccc(OC)c3	C13H12N2O	212.247	Harmine
BIOMOL	NS-710	[C@H]1(c2ccc(F)cc2)CCN[C@H]1COc3ccc4c(OCO4)c3	C19H20FNO3	329.365	Paroxetine HCl
BIOMOL	NS-102	c1(SCCCN(C)C)cccc1NC(=O)C=C1c2ccccc2	C20H24N2OS	340.482	Cinanserin
BIOMOL	DL-470	c(N1C=C(C(=O)O)C2=O)(c2cc(F)c3C4(N)CC4)c3O[C@H]1C	C16H15FN2O4	318.3	Pazufloxacin
BIOMOL	NS-107	c(cccc1)(N(CCN(C)C)C(=O)c(c2N3C)ccccc2)c13	C18H21N3O	295.379	Dibenzepine HCl
BIOMOL	DL-471	C(N(C)C)c1c(c(F)c(N2CCN(C)CC2)c1)C3=O=C3C(=O)O	C17H20FN3O3	333.357	Pefloxacin mesylate
BIOMOL	NS-108	[C@](O)(O[C@@H](C(C)C)NC(=O)[C@H]1CN(C)[C@@H]([H])([H])C1)Cc3c(c4[nH]c3)c2ccc4)C5=O)([C@@H]6([H])N(CCC6)C(=O)[C@H]7Cc8cccc8)N57	C35H41N5O5	611.731	Dihydroergocristine mesylate
BIOMOL	DL-472	c(N=C(N)NC1=O)(n(CCC(CO)CO)cn2)c12	C10H15N5O3	253.258	Penciclovir
BIOMOL	NS-109	C1(N2CCN(C)CC2)=Nc3c(ccc(F)c3)Cc4c1cccc4	C19H20FN3	309.381	Fluperlapine
BIOMOL	DL-473	c(n(C)cn1)(C(=O)N(CCCCC(=O)C)C(=O)N2C)c12	C13H18N4O3	278.307	Pentoxifylline
BIOMOL	NS-140	C(CNC)(O)c1ccc(C(F)(F)F)cc1c2ccccc2	C17H18F3NO	309.326	Fluoxetine HCl
BIOMOL	DL-474	N([C@@H](C([O-]))=O)(C(C)(C)S1)(C(=O)[C@H]2NC(=O)COc3ccccc3)[C@H]12	C16H17N2O5S	349.382	Pencillin v potassium
BIOMOL	NS-145	c1(C(=O)C)(Cn2ccnc2)CC3)c3n(C)c4c1cccc4	C18H19N3O	293.363	Ondansetron
BIOMOL	DL-475	N1(c2ccccc2)C(=O)C(CCCC)C(=O)N1c3ccccc3	C19H20N2O2	308.374	Phenylbutazone
BIOMOL	NS-515	c(cccc1)(NC(=O)N(CCN2CCC(C(=O)c3ccc(F)cc3)CC2)C4=O)c14	C22H22FN3O3	395.427	Ketanserin tartrate
BIOMOL	DL-476	[C@H]([C@H](NC(=O)[C@H](NC(=O)N1CCN(CC)C(=O)C1=O)c2ccccc2)C3=O)(SC(C)(C)[C@@H]4C(O)=O)N34	C23H27N5O7S	517.555	Piperacillin
BIOMOL	DL-562	C(O)(C(=O)O[C@H]1C[C@@H]([H])([N+](C)(C)[C@@H]2([H])C1)[C@H]([C@H]23)O3)(c4scccc4)c5ccccc5.[Br-]	C19H22BrNO4S2	472.416	Tiotropium Br
BIOMOL	DL-477	[C@]12([H])(C=C[C@H](O)[C@@H]1CC[C@@H]3[C@@H]([O])CC(=O)O3)[C@@H](O)C[C@H](O)C[C@H]2O[C@@H](C)C(=O)O	C23H34O6	406.512	Pravastatin lactone
BIOMOL	NS-531	c1(cc(S(=O)(=O)C)cc2)c2Sc3c(cccc3)N1CCC4CCCCN4C	C21H26N2OS2	386.574	Mesoridazine besylate
BIOMOL	GR-341	S(P(=O)(O)O)CCNCCCN	C5H15N2O3PS	214.223	Amifostine
BIOMOL	DL-399	C1(=O)NC(=O)NC=C1F	C4H3FN2O2	130.077	5-fluorouracil
BIOMOL	DL-324	C1(CC)(CCC(=O)NC1=O)c2ccc(N)cc2	C13H16N2O2	232.278	DL-aminoglutethimide
BIOMOL	DL-400	c1(ccc(C(C)C(=O)O)cc1F)c2ccccc2	C15H13FO2	244.261	Flurbiprofen
BIOMOL	DL-325	c1(C(=O)O)cccc(N)cc1O	C7H7NO3	153.135	4-aminosalicylic acid
BIOMOL	DL-401	c(c(F)c(N1CCN(C)CC1)c(F)c2)(N(CCF)C=C(C(=O)O)C3=O)c23	C17H18F3N3O3	369.338	Fleroxacin
BIOMOL	DL-326	c1(C(=O)O)cc(N)ccc1O	C7H7NO3	153.135	5-aminosalicylic acid
BIOMOL	DL-402	c1(ccc([C@@H](O)[C@H](CF)NC(=O)C)Cl)cc1S(C(=O)=O	C12H14Cl2FNO4S	358.213	Florfenicol

BIOMOL	DL-327	<chem>N[C@@H](C(=O)O)C(C)(C)S1(C=O)[C@H]2NC(=O)[C@H](N)c3ccccc3</chem>	C16H19N3O4S	349.405	Ampicillin trihydrate
BIOMOL	DL-403	<chem>[C@H]1(C[C@H](O)[C@@H](CO)O1)N2C=C(F)C(=O)NC2=O</chem>	C9H11FN2O5	246.192	Floxuridine
BIOMOL	DL-328	<chem>C1(O C(C)O C(=O)O CC)=C(C(=O)Nc2ncccc2)N(C)S(=O)(=O)c3c1cccc3</chem>	C20H21N3O7S	447.462	Ampiroxicam
BIOMOL	DL-404	<chem>[C@]1(C(=O)CO)(O C(C)(C)O2)[C@H]2C[C@]3([H])[C@]1(C)C[C@H](O)[C@@]4(F)[C@@]3([H])C[C@H](F)C(=C5)[C@]4(C)C=CC5=O</chem>	C24H30F2O6	452.488	Fluocinolone acetone
BIOMOL	DL-329	<chem>[C@H]([H])(C[C@H](N)[C@H](O)[C@H]1[C@@H](N)C[C@H](N)[C@H](O)[C@H]1O)O2)O[C@H](O[C@H]3[C@H](O)[C@H](O)[C@H](N)[C@H](CO)O3)[C@H](NC)[C@H]4O)[C@]24[H]</chem>	C21H41N5O11	539.577	Apramycin
BIOMOL	DL-405	<chem>c(cc(C(=O)c1ccc(F)cc1)cc2)(nc(NC(=O)OC)[nH]3)c23</chem>	C16H12FN3O3	313.283	Flubendazole
BIOMOL	NP-016	<chem>[C@H]1([C@]1([H])CC[C@H]2C([C@@]2([H])CC3)O[C@]3(C)O4)[C@]4([H])O C(=O)[C@H]1C</chem>	C15H22O5	282.332	Artemisinin
BIOMOL	DL-406	<chem>c1(C(F)(F)F)cc(NC(=O)C(C)C)ccc1[N+](=[O-])=O</chem>	C11H11F3N2O3	276.212	Flutamide
BIOMOL	AC-166	<chem>c1(OCC(O)CNC(C)C)ccc(C(C(=O)N)cc1</chem>	C14H22N2O3	266.336	Atenolol
BIOMOL	DL-407	<chem>c1(ccc(F)cc1F)C(O)(Cn2nccn2)Cn3nccn3</chem>	C13H12F2N6O	306.271	Fluconazole
BIOMOL	DL-332	<chem>c1(cc(OC)c(O)C)c2CC[N+](C)(CCC(=O)O)CCCCCO C(=O)CC[N+](3(C)CC4c(cc(O)C)c(O)C)c4)C3Cc5ccc(O)C)c(O)c5)C1Cc6ccc(O)C)c(O)c6</chem>	C53H72N2O12	929.145	Atracurium besylate
BIOMOL	DL-408	<chem>[C@]([H])([C@]1(C)C=C(O)C(=O)CC1)CC2(C)[C@]3(C)[C@]4([H])CCC3=O)[C@@]24[H]</chem>	C19H26O3	302.408	Formestane
BIOMOL	DL-478	<chem>c(cc(C(C)C(=O)O)cc1)(Cc(c2O3)cccn2)c13</chem>	C15H13NO3	255.269	Pranoprofen
BIOMOL	NS-835	<chem>N1(CCC2CCCCN2C)c3c(cccc3)Sc4c1cc(SC)cc4</chem>	C21H26N2S2	370.575	Thioridazine HCl
BIOMOL	DL-479	<chem>[C@@]1([C@]2(C)C[C@H](O)[C@]3([H])[C@]1(CCC(=C4)[C@]3(C)C=CC4=O)[H])(CC[C@]2(C)CO)=O)[H]</chem>	C21H28O5	360.444	Prednisolone
BIOMOL	PD-125	<chem>c(C=CC(=O)N1)(cc(OCCCC(=O)N(C)C2CCCCC2)cc3)c13</chem>	C20H26N2O3	342.432	Cilostamide
BIOMOL	DL-480	<chem>[C@]([H])([C@]1(C)C=CC(=O)CC1)CC2(C)[C@]3(C)[C@]4([H])CC[C@@H]3C(=O)C)[C@@]24[H]</chem>	C21H30O2	314.462	Progesterone
BIOMOL	PD-130	<chem>c1(cnn2CC)c2ncc(C(=O)OCC)c1Nn=C(C)/C)C</chem>	C14H19N5O2	289.333	Etazolate
BIOMOL	DL-481	<chem>c1(ccc(CNNC)cc1)C(=O)NC(C)C</chem>	C12H19N3O	221.299	Procarbazine HCl
BIOMOL	PD-140	<chem>c1(nc[nH]2)c2C(=O)N(C)C(=O)N1CC(C)C</chem>	C10H14N4O2	222.244	Isobutylmethylxanthine
BIOMOL	DL-482	<chem>c1(CCC)nc(C(=S)N)c1</chem>	C9H12N2S	180.27	Prothionamide
BIOMOL	PD-141	<chem>c1(nc(N)nc(N)n1)c2cc(Cl)ccc2Cl</chem>	C9H7Cl2N5	256.091	Irsogladine maleate
BIOMOL	DL-483	<chem>[C@@]1([C@]2(C)CC(=O)[C@]3([H])[C@]1(CCC(=C4)[C@]3(C)C=CC4=O)[H])(CC[C@]2(C)CO)=O)[H]</chem>	C21H26O5	358.428	Prednisone
BIOMOL	PD-152	<chem>C1(=C(C)NC(=O)C(C#N)=C1)c2ccncc2</chem>	C12H9N3O	211.219	Milrinone
BIOMOL	DL-484	<chem>[C@]([H])([C@]1(C)C[C@H](O)CC1)=CC2(C)[CC[C@@]3(C)[C@@]4([H])CC[C@H]3C(C)=O)[C@@]24[H]</chem>	C21H32O2	316.478	Pregnenolone
BIOMOL	PD-175	<chem>c1(OC2CCCC2)cc(C3CC(=O)NC3)ccc1OC</chem>	C16H21NO3	275.343	Rolipram
BIOMOL	DL-485	<chem>c1(NC(C)CCCN)cc(OC)cc2c1nccc2</chem>	C15H21N3O	259.347	Primaquine phosphate
BIOMOL	PD-179	<chem>c1(ccc(\N=C(/NC)\NC#N)cc1)C2=NNC(=O)CC2C</chem>	C14H16N6O	284.316	Siguzodan
BIOMOL	DL-486	<chem>C1(CN(C(=O)C2CCCCC2)CC3=O)N3CCc4c1cccc4</chem>	C19H24N2O2	312.406	Praziquantel
BIOMOL	PD180	<chem>C1(=C(C)N=C(N)c2c(C)cc(C)cc2C)N(C)C3=O)N3CCc4c1cc(OC)c(O)c4</chem>	C24H27N3O3	405.489	Trequinsin
BIOMOL	DL-487	<chem>c1(c(O)c(C(=O)O)cc(cc2)c1cc2)Cc3c(O)c(C(=O)O)cc4c3cccc4.C5(=NCCC N5C)C=Cc6scoc6</chem>	C34H30N2O6S	594.677	Pyrantel pamoate
BIOMOL	PD-185	<chem>[C@@]([H])([C@@]1(CC)CCC2(N2CC3)c(c3c(c45)cccc4)n5C(C(=O)OCC)=C1</chem>	C22H26N2O2	350.454	Vinpocetine
BIOMOL	DL-333	<chem>N1(CCN(CCCC(=O)c2ccc(F)cc2)CC1)c3ncccc3</chem>	C19H22FN3O	327.396	Azaperone
BIOMOL	DL-409	<chem>N1(C=C(F)C(=O)NC1=O)C2OCCC2</chem>	C8H9FN2O3	200.167	Ftorafur
BIOMOL	T-116	<chem>C1[C@@]([H])([C]C[C@](CC)(O)C2)CN2CCc(c(c3[nH]4)cccc3)c4[C@@]1(C)OC(=O)c5cc6c(N(C)[C@@]([C@@]67[C@](N8CC7)([H])[C@@]9(CC)C=C8)([H])[C@@](O)(C(OC)=O)[C@@H]9OC(C)=O)cc5OC</chem>	C46H58N4O9	810.974	Vinblastine sulfate
BIOMOL	DL-410	<chem>c1(C(=O)O)cc(S(=O)(=O)N)c(C)cc1NCc2cccc2</chem>	C12H11ClN2O5S	330.744	Furosemide
BIOMOL	DL-335	<chem>[C@H]1O[C@@H]2O[C@H](C)[C@H](N(C)C)[C@H]2O)[C@@](O)(C)C[C@@H](C)CN(C)[C@H](C)[C@H](O)[C@@](O)(C)[C@H](CC)OC(=O)[C@H](C)[C@H](O)[C@H]3O[C@H](C)[C@H](O)[C@](C)(OC)C3)[C@@H]1C</chem>	C38H72N2O12	748.984	Azithromycin
BIOMOL	DL-411	<chem>c(N=C(N)NC1=O)(n(COC(CO)CO)cn2)c12</chem>	C9H13N5O4	255.231	Ganciclovir
BIOMOL	DL-336	<chem>[C@@H]1(NC(=O)C(=N/O C(C)(C)C(=O)O))c2nc(N)sc2C(=O)N(S(=O)(=O)O)[C@H]1C</chem>	C13H17N5O8S2	435.433	Aztreonam
BIOMOL	DL-412	<chem>c1(c(OC)c(N2CCNC(C)C2)c(F)c3c3C(=O)C(C(=O)O)=CN1C4CC4</chem>	C19H22FN3O4	375.394	Gatifloxacin
BIOMOL	DL-337	<chem>[C@@]1(OC(=O)CC(C(=O)CO C(=O)CC)[C@@H](C)C[C@]2([H])[C@]1(C)C[C@H](O)C3(F)[C@@]2([H])CCC(=C4)[C@]3(C)C=CC4=O</chem>	C28H37FO7	504.588	Betamethasone

BIOMOL	DL-413	[C@H]1(O[C@H]2O[C@@](O)(C)[C@H](NC)[C@H]2O)[C@H](N)C[C@H](N)[C@H](O)[C@H]3[C@H](N)CC[C@@H]([C@@H](C)NC)O3)[C@@H]1O	C21H43N5O7	477.595	Gentamycin sulfate
BIOMOL	DL-338	C(c1ccccc1)(n2cnc2)c3ccc(c4ccccc4)cc3	C22H18N2	310.392	Bifonazole
BIOMOL	DL-414	c1(OCCCC(C)(C)C(=O)O)cc(C)ccc1C	C15H22O3	250.333	Gemfibrozil
BIOMOL	DL-339	C(c1ccccc1)(c2ccc(O C(=O)O)cc2)c3ccc(O C(=O)O)cc3	C22H19NO4	361.391	Bisacodyl
BIOMOL	DL-415	C(CCC1)(CN(NC(=O)NS(=O)(=O)c2ccc(C)cc2)C3)C13	C15H21N3O3S	323.411	Gliclazide
BIOMOL	DL-340	c1(CN(C)C2CCCC2)cc(Br)cc(Br)c1N N1(C(=O)NCCc2ccc(S(=O)(=O)NC(=O)N[C@@H]3CC[C@H](C)CC3)cc2)CC(C)=C(C)C1=O	C14H20Br2N2	376.13	Bromhexine HCl
BIOMOL	DL-416	C12(CCCC1)CC(=O)N(CCCCN3CCN(c4nccn4)CC3)C(=O)C2	C24H34N4O5S	490.616	Glimepiride
BIOMOL	DL-341	c1(OCC(O)CO)ccccc1OC	C10H14O4	198.216	Guaifenesin
BIOMOL	DL-342	[C@@]12(CCC(=O)O)1CC[C@]3([H])[C@]2(C)CC[C@]4([H])[C@@]3([H])C=CC(=C5)[C@]4(C)CCC5=O	C22H28O3	340.456	Canrenone
BIOMOL	DL-418	[C@@H](CC)(c1ccc(O)cc1)[C@@H](CC)c2ccc(O)cc2	C18H22O2	270.366	Hexestrol
BIOMOL	DL-488	c1(NC(C)CCCN(C)CC)c2c(cc(Cl)cc2)nc3c1cc(OC)cc3	C23H30ClN3O	399.957	Quinacrine 2HCl dihydrate
BIOMOL	PD-190	c1(ccccc1OCCC)C2=NC(=O)c3c(n[nH]3)N2 N1(C(=O)[C@H](C)N[C@H](C(=O)OCC)CCc2ccccc2)Cc(c3C[C@H]1C(=O)O)ccccc3	C13H13N5O2	271.275	Zaprinast
BIOMOL	DL-489	c1(ccc(OC(F)F)c(OC)c1)C2=NNC(=O)C=C2	C25H30N2O5	438.516	Quinapril HCl
BIOMOL	PD-195	C(CSC(=O)C)(C(=O)NCC(=O)O)Cc1ccccc1Cc2ccccc2	C12H10F2N2O3	268.216	Zardaverine
BIOMOL	DL-159	[C@@]1([H])(CCCCCCC(=O)O)C(=O)C[C@H](O)[C@]1([H])C=C[C@@H](O)CCCCC	C21H23NO4S	385.477	Racecadotril
BIOMOL	PG-006 PGE1	c1(OCC(O)CN2CCN(CC(=O)Nc3c(C)cccc3C)CC2)ccccc1OC	C20H34O5	354.481	Alprostadil
BIOMOL	DL-490	[C@H]1(C=C(Cl)C(O)(C)CCC)[C@H](O)CC(=O)[C@@H]1CCCCCCC(=O)OC	C24H33N3O4	427.537	Ranolazine 2HCl
BIOMOL	PG-051	N1(C(=O)[C@H](C)N[C@H](C(=O)OCC)CCc2ccccc2)[C@H](C(=O)O)C[C@@]3([H])[C@]1([H])CCC3	C22H38O5	382.534	Misoprostol
BIOMOL	DL-491	c1(NCC(C)C2)c2ccc1S(=O)(=O)N[C@@H](CCCCN(=N)N)C(=O)N3CC[C@@H](C)C[C@H]3C(=O)O	C23H32N2O5	416.511	Ramipril
BIOMOL	PI-146	c1(cccc2)c2NC(=O)C=C1CC(C(=O)O)NC(=O)c3ccc(Cl)cc3	C23H36N6O5S	508.634	Argatroban
BIOMOL	DL-147	[C@@H]1(C(=O)N(C)C(=O)O)=C/CCCCSC[C@H](N)C(=O)O)CC1(C)C	C19H15ClN2O4	370.786	Rebamipide
BIOMOL	PI-153	[C@@H]1([C@H](O)[C@H](O)[C@@H](CO)O1)n2cnc(C(=O)N)n2	C16H26N2O5S	358.453	Cilastatin
BIOMOL	DL-492	[C@@]([C@]1([H])[C@@]([H])(C)[C@@]([H])(OC(=O)CCC(O)=O)O2)([C@]3([H])[C@]([H])(C)CC1)(O4)[C@]2(O)[C@@]4(C)CC3)[H]	C8H12N4O5	244.205	Ribavirin
BIOMOL	PR-117	[C@@H](N[C@@H]1[C@H]2CCCC1)C[C@H](O)[C@H](CSc3ccccc3)NC(=O)c4cccc(O)c4C(C(=O)NC(C)(C)C)C2.S(=O)(=O)O)C	C19H28O8	384.421	Artesunate
BIOMOL	DL-566	c1(C(=O)NCCc2cnc2)cc(C(=O)NCCc3cnc2)ccc1OC	C33H49N3O7S2	663.888	Nelfinavir Mesylate
BIOMOL	RA-104	[C@@]1([C@@]([H])(C)[C@@]2([H])C1)C[C@@]3([H])C2(C3)C(N)C	C21H20N4O3	376.409	Picotamide
BIOMOL	DL-494	[C@@H](O1)[C@H](O)[C@@H](O)[C@H](O)[C@H]2O)[C@@H]12	C12H21N	179.302	Rimantadine HCl
BIOMOL	S104	c1(cccc2)c2ccc1OCC(O)CNC(C)C	C6H10O5	162.141	Conduritol b epoxide
BIOMOL	ST-405	C(=C1C(=CC(=O)CC1)CC2)([C@@H](c3ccc(N(C)C)cc3)C[C@@]4(C)[C@@]5([H])CC[C@@]4(O)C#CC)[C@@]25[H]	C16H21NO2	259.343	Propranolol
BIOMOL	S-510	c(ccccc1)[n+][O-]c(\C=MNC(=O)OC)[n+][2O-]c12	C29H35NO2	429.594	Mifepristone
BIOMOL	DL-343	[C@@]1([C@]2(C)C[C@H](O)[C@]([C@@]13[H])([H])[C@]4(C)C(=CC(=O)CC4)CC3)(CC[C@@]2(C)CO(=O)O)[H]	C11H10N4O4	262.222	Carbadox
BIOMOL	DL-419	C12(CCC1)C(=O)O[Pt]OC2=O	C21H30O5	362.46	Hydrocortisone
BIOMOL	DL-344	[C@](C)([C@](C(=O)CO C(=O)C)(O)CC1)(C[C@H](O)[C@@]2([H])[C@]3(CCC(=C4)[C@]2(C)CCC4=O)[H])[C@@]13[H]	C6H6O4Pt	337.187	Carboplatin
BIOMOL	DL-420	N1(C(=O)N)c2c(cccc2)C=Cc3c1ccccc3	C23H32O6	404.497	Hydrocortisone 21-acetate
BIOMOL	DL-345	[C@]1([H])(CCC(=C2)[C@]3(C)CCC2=O)[C@]3([H])CC[C@@]4(C)[C@@]1([H])CC[C@]4(O)C(=O)C	C15H12N2O	236.269	Carbamazepine
BIOMOL	DL-421	C1([C@@H](NC([C@H](NC(=O)N2CCN(CC)C(=O)C2=O)c3ccc(O)cc3)=O)[C@]4([H])N1C(C(=O)O)=C(CSc5nnnn5)CS4)=O	C21H30O3	330.461	17- hydroxyprogesterone
BIOMOL	DL-346	[C@@H]1(C[C@H](O)[C@@H](CO)O1)N2C=C(I)C(=O)NC2=O	C25H27N9O8S2	645.667	Cefoperazone acid
BIOMOL	DL-422	N1([C@]2([H])SCC(COC(=O)C)=C1C(=O)O)C(=O)[C@H]2NC(=O)C(=N/O)C)c3ccc(N)n3	C9H11N2O5	354.099	Idoxuridine
BIOMOL	DL-347	N1(CCC)CCCO P1(=O)NCCCl	C16H17N5O7S2	455.465	Cefotaxime acid
BIOMOL	DL-423	N(C(C([O-])=O)=C(C[n+])1ccccc1)CS2)(C(=O)[C@H]3NC(=O)C(=N/O)C(C)C(=O)O)c4nc(N)sc4)[C@H]23	C7H15Cl2N2O2P	261.086	Ifosfamide
BIOMOL	DL-348	c1(n(CC(C)C)n2)c2c(N)nc3c1ccccc3	C22H22N6O7S2	546.576	Ceftazidime
BIOMOL	DL-424		C14H16N4	240.304	Imiquimod

BIOMOL	DL-349	<chem>c1(ccc([N+](O-)=O)cc1)[C@@H](O)[C@@H](CO)NC(=O)C(Cl)Cl</chem>	C11H12Cl2N2O5	323.129	Chloramphenicol
BIOMOL	DL-425	<chem>c1(cccc2)c2CC(C)N1NC(=O)c3ccc(Cl)c(S(=O)(=O)N)c3</chem> <chem>[C@]([C@@]([C@]12[H](C)CC[C@]2[H])([H])[C@@]1([H])C=C(C)C(=C4)[C@]3(C)CCC4O(C(=O)C)(C(=O)C)(O(C(=O)C)CC2</chem>	C16H16ClN3O3S	365.835	Indapamide
BIOMOL	DL-350	<chem>c1(C(=O)NCc2ccc(OCCN(C)C)cc2)ccc(OC)c(C)C1</chem>	C25H33ClO5	448.98	Chlormadinone acetate
BIOMOL	DL-426	<chem>c1(ccc(CCC(C(=O)O)cc1)N(CCC)CCC</chem>	C20H26N2O4	358.431	Itopride HCl
BIOMOL	DL-351	<chem>C1(Cn2ncnc2)(OCC(COc3ccc(N4CCN(c5ccc(N6C=NN(C(C)CC)C6=O)cc5)C4)cc3)O1)c7ccc(Cl)cc7Cl</chem>	C14H19Cl2NO2	304.212	Chlorambucil
BIOMOL	DL-427	<chem>C(CCN(C)C)(c1cccc1)c2ccc(Cl)cc2</chem>	C35H38Cl2N8O4	705.633	Itraconazole
BIOMOL	DL-352	<chem>c1(C(=O)c2ccccc2)cccc([C@H](C)C(=O)O)c1</chem>	C16H19ClN2	274.788	Chlorpheniramine maleate
BIOMOL	EI-288	<chem>c1(CN2CCCC2)cccc(OCCNC(=O)COC(=O)C)c1</chem>	C16H14O3	254.281	Ketoprofen (s)
BIOMOL	DL-496	<chem>[C@]1(C(=O)C)(OC(=O)C)CC[C@]2([H])[C@]1(C)CC[C@]23([H])[C@@]2([H])C=C(C)C(=C4)[C@]3(C)CCC4=O</chem>	C19H28N2O4	348.437	Roxatidine acetate HCl
BIOMOL	S-515	<chem>[C@@H]1(O)[C@@H]2O[C@@H](C)[C@H](O)[C@](C)(OC)C2[C@@H](C)C(=O)O[C@H](CC)[C@](O)(C)[C@H](O)[C@@H](C)C(=N)OCCCCO</chem> <chem>)([C@H](C)C[C@](O)(C)[C@H](O)[C@@H]3O[C@H](C)C[C@H](N(C)C)[C@H]3O)[C@H]1C</chem>	C24H32O4	384.508	Megestrol acetate
BIOMOL	DL-497	<chem>[C@]1(C(=O)C)(OC(=O)C)C(=C)C[C@]2([H])[C@]1(C)CC[C@]23([H])[C@@]2([H])C=C(C)C(=C4)[C@]3(C)CCC4=O</chem>	C41H76N2O15	837.047	Roxithromycin
BIOMOL	S-520	<chem>c(N1C=C(C(=O)O)C2=O)(c2cc(F)c3N4CCN(C)CC4)c3SCC1</chem>	C25H32O4	396.519	Melengestrol acetate
BIOMOL	DL-498	<chem>C/(c1ccccc1)(c2ccc(OCCN(C)C)cc2)=C/(CC)c3ccccc3</chem>	C17H18FN3O3S	363.407	Rufloxacin
BIOMOL	S-650	<chem>c1(cc(N2CCNCC2)c(F)c3c3C(=O)C(C(=O)O)=CN1c4ccc(F)cc4</chem>	C26H29NO	371.515	Tamoxifen citrate
BIOMOL	DL-499	<chem>N(CCC(C)C)(C[C@H](O)[C@H](N(C(=O)O)[C@H]1COCC1)Cc2ccccc2</chem> <chem>)S(=O)(=O)c3ccc(N)cc3</chem>	C20H17F2N3O3	385.364	Sarafloxacin HCl
BIOMOL	DL-532	<chem>[C@@]([H])(O1)[C@]([H])([N+])([C@@]23[H])(C)CCCC)C[C@@H](OC(=O)[C@H](CO)c4ccccc4)C2)[C@@]13[H]</chem>	C25H35N3O6S	505.627	Amprenavir
BIOMOL	DL-500	<chem>C1(CN2CCO[C@H](O)[C@H](C)c3cc(C(F)(F)F)cc(C(F)(F)F)c3)[C@@H]2c4ccc(F)cc4)=NC(=O)NN1</chem>	C21H30NO4	360.467	Scopolamine n-butylbromide
BIOMOL	DL-533	<chem>[C@@]([H])(O1)[C@]([H])(N([C@@]23[H])(C)C[C@H](OC(=O)[C@H](CO)c4ccccc4)C2)[C@@]13[H]</chem>	C23H21F7N4O3	534.427	Aprepitant
BIOMOL	DL-501	<chem>c1(Oc2ccccc2OC)c(OCCO)nc(c3ncccn3)nc1NS(=O)(=O)c4ccc(C(C)(C)C)c4</chem>	C17H21NO4	303.353	Scopolamine HBr
BIOMOL	DL-534	<chem>n1(CC(O)C)c(C)nc1[N+](O-)=O</chem>	C27H29N5O6S	551.614	Bosentan
BIOMOL	DL-502	<chem>[C@@]1(C#CC2CC2)(c3c(ccc(Cl)c3)NC(=O)O1)C(F)(F)F</chem>	C7H11N3O3	185.181	Secnidazole
BIOMOL	DL-535	<chem>C1(CCC1)(C(N(C)C)CC(C)C)c2ccc(Cl)cc2</chem>	C14H9ClF3NO2	315.675	Efavirenz
BIOMOL	DL-503	<chem>[C@]1([H])([C@H](O)C[C@]2([H])[C@]3(C)CC[C@H](O)C2)[C@]3([H])C[C@H](O)[C@@]4(C)[C@@]1([H])CC[C@H]4[C@H](C)CCC(=O)NC</chem> <chem>CS(=O)(=O)O</chem>	C17H26ClN	279.848	Sibutramine HCl
BIOMOL	DL-536	<chem>c(c(F)c(N1C[C@H](C)N[C@H](C)C1)c(F)c2N(N(C3CC3)C=C(C(=O)O)C4=O)c24</chem>	C26H45NO7S	515.703	Taurocholic acid, sodium salt hydrate
BIOMOL	DL-149	<chem>N1(CCCC)C[C@H](O)[C@@H](O)[C@H](O)[C@H]1CO</chem>	C19H22F2N4O3	392.4	Sparfloxacin
BIOMOL	SL-230	<chem>[C@@]12(CCC(=O)O1)CC[C@]3([H])[C@]2(C)CC[C@]4([H])[C@@]3([H])[C@H](S(C(=O)C)CC(=C5)[C@]4(C)CCC5=O</chem>	C10H21NO4	219.278	Miglustat
BIOMOL	DL-504	<chem>[C@@]([H])([C@@]1([H])[C@]([C@H](O)CC1)CC2)([C@H](CCCCCCCCS(=O)O)CCCC(F)(F)C(F)(F)Cc3c4ccc(O)c3)[C@]24[H]</chem>	C24H32O4S	416.573	Spironolactone
BIOMOL	DL-104	<chem>c(ccc(Cl)c1)(c(NC(C)CCN(CC)CC)ccn2)c12</chem>	C32H47F5O3S	606.771	Fulvestrant
BIOMOL	DL-353	<chem>[C@H]1(N=C(N2C1)SCC2)c3ccccc3</chem>	C18H26ClN3	319.872	Chloroquine phosphate
BIOMOL	DL-429	<chem>N1(C(=O)C)c(c2C1=O)cccc2)C3CCC(=O)N3C=O</chem>	C11H12N2S	204.291	Levamisole HCl
BIOMOL	T-115	<chem>[C@](CC)([C@](O)(C#C)CC1)(CC[C@]2([H])[C@@]3([H])CCC(=C4)[C@@]2([H])CCC4=O)[C@@]13[H]</chem>	C13H10N2O4	258.229	Thalidomide
BIOMOL	DL-430	<chem>c1(cc(N2CCNCC2)c(F)c3c3C(=O)C(C(=O)O)=CN1C4CC4</chem>	C21H28O2	312.446	Levonorgestrel
BIOMOL	DL-355	<chem>c1(O)cc(C[C@H](N)C(=O)O)ccc1O</chem>	C17H18FN3O3	331.342	Ciprofloxacin
BIOMOL	DL-431	<chem>C1(CCCN(C)C)(c2ccc(F)cc2)OCc3c1ccc(C#N)c3</chem>	C9H11NO4	197.188	Levodopa
BIOMOL	AR-116	<chem>c(N1C=C(C(=O)O)C2=O)(c2cc(F)c3N4CCN(C)CC4)c3OC[C@H]1C</chem>	C20H21FN2O	324.392	Citalopram
BIOMOL	DL-432	<chem>[C@@H]1(O)[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@@H](C)[C@H](O)[C@@H]3O[C@@H](C)[C@H](O)[C@](C)(OC)C3[C@@H](C)C(=O)O[C@H](CC)[C@](O)(C)[C@H](O)[C@@H](C)C(=O)[C@H](C)C[C@@]1(C)OC</chem>	C18H20FN3O4	361.368	Levofloxacin HCl
BIOMOL	DL-357	<chem>c1(cnoc1C)C(=O)Nc2ccc(C(F)(F)F)cc2</chem>	C38H69NO13	747.953	Clarithromycin
BIOMOL	DL-433	<chem>C(C(=O)C(C)C)(Oc1ccc(Cl)cc1)n2ncnc2</chem>	C12H9F3N2O2	270.207	Leflunomide
BIOMOL	DL-358	<chem>N1(C(=O)[C@H](CCCC)N[C@H](C(=O)O)CCc2ccccc2)CCC[C@H]1C(=O)O</chem>	C15H17ClN2O2	292.761	Climbazole
BIOMOL	DL-434		C21H31N3O5	405.488	Lisinopril

BIOMOL	DL-359	c1(c(Cl)c(N2CCC(N)C2)c(F)c3)c3C(=O)C(C(=O)O)=CN1C4CC4	C17H17ClFN3O3	365.787	Clinafloxacin HCl
BIOMOL	DL-435	c(c(F)c(N1CCNC(C)C1)c(F)c2)(N(CC)C=C(C(=O)O)C3=O)c23	C17H19F2N3O3	351.348	Lomefloxacin HCl
BIOMOL	DL-360	C(=C(/C/))c1cccc1)/(c2cccc2)/c3ccc(OCCN(CC)CC)cc3	C26H28ClNO	405.96	Clomiphene citrate
BIOMOL	DL-436	C(=C(\CCN(C(=O)O)CC)C1)/C1)/(c2c(cccn2)CC3)/c(ccc(Cl)c4)c34	C22H23ClN2O2	382.883	Loratadine
BIOMOL	DL-361	c1(O)c(Cl)c(C)nc(C)c1Cl	C7H7Cl2NO	192.043	Clopidol
BIOMOL	DL-437	C(CCC(=O)O)(N(C(=O)c1ccc(Cl)c(Cl)c1)C(=O)N(CCCCC)CCCC	C22H32Cl2N2O4	459.406	Lorglumide
BIOMOL	AC-1290	N1(CCc2c(ccs2)C1)[C@H](C(=O)O)C3cccc3Cl	C16H16ClNO2S	321.822	Clopidogrel sulfate
BIOMOL	DL-438	c1(c2nnnn2[K])cccc1c3ccc(Cn4c(CO)c(Cl)nc4CCCC)cc3	C22H22ClKN6O	461.001	Losartan potassium
BIOMOL	DL-505	[C@]([H])([C@]1(C)[C@]([H])(Cc2C1)[nH]nc2)CC3)(CC[C@]4(C)[C@ @]5([H])CC[C@]4(O)C)[C@]35[H]	C21H32N2O	328.492	Stanozolol
BIOMOL	DL-538	c(c1n(C)c2)(c2[C@]3([H])C4=C[C@]@H(C(=O)N[C@H](CO)CC)CN3C)c4 ccc1	C21H27N3O2	353.458	Methysergide
BIOMOL	DL-506	[C@]@H]1(O)[C@]@H]2O[C@]@H](CO)[C@H](O)[C@]@H](O)[C@]@H]2N C)[C@]@](O)(C=O)[C@H](C)O[C@H]1O[C@]@H]3[C@]@H](O)[C@H](O) [C@]@H](NC(=N)N)[C@H](O)[C@H]3NC(=N)N	C21H39N7O12	581.574	Streptomycin sulfate
BIOMOL	DL-107	c1(OCC(O)CNC(C)C)ccc(CCC(=O)O)Ccc1	C16H25NO4	295.374	Esmolol
BIOMOL	DL-507	c1(NS(=O)(=O)c2ccc(N)cc2)ncnc(O)c1OC	C12H14N4O4S	310.329	Sulfadoxine
BIOMOL	DL-123	[C@H](O)(C(=O)NCCC(=O)O)C(C)C(CO	C9H17NO5	219.235	Pantothenic acid
BIOMOL	DL-508	c1(ccc(N)cc1)S(=O)(=O)Nc2ncccn2	C10H10N4O2S	250.277	Sulfadiazine
BIOMOL	DL-146	c1(C(=O)CCc2ccc(O)cc2)c(O)cc(O)cc1O[C@H]3[C@H](O)[C@]@H](O)[C @H](O)[C@]@H](CO)O3	C21H24O10	436.409	Phloridzin
BIOMOL	DL-509	c1(nc(OC)nc(OC)c1)NS(=O)(=O)c2ccc(N)cc2	C12H14N4O4S	310.329	Sulfadimethoxine
BIOMOL	DL-225	c1(ccccc1)[C@]@H](O)[C@]@H](N)C	C9H13NO	151.206	Phenylpropanolamine
BIOMOL	DL-510	c1(ccc(N=Nc2ccc(O)c(C(=O)O)c2)cc1)S(=O)(=O)Nc3ncccc3	C18H14N4O5S	398.393	Sulfasalazine
BIOMOL	DL-234	[N+](C)(C)(C)CCOC(=O)CCC(=O)OCC[N+](C)(C)C	C14H30N2O4	290.399	Succinylcholine
BIOMOL	DL-160	c1(S(=O)(=O)N)cc(C[C@]@H](C)NCCOC2cccc2OCC)ccc1OC	C20H28N2O5S	408.512	Tamsulosin HCl
BIOMOL	DL-195	c1(ccccc(C(F)(F)F)c1)C2(O)CCN(CCC(=O)c3ccc(F)cc3)CC2	C22H23F4NO2	409.417	Trifluoperidol 2HCl
BIOMOL	DL-511	c1(cc(c2nc(c3n2C)cccc3)cc4C)c4nc(CCC)n1Cc5ccc(c6ccccc6C(=O)O)cc5	C33H30N4O2	514.617	Telmisartan
BIOMOL	DL-540	c1(cc(l)c(O)c(l)c1)Oc2c(l)c1)cc(C[C@H](N)C(=O)O)cc2l	C15H11I4NO4	776.87	L-thyroxine [(3-[4-(4-hydroxy-3,5-diiodophenoxy)-3,5-diiodophenyl]-l-alanine]
BIOMOL	DL-512	c(scc1)(C(O)=C(C(=O)Nc2ncccc2N(C)S3(=O)=O)c13	C13H11N3O4S2	337.374	Tenoxicam
BIOMOL	DL-136	C(=C(\CCN(C)C1)/C1)/(c2c(cccc2)C=C3)/c(cccc4)c34	C21H21N	287.398	Cyproheptadine
BIOMOL	DL-513	c(cc(OC)c(C)O)c1)(c(N)nc(N2CCN(C(=O)C3OCCCC)CC2)n4)c14	C19H25N5O4	387.433	Terazosin HCl
BIOMOL	DL-559	c(cccc1)(n(Cc2cccc2)nc3OCCCN(C)C)c13	C19H23N3O	309.405	Benzylamine
Selleck	Chemicals S1011	c1(F)ccc(Nc2c3c(cc(O)[C@]@H]4COCC4)c(NC(=O)C=CCN(C)C)c3)ncn2)cc 1Cl	C24H25ClFN5O3	485.938	Afatinib (BIBW2992)
Selleck	Chemicals S1888	C1=C[C@]@]2(C)C(C(C[C@]3([H])([C@]@]2([H])([C@H](O)C[C@]@]4(C)[C @]@]3([H])C[C@]5([H])([C@]4(C(=O)CO)C(=O)C)N=C(C)O5)=CC1=O	C25H31NO6	441.517	Deflazacort
Selleck	Chemicals S1198	N1(C2CCN(C(Oc3ccc(c4c3)nc5c(CN(C5=C6)C(=O)C7=C6[C@]@](CC)(O)C (=O)O)C7)c4CC)=O)CC2)CCCCC1	C33H38N4O6	586.678	Irinotecan
Selleck	Chemicals S1941	c1cc(C[C@]@H](C(=O)OCC)N[C@]@H](C)C(=O)N2CCC[C@H]2C(=O)O) ccc1.C(=O)(C=CC(=O)=O)O	C24H32N2O9	492.519	Enalapril Maleate
Selleck	Chemicals S1274	N1(C(Nc2cccc(Nc3ncc(l)c(NCCCNC(=O)c4sccc4)n3)c2)=O)CCCC1	C23H26ClN7O2S	591.468	BX-795
Selleck	Chemicals S2013	N1c(c2CCC1=O)ccc(Nc3ncc(C(F)(F)F)c(NCc4cccc(S(C(=O)=O)c4)n3)c2 C1([C@]@H]2[C@H]3C(C)(C)C(C34[C@]@]([H])(O)C(=O)[C@H]4O)O5)[C@]@]5(C(=O)O2)[C@]6(O)[C@]@]([H])(O)C(=O)[C@]@H]6C)[C@H]1O	C22H20F3N5O3S	491.486	PF-573228
Selleck	Chemicals S1343		C20H24O10	424.399	Ginkgolide B
Selleck	Chemicals S2054	c1(ccccc1)C(c2c(C)cccc2)OCCN(C)C.Oc(=O)CC(O)(C(=O)O)CC(=O)O	C24H31NO8	461.505	Orphenadrine Citrate
Selleck	Chemicals S1389	c1cc2c(nc(S(Cc3ncc(C)c(OC)c3C)=O)[nH]2)cc1OC	C17H19N3O3S	345.416	Omeprazole
Selleck	Chemicals S2096	c1(CS(=O)(=O)N2CCCC2)cc3c([nH]cc3CCN(C)C)cc1.C(O)(=O)C(O)CC(=O)O	C21H31N3O7S	469.552	Almotriptan Malate
Selleck	Chemicals S1544	c1ccc2c(c(C(=O)c3c(l)ccc([N+])([O-])=O)c3)cn2CC4CCCCN4C)c1	C22H22I3O3	503.333	AM1241
Selleck	Chemicals S2153	c(ncn1[C@H]2[C@]@H](O)[C@H](O)[C@]@H](C(=O)NCC)O2)(c(N)nc(NC Cc3ccc(CCC(=O)O)cc3)n4)c14.Cl	C23H30ClN7O6	535.981	CGS 21680 HCl
Selleck	Chemicals S1638	c1cc(C(C)C(=O)O)ccc1CC(C)C	C13H18O2	206.281	Ibuprofen

Selleck		<chem>C1CCN(C2CCN(C(=O)O)c3cc4c(nc5c(CN6C5=CC7=C(COC(=O)[C@]7(O)C</chem>			
Chemicals	S2217	<chem>C)C6=O)c4CC(cc3)CC2)CC1.Cl.O.O.O</chem>	C33H45ClN4O9	677.185	Irinotecan HCl Trihydrate
Selleck		<chem>C1C[C@@]2(C)C(C[C@]3([H])[C@@]2([H])[C@H](O)C[C@@]4(C)[C@</chem>			
Chemicals	S1696	<chem>@]3([H])C[C@]4(O)C(CO)=O)=CC1=O</chem>	C21H30O5	362.46	Hydrocortisone
Selleck					
Chemicals	S2293	<chem>OC(=O)CC(C[N+](C)(C)C)O.[Cl-]</chem>	C7H16ClNO3	197.66	DL-Carnitine HCl
Selleck		<chem>OC(=O)C=CC(=O)O.c1cc2c(Sc3c(cccc3)C(N4CCN(CCOCCO)CC4)=N2)cc</chem>			
Chemicals	S1763	<chem>1.c5cc6c(Sc7c(cccc7)C(N8CCN(CCOCCO)CC8)=N6)cc5</chem>	C46H54N6O8S2	883.086	Quetiapine Fumarate
Selleck		<chem>c1(O)cc2c(C(=O)C(O)[C@H]3[C@@H](O)[C@H](O)[C@@H](O)[C@H](C</chem>			
Chemicals	S2327	<chem>O3)=C(c4cc(O)c(O)c(O)c4)O2)c(O)c1</chem>	C21H20O12	464.376	Myricitrin
Selleck		<chem>c(C(=O)C=C(c1[nH]nnn1)O2)(ccc(NC(=O)c3ccc(OCCCCc4ccccc4)cc3)c5)c</chem>			
Chemicals	S1829	<chem>25</chem>	C27H23N5O4	481.503	Pranlukast
Selleck					
Chemicals	S2363	<chem>c1(O)c(O)c(O)c2c(C(=O)C=C(c3ccc(O)C)cc3)O2)c(O)c1OC</chem>	C20H20O7	372.369	Tangeretin
Selleck					
Chemicals	S2393	<chem>OC[C@@H](O)[C@@H](O)[C@H](O)[C@@H](O)CO</chem>	C6H14O6	182.172	Sorbitol
Selleck					
Chemicals	S2872	<chem>c1c(l)ccc2c1C(=Cc3cc(Br)c(O)c(Br)c3)C(=O)N2</chem>	C15H8Br2INO2	520.942	GW5074
Selleck					
Chemicals	S2450	<chem>C1Oc2c(ccc(O)c2)C[C@H]1c3ccc(O)cc3</chem>	C15H14O3	242.27	Equol
Selleck					
Chemicals	S2886	<chem>c1(cc(NC(=O)CN(C)C)cc2)c2NC(=O)c3c1cccc3</chem>	C17H17N3O2	295.336	PJ34
Selleck		<chem>O1C(=O)C(O)=C(O)[C@@]1([H])[C@@H](O)COC(=O)CCCCCCCCCCC</chem>			
Chemicals	S2532	<chem>CCC</chem>	C22H38O7	414.533	L-Ascorbyl 6-palmitate
Selleck		<chem>c1(nc(C(C)C)sc1)CN(C)C(=O)N[C@@H](CCN2CCOCC2)C(=O)N[C@@H](</chem>			
Chemicals	S2900	<chem>Cc3cccc3)C[C@H](Cc4ccccc4)NC(=O)OCc5scnc5</chem>	C40H53N7O5S2	776.023	Cobicistat (GS-9350)
Selleck					Brompheniramine
Chemicals	S2585	<chem>c1(ccc(Br)cc1)C(c2ncccc2)CCN(C)C.OC(=O)C=CC(=O)O</chem>	C20H23BrN2O4	435.312	hydrogen maleate
Selleck					
Chemicals	S2910	<chem>C1(C)(C)CC(O)CC(C)(C)N1[O]</chem>	C9H18NO2	172.245	Tempol
Selleck					
Chemicals	S2691	<chem>c1cc(N2CCN(CCN3C(=O)CC4(CCCC4)CC3=O)CC2)c(O)C)cc1.Cl.Cl</chem>	C22H33Cl2N3O3	458.422	BMV 7378
Selleck					
Chemicals	S2919	<chem>C(O)(=O)CNC(C1=C(O)c(c2N(Cc3cccc3)C1=O)cccc2)=O</chem>	C19H16N2O5	352.341	IOX2
Selleck					
Chemicals	S2804	<chem>C(NC(c1cccc1)C)(=O)c2cccc2N=Cc3c(c4ccc3O)cccc4</chem>	C26H22N2O2	394.465	Sirtinol
Selleck					
Chemicals	S2930	<chem>c1cc(C#CS(=O)(=O)N)ccc1</chem>	C8H7NO2S	181.212	Pifithrin-?
Selleck					
Chemicals	S2819	<chem>n1(c2ccc(Cl)cc2Cl)c(c3ccc(l)cc3)c(C)c(C(NN4CCCC4)=O)n1</chem>	C22H21Cl2IN4O	555.239	AM251
Selleck		<chem>c1([C@@H]2N(CC(NC(=O)N3P(O)(=O)O)=N3)CCO[C@@H]2O[C@H](C</chem>			
Chemicals	S3038	<chem>c4cc(C(F)(F)F)cc(C(F)(F)F)c4ccc(F)cc1.CNC[C@H](O)[C@@H](O)[C@</chem>			
Selleck		<chem>H](O)[C@H](O)CO.CNC[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO</chem>	C37H56F7N6O16P	1004.834	Fosaprepitant dimethylamine salt
Chemicals	S2842	<chem>c(ccc(C#C[C@@])(CO)C(O)n1)(C(=O)C(C(=O)NC)=C(N)N2CC)c12</chem>	C18H22N4O4	358.392	SAR131675
Selleck		<chem>c(C=C1CCN(Cc2cc(C)cnc2)CC1)c3c(cc(Cl)cc3)CC4)(ncccc)c45.C(O)(=O)C</chem>			
Chemicals	S3052	<chem>=CC(O)=O</chem>	C30H30ClN3O4	532.03	Rupatadine Fumarate
Selleck					
Chemicals	S2855	<chem>C(NCCCCNC(=S)Nc1cccc(N=C=S)c1)(=S)Nc2cccc(N=C=S)c2</chem>	C20H20N6S4	472.673	MRS 2578
Selleck					
Chemicals	S3067	<chem>C(Nc1ccc(Cl)cc1)(=N)NC(=N)NCCCCCNC(=N)NC(Nc2ccc(Cl)cc2)=N.Cl.Cl</chem>	C22H32Cl4N10	578.368	Chlorhexidine HCl
Selleck					
Chemicals	S2863	<chem>c1cc2c(nc(N)n2S(=O)(c3ccc(C)cc3)=O)cc1</chem>	C14H13N3O2S	287.337	ML130 (Nodinitib-1)
Selleck		<chem>[C@H]1(c2ccc(N(C)C)cc2)C[C@@]3(C)[C@@]([H])(CC[C@@]3(O)C(=O)C</chem>			
Chemicals	S3081	<chem>)C(C)=O)[C@@]4([H])C1=C5C(=CC(=O)CC5)CC4</chem>	C30H37NO4	475.619	Ulipristal
Selleck					
Chemicals	S1014	<chem>n1c(c2c(Nc3cc(O)C(Cl)cc3Cl)c(C#N)c1)cc(OCCCN4CCN(C)CC4)c(O)C2</chem>	C26H29Cl2N5O3	530.446	Bosutinib (SKI-606)
Selleck					
Chemicals	S1890	<chem>s1cc(CSCCNC(NC)=C[N+](O-)=O)nc1CN(C)C</chem>	C12H21N5O2S2	331.457	Nizatidine
Selleck		<chem>S([O-])</chem>			
Chemicals	S1214	<chem>)](O)(=O)=O.[C@@H](NC(=O)c1c(C)c(N)nc([C@H](CC(=O)N)NC[C@@H</chem>			
Selleck		<chem>](N)C(=O)N)n1)(C(=O)N[C@@H](C)[C@H](O)[C@@H](C)C(=O)N[C@@</chem>			
Chemicals	S1958	<chem>H](C(=O)NCCC2sc(C3sc(C(=O)NCCC[S+](C)C)n3n2)[C@H](O)C)C(O)[C</chem>			
Selleck		<chem>@H]4O[C@H](CO)[C@H](O)[C@@H](O)[C@@]4([H])O[C@H]5O[C@H](</chem>			
Chemicals	S1214	<chem>CO)[C@@H](O)[C@H](OC(=O)N)[C@@H]5O)c6c[nH]cn6</chem>	C55H85N17O25S4	1512.622	Bleomycin Sulfate
Selleck					
Chemicals	S1958	<chem>C1(=O)N2[C@]([H])(S(=O)(=O)C(C)(C)[C@]2(C(=O)O)[H])C1</chem>	C8H11NO5S	233.242	Sulbactam

Selleck Chemicals	S1284	<chem>N1(CC(=O)O)c2c(cccc2)CC[C@H](N[C@@H](CCc3ccccc3)C(=O)OCC)C1=O.Cl</chem>	C24H29ClN2O5	460.95	Benazepril HCl
Selleck Chemicals	S2017	<chem>c1(cccc([N+])([O-])=O)c1[C@@H]2C(C(=O)OC)=C(C)NC(C)=C2C(=O)O[C@H]3CN(Cc4ccc4)CC3.Cl</chem>	C28H32ClN3O6	542.023	Benidipine HCl
Selleck Chemicals	S1351	<chem>[C@](O)(C1=CC=C[C@H](C)[C@H](O[C@]2([H])O[C@@H](C)[C@H](O[C@]3([H])O[C@@H](C)[C@H](O)[C@@H](OC)C3)[C@@H](OC)C2)C(C)=CC[C@]([H])(C[C@@H]4OC5=O)O[C@@]6(CC[C@H](C)[C@@]([H])([C@H](CC(C)O6)C4)([C@]5([H])C=C(C)[C@H]7O)[C@]7([H])OC1NC(=N)NCCC[C@]([H])(NS(=O)=O)(=O)c1c2c(CC(C)CN2)ccc1)C(=O)N3[C@H](C(O)=O)C[C@H](C)CC3</chem>	C48H74O14	875.093	Ivermectin
Selleck Chemicals	S2069	<chem>C1(=C2CCN(C)CC2)c3c(cccc3)CCc4c1ccs4.C(O)(=O)C(O)CC(O)=O</chem>	C23H27NO5S	429.529	Pizotifen Malate
Selleck Chemicals	S2099	<chem>c1ccc(C[C@@H](C(=O)OCC)N[C@H]2CS[C@H](c3cccs3)CN(CC(=O)O)C2=O)ccc1.Cl</chem>	C23H29ClN2O5S2	513.07	Temocapril HCl
Selleck Chemicals	S1578	<chem>c1(Cn2c(OCC)nc3c2c(C(=O)O)ccc3)ccc(c4c(c5[nH]nn5)cccc4)cc1</chem>	C24H20N6O3	440.454	Candesartan
Selleck Chemicals	S2160	<chem>c1cccc([C@H](N2[C@@H](CCc3ccc(C(F)(F)F)cc3)c4c(cc(OC)c(O)c4)CC2)C(=O)NC)c1.Cl</chem>	C29H32ClF3N2O3	549.024	Almorexant HCl
Selleck Chemicals	S1640	<chem>c1(SCCC)cc2c(nc(NC(=O)OC)[nH]2)cc1</chem>	C12H15N3O2S	265.331	Albendazole
Selleck Chemicals	S2228	<chem>c1(C(=O)N[C@@H](C(C)(C)C)N2CCC[C@H]2C(=O)N[C@@H]3[C@@H](OCC)OC(=O)C3=O)ccc(N)c(Cl)c1</chem>	C24H33ClN4O6	508.995	VX-765
Selleck Chemicals	S1703	<chem>C(CCC)(CCC)C(=O)[O-].[Na+].C(O)(=O)C(CCC)CCC</chem>	C16H31NaO4	310.405	Divalproex Sodium
Selleck Chemicals	S2303	<chem>c1(C=O)c2c(cc(C)c(c3c(C)cc4c(c(C=O)c(O)c(O)c4(C)C)c3O)c2O)c(C(C)C)c(O)c1O</chem>	C30H30O8	518.554	Gossypol
Selleck Chemicals	S1771	<chem>c1cc2c(C(=CCN(C)C)c3c(ccc(C)C3)S2)cc1</chem>	C18H18ClNS	315.86	Chlorprothixene
Selleck Chemicals	S2329	<chem>c1c(O)c2c(O[C@H](c3ccc(O)cc3)CC2=O)cc1O[C@H]4[C@@H](O[C@H]5[C@@H](O)[C@H](O)[C@@H](O)[C@H](C)O5)[C@@H](O)[C@H](O)[C@@H](O)[C@H](CO)O4</chem>	C27H32O14	580.535	Naringin
Selleck Chemicals	S1832	<chem>c1(O)c2c(C(Cc3cc(OC)c(OC)cc3)[N+](C)(CCC(=O)O)CCCCCO C(=O)CC[N+](4(C)CCc(c5C4c6cc(OC)c(OC)cc6)cc(OC)c(OC)c5)CC2)cc1O.C.c7c(S(=O)(=O)[O-])cccc7.c8c(S(=O)(=O)[O-])cccc8</chem>	C65H82N2O18S2	1243.479	Atracurium Besylate
Selleck Chemicals	S2369	<chem>c1c(O)c2c(Oc(c3ccc(OCCO)c(OCCO)c3)=C(O)[C@H]4[C@H](O)[C@@H](O)[C@H](O)[C@H](CO[C@@H]5O[C@@H](C)[C@H](O)[C@@H](O)[C@H]5O)O4)C2=O)cc1OCCO</chem>	C33H42O19	742.675	Troloxerutin
Selleck Chemicals	S2397	<chem>c1cc2c(c[n+]3c(c4c(cc(OC)c(OC)c4)CC3)c2c(OC)c1OC.[Cl-]</chem>	C21H22ClNO4	387.857	Palmitine chloride
Selleck Chemicals	S2874	<chem>c1(ccc(NC(=N)N)cc1)C(=O)Oc2ccc(CC(=O)OCC(=O)N(C)C)cc2.S(=O)(=O)(O)C</chem>	C21H26N4O8S	494.518	Camostat Mesilate
Selleck Chemicals	S2454	<chem>c1c(C)c(NC(=O)C2CCCCN2CCCC)c(C)cc1.Cl</chem>	C18H29ClN2O	324.889	Bupivacaine HCl
Selleck Chemicals	S2890	<chem>c1ccc(CNc2nc(Nc3cc4c(NC(=O)C4)cc3)ncc2C(F)(F)F)c(N(S(C(=O)O)O)C)n1</chem>	C21H20F3N7O3S	507.489	PF-562271
Selleck Chemicals	S2538	<chem>CC(Nc1ccccc1)=O</chem>	C8H9NO	135.163	Acetanilide
Selleck Chemicals	S2901	<chem>c1(F)ccc(CN2C(=O)SN(c3ccc(C)cc3)C2=O)cc1</chem>	C16H13FN2O2S	316.35	CCG 50014
Selleck Chemicals	S2590	<chem>c1(CC)cnc(CCOc2ccc(CC3SC(=O)NC3=O)cc2)cc1</chem>	C19H20N2O3S	356.439	Pioglitazone
Selleck Chemicals	S2911	<chem>c1(OC)cc2c(n(CCCN(C)C)cc2C3=C(c4c[nH]c5c4cccc5)C(=O)NC3=O)cc1</chem>	C26H26N4O3	442.51	Go 6983
Selleck Chemicals	S2693	<chem>c1cc(CN(C)C)ccc1S(=O)(=O)n2cc(C=CC(=O)NO)cc2</chem>	C16H19N3O4S	349.405	Resminostat
Selleck Chemicals	S2921	<chem>c1(cnn(C)c1c2ccc(C)cc2)c3nn(C)c4c3c(N5CC[C@H](N6CCCC6)C5)ncn4</chem>	C26H32N8	456.586	PF-4981517
Selleck Chemicals	S2806	<chem>c1(N2CCN(C)CC2)cc(Nc3nn4c(c(c5ccc(S(=O)(C)=O)cc5)ccc4)n3)ccc1</chem>	C24H26N6O2S	462.567	CEP-33779
Selleck Chemicals	S3002	<chem>c1cc(N2CCOCC2=O)ccc1N3CC(CNC(=O)c4ccc(Cl)s4)OC3=O</chem>	C19H18ClN3O5S	435.881	Rivaroxaban
Selleck Chemicals	S2821	<chem>[C@@]([H])(C(=O)O)(Cc1c[nH]c2c1cccc2)N3C(=O)c(c4C3=O)cccc4</chem>	C19H14N2O4	334.325	RG108
Selleck Chemicals	S3042	<chem>c(n(C1CCCC1)cn2)(nc(Oc3cccc4c3cccc4)nc5Nc6ccc(N7CCOCC7)cc6)c25</chem>	C31H32N6O2	520.625	Purmorphamine
Selleck Chemicals	S2843	<chem>c1(O)c(F)cc(Nc2ncc3c(N(CCC(C)C)C(C)C(=O)N3C)n2)cc1F</chem>	C19H23F2N5O2	391.415	BI-D1870

Selleck		<chem>C(N)(NC(C)=C(C(OC(C)C)=O)C1c2cccc([N+])([O-])=O)c2)=C1C(O C3CN(C(c4cccc4)c5cccc5)C3)=O</chem>	<chem>C33H34N4O6</chem>	582.646	Azelinidipine
Chemicals	S3053				
Selleck		<chem>c(ccc(C)C1)(sc(S(Nc2ccc(OC)c(N3CCNCC3)c2)(=O)=O)c4C)c14</chem>	<chem>C20H22ClN3O3S2</chem>	451.99	SB271046
Chemicals	S2856				
Selleck		<chem>C(=O)c1ccc(O)c(OC)c1</chem>	<chem>C8H8O3</chem>	152.147	Vanillin
Chemicals	S3071				
Selleck		<chem>c1c(O)c(C(=O)Nc2cc(C(F)(F)F)cc(C(F)(F)F)c2)cc(Cl)c1</chem>	<chem>C15H8ClF6NO2</chem>	383.673	IMD 0354
Chemicals	S2864				
Selleck		<chem>N1c(c2C=CC1=O)c(O)ccc2[C@@H](O)CNC3Cc(c4C3)cc(Cc(C)CC)c4.C(=CC(O)=O)C(O)=O</chem>	<chem>C28H32N2O7</chem>	508.563	Indacaterol Maleate
Chemicals	S3083				Dovitinib (TKI-258, CHIR-258)
Selleck		<chem>c1c2c(C(N)=C(c3nc4c(cc(N5CCN(C)CC5)cc4)[nH]3)C(=O)N2)c(F)cc1</chem>	<chem>C21H21FN6O</chem>	392.429	
Chemicals	S1018				
Selleck		<chem>c1(CN(C(CCCC)=O)[C@]([H])([H])(C(O)=O)C(C)C)ccc(c2c(c3n[nH]nn3)cccc2)c1</chem>	<chem>C24H29N5O3</chem>	435.519	Valsartan
Chemicals	S1894				
Selleck		<chem>c1(NS(c2cccc2OC)(=O)=O)cc3c(NC(=O)N(C)C3)cc1</chem>	<chem>C16H17N3O4S</chem>	347.389	PFI-1 (PF-6405761)
Chemicals	S1216				
Selleck		<chem>c1(ccccc1C(=O)O)Nc2c(C)c(Cl)ccc2</chem>	<chem>C14H12ClNO2</chem>	261.704	Tolfenamic Acid
Chemicals	S1959				
Selleck		<chem>c1c(C2C(C(=O)O)CCOC)=C(C)NC(C)=C2C(=O)OCC=Cc3cccc3)cc([N+])([O-])=O)c1</chem>	<chem>C27H28N2O7</chem>	492.52	Cilnidipine
Chemicals	S1293				
Selleck		<chem>OC(=O)C=CC(=O)O.c1cc(C[C@H](C)NC[C@@H](O)c2cc(NC=O)c(O)cc2)ccc1OC.c3cc(C[C@H](C)NC[C@@H](O)c4cc(NC=O)c(O)cc4)ccc3OC</chem>	<chem>C42H52N4O12</chem>	804.882	Formoterol Hemifumarate
Chemicals	S2020				
Selleck		<chem>c1(N2CCN(C(C=O)CC2)ccc(O[C@H]3CO[C@@](c4c(Cl)cc(Cl)cc4)(Cn5cncc5)O3)cc1</chem>	<chem>C26H28Cl2N4O4</chem>	531.431	Ketoconazole
Chemicals	S1353				
Selleck		<chem>c1(OC)cc2c(CN(C[C@@H](N[C@@H](CCc3cccc3)C(OCC)=O)C)=O)[C@@H](C(=O)O)C2)cc1OC.Cl</chem>	<chem>C27H35ClN2O7</chem>	535.029	Moexipril HCl
Chemicals	S2079				
Selleck		<chem>c1(CS(=O)(=O)NC)cc2c([nH]cc2CCN(C)C)cc1.Oc(=O)CCC(=O)O</chem>	<chem>C18H27N3O6S</chem>	413.488	Sumatriptan Succinate
Chemicals	S1432				
Selleck		<chem>c1cc2c(C[C@@H]2NCC#C)cc1.O=S(O)(C)=O</chem>	<chem>C13H17NO3S</chem>	267.344	Rasagiline Mesylate
Chemicals	S2102				
Selleck		<chem>n1(c(C(=O)O)CC2=C(C)OC(=O)O2)c(C(C)C(O)nc1CCC)Cc3ccc(c4c(c5nn[nH]n5)cccc4)cc3</chem>	<chem>C29H30N6O6</chem>	558.585	Olmesartan Medoxomil
Chemicals	S1604				
Selleck		<chem>[nH]1c2c(cc(C(F)(F)F)cc2)nc1CN3CCN(c4c(CC)cncn4)CC3</chem>	<chem>C19H21F3N6</chem>	390.405	PF-4708671
Chemicals	S2163				
Selleck		<chem>c1c2c([nH]cc2CCN(C)C)ccc1C[C@H]3COc(=O)N3</chem>	<chem>C16H21N3O2</chem>	287.357	Zolmitriptan
Chemicals	S1649				
Selleck		<chem>c1(O)c2c([n-]c(S(=O)Cc3c(C)c(O)C)c(C)n3)n2)cc1.[Na+]</chem>	<chem>C17H18N3NaO3S</chem>	367.398	Esomeprazole Sodium
Chemicals	S2233				
Selleck		<chem>C1CC(NC(=O)NS(=O)(=O)c2ccc(CCNC(=O)c3cc(Cl)ccc3OC)cc2)CCC1</chem>	<chem>C23H28ClN3O5S</chem>	494.004	Glyburide
Chemicals	S1716				
Selleck		<chem>c(c(CN(C)C)c[nH]1)(cccc2)c12</chem>	<chem>C11H14N2</chem>	174.242	Gramine
Chemicals	S2304				
Selleck		<chem>c1cc(C(=C(CCl)c2cccc2)c3cccc3)ccc1OCCN(C)C.Oc(=O)CC(O)(C(O)=O)CC(O)=O</chem>	<chem>C32H36ClNO8</chem>	598.083	Toremifene Citrate
Chemicals	S1776				
Selleck		<chem>c1c(O)c2c(O[C@H](c3cc(O)cc(O)C3)CC2=O)cc1O[C@H]4[C@@H](O)[C@@H]5[C@@H](O)[C@H](O)[C@@H](O)[C@H](O)5][C@@H](O)[C@H](O)[C@@H](CO)O4</chem>	<chem>C28H34O15</chem>	610.561	Neohesperidin
Chemicals	S2332				
Selleck		<chem>c1(C)[nH]cnc1CSCCN(C)C(=NC#N</chem>	<chem>C10H16N6S</chem>	252.339	Cimetidine
Chemicals	S1845				
Selleck		<chem>c1cc(CCC(=O)C)cc(OC)c1O</chem>	<chem>C11H14O3</chem>	194.227	Vanillylacetone
Chemicals	S2371				
Selleck		<chem>[C@H]1(O)[C@@H](O)[C@@H](O)[C@H](O)[C@H]2[C@]3([H])[C@]([H])(CC=C3CO)C(C(OC)=O)=CO2)O[C@@H]1CO</chem>	<chem>C17H24O10</chem>	388.366	Geniposide
Chemicals	S2411				
Selleck		<chem>c1(C(=O)NC2CCN(CCCOC)CC2)cc(Cl)c(N)c3c1OCC3</chem>	<chem>C18H26ClN3O3</chem>	367.87	Prucalopride
Chemicals	S2875				
Selleck		<chem>c1cc([N+])(=O)[O-])cc(C2C(C(OC)=O)=C(C)NC(C)=C2C(OCC)=O)c1</chem>	<chem>C18H20N2O6</chem>	360.361	Nitrendipine
Chemicals	S2491				
Selleck		<chem>c1(C(Nc2ccc(Cl)c(O)C2)=O)ncccc1</chem>	<chem>C13H11ClN2O2</chem>	262.692	VU 0361737
Chemicals	S2892				
Selleck		<chem>c1cc(O)c([C@H](CCN(C(C)C)C(C)C)c2cccc2)cc1C.O=C([C@H](O)[C@@H](O)C(=O)O)O</chem>	<chem>C26H37NO7</chem>	475.574	Tolterodine tartrate
Chemicals	S2550				S-Ruxolitinib
Selleck		<chem>n1cnc(c2cnn([C@@H](CC#N)C3CCCC3)c2)c4c1[nH]cc4</chem>	<chem>C17H18N6</chem>	306.365	(INCB018424)
Chemicals	S2902				
Selleck		<chem>c1cc2c(C(=O)O)nn2Cc3ccc(Cl)cc3Cl)cc1</chem>	<chem>C15H10Cl2N2O2</chem>	321.158	Londamine
Chemicals	S2610				
Selleck		<chem>c1(CNc2cccc2)ccc(CNc3cccc3)cc1</chem>	<chem>C18H18N4</chem>	290.362	WZ811
Chemicals	S2912				

Selleck							
Chemicals	S2694	c1cc2c([nH]c3c2C(C)(C)CN(C(=O)c4cc(F)c(F)cc4)C=C3C(OC(C)C)=O)cc1	C25H24F2N2O3	438.466	XL335		
Selleck							
Chemicals	S2922	c1c(Nc2c3c(cc4c(OCOCOCOCOC4)c3)ncn2)cccc1C#C	C22H21N3O4	391.42	Icotinib		
Selleck							
Chemicals	S2809	c1(C)nc(C#Cc2ccccc2)ccc1	C14H11N	193.244	MPEP		
Selleck		[C@H]1(NC([C@H](N)c2ccc(O)cc2)=O)[C@@]3([H])N([C@H](C(O)=O)C(C)(C)S3)C1=O	C16H19N3O5S	365.404	Amoxicillin		
Selleck							
Chemicals	S2822	c1(F)cc2c(n(CC(=O)O)c(C)c2Cc3nc4c(cccc4)cc3)cc1	C21H17FN2O2	348.37	OC000459		
Selleck							
Chemicals	S3043	c1cc(C(COC2=O)=C2c3ccccc3)ccc1S(=O)(=O)C	C17H14O4S	314.356	Rofecoxib		
Selleck							
Chemicals	S2845	c1cc2c(NC(=O)C2=Cc3c(C)cc(C)[nH]3)cc1	C15H14N2O	238.284	Semaxanib (SU5416)		
Selleck							
Chemicals	S3054	c1(CCCN(CC)CCCc2ccccc2)ccccc1.C(C(O)=O)C(O)(C(O)=O)CC(O)=O	C26H35NO7	473.559	Alverine Citrate		
Selleck							
Chemicals	S2857	c(cccc1)(C[C@@H](N[C@]23C)c4c2ccccc4)c13	C16H15N	221.297	MK-801 (Dizocilpine)		
Selleck		[C@@H]1(O)C[C@]2([H])N(C(=O)[C@]([H])([C@H](O)C)NC(=O)[C@@H](NC(=O)CCCCCCC[C@H](C)C[C@H](C)CC)[C@H](O)[C@H](NCN)NC(=O)[C@@]3([H])N(CC[C@H]3O)C(=O)[C@@]([H])([C@H](O)CCN)NC(=O)[C@]([H])([C@H]([C@H](c4ccc(O)cc4)O)O)NC2=O)C1.C(C(O)=O.CC(O)=O	C56H96N10O19	1213.417	Caspofungin Acetate		
Chemicals	S3073						
Selleck							
Chemicals	S2865	c1cc2c(nc(Cl)c(N3CCN(C)CC3)n2)cc1	C13H15ClN4	262.738	VUF 10166		
Selleck							
Chemicals	S3100	N1C=CC(=O)NC1=S	C4H4N2OS	128.152	2-Thiouracil		
Selleck		N1(C(N2CC(=O)NCC2)=O)C(c3ccc(OC)cc3OC(C)C)=NC(c4ccc(Cl)cc4)C1c5ccc(Cl)cc5	C30H30Cl2N4O4	581.49	Nutlin-3		
Chemicals	S1061						
Selleck							
Chemicals	S1897	[K+].[I-]	IK	166.003	Potassium Iodide		
Selleck		c1c(OC)c2c(C(=O)c3c(c(O)c4c(C[C@@](O)(C(=O)CO)C[C@H]4O[C@]5([H])O[C@@H](C)[C@H](O)[C@@H](N)C5)c3O)C2=O)cc1.Cl	C27H30ClNO11	579.98	Epirubicin HCl		
Chemicals	S1223						
Selleck							
Chemicals	S1960	c1cc2c(OC3c(cc(C(C)C(=O)O)cc3)C2)nc1	C15H13NO3	255.269	Pranoprofen		
Selleck							
Chemicals	S1305	N(C(=S)c1c(nc[nH]1)N2)=C2	C5H4N4S	152.177	Mercaptopurine (6-MP)		
Selleck							
Chemicals	S2025	N1(C)C(=O)C=C(NCCCN2CCN(c3c(OC)ccccc3)CC2)N(C)C1=O.Cl	C20H30ClN5O3	423.937	Urapidil HCl		
Selleck							
Chemicals	S1357	c1c(C)c(NC(=O)CN(CC)CC)c(C)cc1	C14H22N2O	234.337	Lidocaine		
Selleck							
Chemicals	S2080	CCCC(=O)OCOC(=O)C(C(c1c(Cl)c(Cl)ccc1)C(C(=O)OC)=C(C)N2)=C2C	C21H23Cl2NO6	456.316	Clevidipine Butyrate		
Selleck							
Chemicals	S1436	c(cccc1)(N(C)S(=O)(=O)c2c(ccc(Cl)c2)C3NCCCCC([O-])=O)c13.[Na+]	C21H24ClN2NaO4S	458.934	Tianeptine sodium		
Selleck							
Chemicals	S2104	c1c(S(=O)(N)=O)cc(C(NC[C@@H]2CCCC2CC)=O)c(OC)c1	C15H23N3O4S	341.426	Levosulpiride		
Selleck							
Chemicals	S1608	c1[n+](C)cccc1OC(=O)N(C)C.[Br-]	C9H13BrN2O2	261.116	Pyridostigmine Bromide		
Selleck							
Chemicals	S2168	c1(O)cc2c(OC[C@@]3([H])[C@]2([H])OCCN3CCC)cc1	C14H19NO3	249.306	PD128907 HCl		
Selleck							
Chemicals	S1654	N1(c2ccccc2)C(=O)C(CCCC)C(=O)N1c3ccccc3	C19H20N2O2	308.374	Phenylbutazone		
Selleck		c1ccccc1[C@H](c2cc(CO)ccc2OC(=O)C(C)C)CCN(C(C)C)C(C)C.C(C(=O)O)=CC(=O)O	C30H41NO7	527.649	Fesoterodine Fumarate		
Chemicals	S2240						
Selleck		C1[C@@]2([H])C(CC[C@@]3([H])[C@@]2([H])CC[C@@]4(CC)[C@@]3([H])CC[C@@]4(C#C)O)=CC1=O	C21H28O2	312.446	Levonorgestrel		
Chemicals	S1727						
Selleck		C1[C@@]2(C)[C@@]([H])(CC[C@]3(C)[C@@]2([H])C[C@H](O)[C@@]4([H])[C@@]3(C)CC[C@H]4[C@@](CCC=C(C)C)(CO[C@H]5[C@@H](O)[C@@H](O)[C@H](O)[C@@H](CO[C@H]6[C@@H](O)[C@H]7C[C@H](O)[C@H](O)[C@H](O)[C@@H](CO)O7	C47H80O17	917.128	Gynostemma Extract		
Chemicals	S2306						
Selleck							
Chemicals	S1782	[C@H]1(O)[C@H](O)[C@H](N2C=NC(N)=NC2=O)O[C@@H]1CO	C8H12N4O5	244.205	Azaciditine		
Selleck							
Chemicals	S2333	c1(OC)c(OC)c2c(C(=O)C=C(c3ccc(OC)c(OC)c3)O2)c(OC)c1OC	C21H22O8	402.395	Nobiletin		
Selleck							
Chemicals	S1854	c1cc(C(n2ccnc2)c3ccc(c4ccccc4)cc3)ccc1	C22H18N2	310.392	Bifonazole		

Selleck					
Chemicals	S2372	<chem>c1cc2c(Oc3c(cccc3)C2=O)cc1</chem>	C13H8O2	196.201	Xanthone
Selleck					
Chemicals	S2425	<chem>c1(OC)c(O)ccc(C(=O)C)c1</chem>	C9H10O3	166.174	Apocynin
Selleck					
Chemicals	S2876	<chem>[C@]1(C)(N[C@]2([H])c3c1cccc3)c4c(cccc4)C2.C(C(=O)O)=CC(=O)O</chem>	C20H19NO4	337.369	(-)-MK 801 Maleate
Selleck					
Chemicals	S2516	<chem>c1c(C)c(NC2=NCCCS2)c(C)cc1.Cl</chem>	C12H17ClN2S	256.795	Xylazine HCl
Selleck					
Chemicals	S2894	<chem>c1c(S(=O)(=O)c2cc(c3nc2)cccc3N4CCNCC4)cccc1</chem>	C19H19N3O2S	353.438	SB742457
Selleck					
Chemicals	S2551	<chem>C1(=O)N2[C@]([H])(S(=O)(=O)C(C)(C)[C@]2(C(=O)[O-])[H])C1.[Na+]</chem>	C8H10NNaO5S	255.223	Sulbactam sodium
Selleck					
Chemicals	S2903	<chem>c1c(Cl)c(Nc2c(CC(=O)O)cc(C)cc2)c(F)cc1</chem>	C15H13ClFNO2	293.721	Lumiracoxib
Selleck					
Chemicals	S2625	<chem>c1(OC)cc(Nc2nc(Nc3nc4c(O C(C)(C)C(=O)N4COP(=O)(O)O)cc3)c(F)cn2)c c(OC)c1OC</chem>	C23H26FN6O9P	580.46	Fostamatinib (R788)
Selleck					
Chemicals	S2913	<chem>c1(ccc(C)cc1)S(=O)(=O)C=CC#N</chem>	C10H9NO2S	207.249	BAY 11-7082
Selleck					
Chemicals	S2698	<chem>c1c(c2nc(N)nc(C(C)C)c2)c3c(cccc3)c(F)c1</chem>	C17H16FN3	281.327	RS-127445
Selleck					
Chemicals	S2923	<chem>c1(nccc2)c2cccc1NC(=S)NC(C(Cl)(Cl)Cl)NC(=O)C=Cc3cccc3</chem>	C21H17Cl3N4OS	479.81	Salubrial
Selleck					
Chemicals	S2812	<chem>c1(O)c(c2cc(C)c1c3c(C)cc(c4c3O)c(C(C)C)c(O)c(O)c4C=O)c(C=O)c(O)c(O)c2C(C)C.C(O)(=O)C</chem>	C32H34O10	578.606	AT101
Selleck					
Chemicals	S3033	<chem>C1CC[C@H](C#N)N1C(=O)CNC2(CC(O)(CC3C2)CC4C3)C4</chem>	C17H25N3O2	303.399	Vildagliptin (LAF-237)
Selleck					
Chemicals	S2824	<chem>c1(NC(N)=O)sc(c2ccc(F)cc2)cc1C(N)=O</chem>	C12H10FN3O2S	279.29	TPCA-1
Selleck					
Chemicals	S3045	<chem>N1(CC(N2CCCC2)=O)CCN(C(=O)C=Cc3cc(OC)c(O C)c(OC)c3)CC1.C(=O)(O)C=CC(=O)O</chem>	C26H35N3O9	533.571	Cinepazide maleate
Selleck					
Chemicals	S2847	<chem>n1(C)c(C(N[C@@H](Cc2cccc(Cl)c2)C(NCC#N)=O)=O)cc(C(C)C)C)n1</chem>	C20H24ClN5O2	401.89	Cathepsin Inhibitor 1
Selleck					
Chemicals	S3057	<chem>c1(OCC)n(Cc2ccc(c3cccc3C4=NC(=O)ON4)cc2)c5c(cccc5C(OC)C6=C(C)OC(=O)O6)=O)n1</chem>	C30H24N4O8	568.534	Azilsartan Medoxomil
Selleck					
Chemicals	S2858	<chem>c1(O)ccc(CCNc2c(c3nc(c4csc5c4cccc5)n2)ncn3C(C)C)cc1</chem>	C24H23N5OS	429.537	StemRegenin 1 (SR1)
Selleck					
Chemicals	S3075	<chem>c1ccc(C)c(C)c1[C@H](C)c2cnc[nH]2</chem>	C13H16N2	200.28	Dexmedetomidine
Selleck					
Chemicals	S2866	<chem>N(c1ccc(F)cc1)C(=O)Nc2ccc(S(=O)(=O)N)cc2</chem>	C13H12FN3O3S	309.316	U-104
Selleck					
Chemicals	S3104	<chem>c1cccc(OC)c1OCC2SCCN2C(CC(=O)OCC)=O</chem>	C16H21NO5S	339.407	Moguisteine
Selleck					
Chemicals	S1121	<chem>c1c(C(C)(C)C)c(S(=O)(=O)c2ccc(NC(=O)C3cc(C4c(C)C)cccc4)c(O)c(O)c3O)cc2)ccc1</chem>	C33H35NO6S	573.699	TW-37
Selleck					
Chemicals	S1905	<chem>N1C(C)=C(C(OC)=O)C(c2ccccc2Cl)C(C(=O)OCC)=C1COCCN</chem>	C20H25ClN2O5	408.876	Amlodipine
Selleck					
Chemicals	S1228	<chem>c1cc2c(C(=O)C3c(c(O)c4c(C[C@@](O)(C(=O)C)C[C@H]4O[C@H]5C[C@H](N)[C@H](O)[C@H](C)O5)c3O)C2=O)cc1.Cl</chem>	C26H28ClNO9	533.955	Idarubicin HCl
Selleck					
Chemicals	S1972	<chem>c1(OCCN(C)C)ccc(C(c2ccccc2)=C(c3ccccc3)CC)cc1.C(O)(=O)CC(O)(C(O)=O)CC(O)=O</chem>	C32H37NO8	563.638	Tamoxifen Citrate
Selleck					
Chemicals	S1319	<chem>C1C=C(C)CC[C@H]2[C@H](OC(=O)C2=C)C=C(C)C1</chem>	C15H20O2	232.318	Costunolide
Selleck					
Chemicals	S2037	<chem>C1CC(O C(=O)O C(C)O C(c2c3c(nc(OCC)n3Cc4ccc(c5cccc5c6[nH]nnn6)cc4)ccc2)=O)CCC1</chem>	C33H34N6O6	610.66	Candesartan Cilexetil Losartan Potassium (DuP 753)
Selleck					
Chemicals	S1359	<chem>c1c(c2cccc2c3nn[nH]3)ccc(Cn4c(CCCC)nc(Cl)c4CO)c1.[K]</chem>	C22H23ClKN6O	462.009	
Selleck					
Chemicals	S2081	<chem>c1ccc(CC[C@H](C(OC)C)=O)N[C@H]2C(=O)N3N(CCC[C@H]3C(=O)O)CCC2)cc1.O</chem>	C22H33N3O6	435.514	Cilazapril Monohydrate
Selleck					
Chemicals	S1468	<chem>C1C(=CC=C2CC[C@]3(C)[C@@]2([H])C[C@H]3[C@H](C)CCCC(C)C)C(=C)[C@H]1(O)C[C@H]1O</chem>	C27H44O2	400.637	Alfacalcidol
Selleck					
Chemicals	S2108	<chem>c1(Nc2ccc(C(F)(F)F)c2)ncccc1C(O)=O.N(C)C[C@H]([C@H]([C@@H]([C@@H](CO)O)O)O)O</chem>	C21H28F3N3O7	491.458	Flunixin Meglumine
Selleck					
Chemicals	S1609	<chem>N1C(=S)N(C)C=C1</chem>	C4H6N2S	114.169	Methimazole
Selleck					
Chemicals	S2169	<chem>[Ca+2].n1c(C(C)C)c(C=C[C@H](C[C@@H](O)CC(=O)[O-])O)c(c2ccc(F)cc2)nc1N(C)S(=O)(=O)C.n3c(C(C)C)c(C=C[C@H](C[C@@H](O)CC(=O)[O-])O)c(c4ccc(F)cc4)nc3N(C)S(=O)(=O)C</chem>	C44H54CaF2N6O12S	1001.137	Rosuvastatin Calcium

Selleck Chemicals	S1657	<chem>c1cc(Cc1C@H)(N[C@@H](C)C(=O)N2CCC[C@H]2C(O)=O)C(=O)O)ccc1.O.O</chem>	C18H28N2O7	384.424	Enalaprilat Dihydrate
Selleck Chemicals	S2250	<chem>c1(O)cc(C(=O)O)[C@@H]2Cc3c(cc(O)cc3O)O[C@@H]2c4cc(O)c(O)c(O)c4)cc(O)c1O</chem>	C22H18O11	458.372	(-)-Epigallocatechin Gallate
Selleck Chemicals	S1740	<chem>c1ccc(OC(C(O)CO)c(OC)c1</chem>	C10H14O4	198.216	Guaifenesin
Selleck Chemicals	S2313	<chem>c1c2c([nH]cc2CO)ccc1</chem>	C9H9NO	147.174	Indole-3-carbinol
Selleck Chemicals	S1801	<chem>N(C)(C)Cc1cc(CSCCNC(NC)=C[N+](O-)=O)cc1.Cl</chem>	C13H23ClN4O3S	350.865	Ranitidine
Selleck Chemicals	S2336	<chem>C(C(=O)NC(=O)N1)=C1C(=O)O[C@@H](O)([C@@H](O)C(=O)O)C(=O)O.O.c1cc(OC(C(O)CNC(C)C)ccc1C</chem>	C5H4N2O4	156.096	Orotic acid (6-Carboxyuracil)
Selleck Chemicals	S1856	<chem>CO.C.c2cc(OC(C(O)CNC(C)C)ccc2CCOC[C@@]1(C(=O)O)(C)C[C@]2([H])([C@@](C)(CC[C@]3(C)C2=CC(=O)[C@@]4([H])(C@@]3(C)CC[C@]5([H])(C@@]4(C)CC[C@H](O)[C@@]6([H])(C@@]@H)(O)[C@]7([H])O[C@H](C(=O)=O)[C@@H](O)[C@H](O)[C@H]7O)[C@@]@H)(O)[C@H](O)[C@@H](C(=O)O)O6)C5(C)C)CC1.N</chem>	C34H56N2O12	684.815	Metoprolol Tartrate
Selleck Chemicals	S2376	<chem>C42H65NO16</chem>		839.963	Ammonium Glycyrhizinate
Selleck Chemicals	S2439	<chem>c1(N=C(N)NC2=O)c2ncn1[C@H]3[C@H](O)[C@H](O)[C@H](CO)O3</chem>	C10H13N5O5	283.241	Guanosine
Selleck Chemicals	S2882	<chem>c1(C1N2CCC(N3CCCC3)CC2)=O)ccc(Nc4nccc(c5sc6c(cccc6)c5)n4)cc1</chem>	C28H29N5OS	483.628	IKK-16 (IKK Inhibitor VII)
Selleck Chemicals	S2519	<chem>c1(cccc2)c2c(CC(NCC3)=N3)ccc1.Cl</chem>	C14H15ClN2	246.735	Naphazoline HCl
Selleck Chemicals	S2895	<chem>c1(C(C)(C)C)cc(C=C(C#N)C#N)cc(C(C)(C)C)c1O</chem>	C18H22N2O	282.38	Tyrphostin 9
Selleck Chemicals	S2553	<chem>NCC(=O)CCC(=O)O.O.Cl</chem>	C5H10ClNO3	167.591	5-Aminolevulinic acid HCl
Selleck Chemicals	S2904	<chem>c1c2c(c3C=NNC2=O)c([nH]c3c4cn(C)nc4)cc1NC(=O)[C@H](N)C5CCCCC5</chem>	C22H25N7O2	419.48	PF-477736
Selleck Chemicals	S2637	<chem>c1ccc(COc2cc3c([C@H](CC(O)=O)CO3)cc2)cc1c4c(C)cc(OC(CS(=O)O)(C)=O)cc4C.O.c5ccc(COc6cc7c([C@H](CC(O)=O)CO7)cc6)cc5c8c(C)cc(OC(CS(=O)O)(C)=O)cc8C</chem>	C58H66O15S2	1067.266	TAK-875
Selleck Chemicals	S2914	<chem>n1c(Nc2c(C)cc(C)cc2C)ccnc1Nc3ccc(C#N)cc3</chem>	C20H19N5	329.398	Dapivirine (TMC120)
Selleck Chemicals	S2721	<chem>C1(C)=C(C(O(C(C)C)=O)C)c2cc([N+](O-))=O)ccc2C(C(=O)O)C=C(C#N)N1</chem>	C19H19N3O6	385.371	Nilvadipine
Selleck Chemicals	S2925	<chem>c1(C(F)(F)F)cc(CN(c2nn(C)nn2)[C@]3([H])c4c(c(C)cc(C)c4)N(C[C@]5([H])CC[C@]6([H])(C(=O)O)CC5)CCC3)cc(C(F)(F)F)c1</chem>	C31H36F6N6O2	638.647	Evacetrapib (LY2484595)
Selleck Chemicals	S2813	<chem>C(C1CC1)(c2ccc(OC(Cc3[nH]cn3)cc2)=O.O)(C(=O)C=CC(O)=O</chem>	C20H22N2O6	386.398	Ciproxifan
Selleck Chemicals	S3034	<chem>c1(C(Cc2c(C)cc(c3c2)OCO3)=O)sccc1S([N-]c4onc(C)c4Cl)(=O)=O.[Na+]</chem>	C18H14ClN2NaO6S2	476.886	Sitaxentan sodium
Selleck Chemicals	S2825	<chem>c1ccc2c(cccc2CNc3ccc(OC)cc3)c1.Cl</chem>	C19H20ClNO	313.821	ML133 HCl
Selleck Chemicals	S3046	<chem>c1(OC)n(Cc2ccc(c3ccccc3C4=NC(=O)ON4)cc2)c5c(cccc5C(O)=O)n1</chem>	C25H20N4O5	456.45	Azilsartan
Selleck Chemicals	S2849	<chem>N1(S(c2cccc(O)c2)(=O)=O)CCC[C@@H]1CCN3CCC(C)CC3.Cl</chem>	C18H29ClN2O3S	388.952	SB269970 HCl
Selleck Chemicals	S3060	<chem>c1(C(C)c2c([nH]cn2)cccc(C)c1C.Cl</chem>	C13H17ClN2	236.74	Medetomidine HCl
Selleck Chemicals	S2859	<chem>c1c(F)c(NC(=O)C2(CC2)C(=O)Nc3ccc(F)cc3)ccc1Oc4ccnc(NC(=O)N5CCC(N6CCN(C)CC6)CC5)c4</chem>	C33H37F2N7O4	633.688	Golvatinib (E7050)
Selleck Chemicals	S3076	<chem>P(=O)([O-])([O-])C([O-])=O.[Na+].[Na+].[Na+]</chem>	ClNa3O5P	191.951	Foscarnet Sodium
Selleck Chemicals	S2867	<chem>n1c(c2c(Nc3ccc(O)c(Br)c3)nc1)cc(OC)c(OC)c2</chem>	C16H14BrN3O3	376.205	WHI-P154
Selleck Chemicals	S3105	<chem>c1(cc(F)c2N3CCC(O)CC3)c(N4C=C(C(O)=O)C1=O)c2CCC4C</chem>	C19H21FN2O4	360.379	Nadifloxacin
Selleck Chemicals	S1138	<chem>c([nH]c(C)c1)(ccc(Oc2c3n(cc(O[C@H](O(C(=O)[C@H](C)N)C)c3C)ncn2)c4F)c14</chem>	C22H24FN5O4	441.455	Brivanib Alaninate (BMS-582664)
Selleck Chemicals	S1913	<chem>c1cc(C(C(N(Cc2ccnc2)CC)=O)CO)ccc1</chem>	C17H20N2O2	284.353	Tropicamide
Selleck Chemicals	S1235	<chem>c1c(C(c2ccc(C#N)cc2)n3cncn3)ccc(C#N)c1</chem>	C17H11N5	285.303	Letrozole
Selleck Chemicals	S1973	<chem>C(N1C(O[C@H]2[C@H]1O[C@H](CO)[C@@H]2O)=NC3=N=C3.Cl</chem>	C9H12ClN3O4	261.662	Cyclocytidine HCl

Selleck		<chem>C1=C[C@@]2(C)C(C)[C@]3([H])[C@@]2(F)[C@H](O)C[C@@]4(C)[C@@]3([H])[C@H](C)[C@@]4(O)C(CO)=O)=CC1=O</chem>	C22H29FO5	392.461	Dexamethasone (DHAP)
Chemicals	S1322				
Selleck					
Chemicals	S2041	<chem>c1cc(C(=O)CCN2CCCCC2)ccc1OCCCC.Cl</chem>	C18H28ClNO2	325.873	Dyclonine HCl
Selleck					
Chemicals	S1362	<chem>c1(C=CS(=O)(=O)Cc2cc(NCC(=O)[O-])c(OC)cc2)c(OC)cc(OC)cc1O.[Na+]</chem>	C21H24NNaO8S	473.472	Rigosertib (ON-01910)
Selleck					
Chemicals	S2082	<chem>C(=O)(OCCN(CC)CC)C(c1cccc1)c2cccc2.Cl</chem>	C20H26ClNO2	347.879	Adiphenine HCl
Selleck					
Chemicals	S1469	<chem>C1C(=CC=C2CC[C@]3(C)[C@@]2([H])CC[C@]3([H])[C@H](C)CCC(C(O)(C)C)C(=C)CC[C@H]1O</chem>	C27H44O2	400.637	Calcifediol
Selleck					
Chemicals	S2109	<chem>CCO[C](C@H)(CCc1cccc1)N[C@@H](C)C(=O)N2[C@@H](C(O)=O)CN(C)C2=O=O</chem>	C20H27N3O6	405.445	Imidapril HCl
Selleck					
Chemicals	S1611	<chem>C1(CSc2n(C)mn2)=C(C(O)=O)N3[C@@]([H])([C@H](NC([C@H](NC(=O)N4CCN(CC)C(=O)C4=O)c5ccc(O)cc5)=O)C3=O)SC1</chem>	C25H27N9O8S2	645.667	Cefoperazone
Selleck					
Chemicals	S2173	<chem>c1cc(c2nc(N)nc(O[C@@H](C(F)(F)F)c3c(n4ccc(C)n4)cc(Cl)cc3)c2)ccc1C[C@H](N)C(=O)OCC.c5cc(C(=O)NCC(=O)O)ccc5</chem>	C36H35ClF3N7O6	754.155	Telotristat Etiprate (LX 1606 Hippurate)
Selleck					
Chemicals	S1675	<chem>C1(=O)[C@@H](CCCCC(=O)O)[C@@H](CCC(=O)C(F)(F)CCCC)[C@H](O)C1</chem>	C20H32F2O5	390.462	Lubiprostone
Selleck					
Chemicals	S2258	<chem>c1(O)cc2c(C=CC(=O)O2)cc1O[C@H]3[C@@H](O)[C@H](O)[C@H](O)[C@@H](CO)O3</chem>	C15H16O9	340.282	Esculin
Selleck					
Chemicals	S1748	<chem>C(C)(NC(C)=C(C(=O)OC)C1c2c([N+])([O-])=O)cccc2)=C1C(=O)OCC(C)C</chem>	C20H24N2O6	388.414	Nisoldipine
Selleck					
Chemicals	S2316	<chem>c(nc[nH]1)(ncnc2NCc3ccc3)c12</chem>	C10H9N5O	215.211	Kinetin
Selleck					
Chemicals	S1805	<chem>CC(=O)OCC([N+](C)(C)C.[Cl-])C(c1ccc(O)c(O)c1)(Oc2c(c(O)cc(O)c2)C3=O)=C3O[C@H]4[C@@H](O)[C@@H](O)[C@H](O)[C@@H](CO[C@H]5[C@@H](O)[C@H](O)[C@@H](O)[C@H](CO5)O4</chem>	C7H16ClNO2	181.66	Acetylcholine Chloride
Selleck					
Chemicals	S2350	<chem>c1(cccc2c2S[C@@H](c3ccc(OC)cc3)[C@@H](OC(=O)C)C(=O)N1CCN(C)C.Cl</chem>	C27H30O16	610.518	Rutin
Selleck					
Chemicals	S1865		C22H27ClN2O4S	450.979	Diltiazem HCl
Selleck					
Chemicals	S2383	<chem>[C@@H]1(O)[C@H](CO)O[C@@H](Oc2ccc(CO)cc2)[C@H](O)[C@H]1O</chem>	C13H18O7	286.278	Gastrodin
Selleck					
Chemicals	S2442	<chem>O1[C@H](n2cnc3c2N=CNC3=O)[C@H](O)[C@H](O)[C@H]1CO</chem>	C10H12N4O5	268.226	Inosine
Selleck					
Chemicals	S2883	<chem>C(O)(=O)CNC(c1ccc(N)cc1)=O</chem>	C9H10N2O3	194.187	4-Aminhippuric Acid
Selleck					
Chemicals	S2521	<chem>c1(O)cc([C@H](CNC)O)ccc1O.C(O)(=O)[C@@H]([C@H](C(O)=O)O)O</chem>	C13H19NO9	333.291	Epinephrine Bitartrate
Selleck					
Chemicals	S2896	<chem>c1(O)cc(Nc2c(c3ncn2)ccc(OCc4ccccc4)c3)c(F)cc1C.Cl</chem>	C22H19ClFN3O2	411.857	ZM 323881 HCl
Selleck					
Chemicals	S2573	<chem>c1cc(C(=O)OCCN(C)C)ccc1NCCCC.Cl</chem>	C15H25ClN2O2	300.824	Tetracaine HCl
Selleck					
Chemicals	S2905	<chem>c1(Cl)cc2c([nH]c(C(=O)N3CCN(C)CC3)c2)cc1</chem>	C14H16ClN3O	277.749	JNJ-7777120
Selleck					
Chemicals	S2662	<chem>c1ccc(CNC(=O)N2CCC(=O)N3[C@]2([H])CN(Cc4c5c(cccc5)ccc4)C(=O)[C@H]3Cc6ccc(O)cc6)cc1</chem>	C33H32N4O4	548.632	ICG-001
Selleck					
Chemicals	S2915	<chem>c1(C(=O)Nc2ccccc2)c(Cl)ccc([N+])([O-])=O)c1</chem>	C13H9ClN2O3	276.675	GW9662
Selleck					
Chemicals	S2769	<chem>N1c(c2C(N)=C(c3[nH]c4c(ccc(N5CCN(C)CC5)c4)n3)C1=O)cccc2F.CC(O)C(=O)O.CC(O)C(=O)O</chem>	C27H33FN6O7	572.585	Dolactac Acid
Selleck					
Chemicals	S2927	<chem>c(C(=O)C(=O)N1Cc2ccc(Cl)c(Cl)c2)(cccc3)c13</chem>	C15H9Cl2NO2	306.143	Apoptosis Activator 2
Selleck					
Chemicals	S2816	<chem>C(=S)(N)C(C#N)=Cc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1</chem>	C18H24N2OS	316.461	Tyrphostin AG 879
Selleck					
Chemicals	S3035	<chem>c1c(OC)C2c(C(=O)Cc3c(c(O)c4c(C[C@@]([C](=O)C)(O)C[C@H]4O[C@]5([H])O[C@@H](C)[C@@H](O)[C@@H](N(C)C5)c3O)C2=O)cc1.Cl</chem>	C27H30ClNO10	563.981	Daunorubicin HCl
Selleck					
Chemicals	S2828	<chem>N1(c2snc(c3ccccc3)n2)CCN(C(Nc4ccccc4)=O)CC1</chem>	C19H19N5OS	365.452	JNJ-1661010
Selleck					
Chemicals	S3047	<chem>C([N+](CC)(CC)C)CO C(=O)c1ccc(NC(=O)c2ccccc2OCCCCCCCC)cc1.[Br-]</chem>	C29H43BrN2O4	563.567	Otilonium Bromide
Selleck					
Chemicals	S2851	<chem>CCS(N1CC(n2ncc(c3ncnc(c34)[nH]cc4)c2)(CC#N)C1)=O=O</chem>	C16H17N7O2S	371.417	INC028050)
Selleck					
Chemicals	S3063	<chem>c1c(Cl)c(Nc2Cc(C(=O)O)cccc2)c(Cl)cc1.N(CC)CC</chem>	C18H22Cl2N2O2	369.285	Diclofenac Diethylamine
Selleck					
Chemicals	S2860	<chem>C(N)CCCCNCC1(CC(CC2C1)CC3C2)C3.Br.Br</chem>	C16H32Br2N2	412.247	IEM 1754 dihydrobroMide

Selleck		<chem>C1=C[C@@]2(C)C(CC[C@]3([H])[C@@]2(C)[C@H](O)C[C@@]4(C)[C@</chem>			Beclomethasone
Chemicals	S3078	<chem>@]3([H])C[C@H](C)[C@@]4(OC(CC)=O)C(=O)CO C(CC)=O)=CC1=O</chem>	C28H37ClO7	521.042	dipropionate
Selleck					
Chemicals	S2868	<chem>C(#N)c1cccc1CN2C(=O)N(C)C(=O)C=C2N3C[C@H](N)CCC3</chem>	C18H21N5O2	339.392	Alogliptin
Selleck					
Chemicals	S3106	<chem>S1C[C@H](C(O)=O)N(C)[C@H]2CCC(=O)N2=O)C1</chem>	C9H12N2O4S	244.268	Pidotimod
Selleck		<chem>c1c(C(O)[C@@H]2C([C@@]3(C)C(=O)[C@H](O)C(C([C@@]24O)(C)C)=C</chem>			
Chemicals	S1148	<chem>(C)[C@H](OC(=O)[C@H](O)[C@H](NC(=O)OC(C)(C)C)c5cccc5)C4)[C</chem>	C43H53NO14	807.879	Docetaxel
Selleck		<chem>@]6(OC(=O)C)[C@H](OC6)C[C@H]3O)=O)cccc1</chem>			
Chemicals	S1921	<chem>c1cc2c(C(=O)C(c3cccc3)C2=O)cc1</chem>	C15H10O2	222.239	Phenindione
Selleck					
Chemicals	S1252	<chem>N(C(=O)c1c(n([C@@H]2C(=C)[C@H](CO)[C@H](O)C2)cn1)N3)=C3N.O</chem>	C12H17N5O4	295.294	Entecavir Hydrate
Selleck					
Chemicals	S1983	<chem>c([nH]cn1)(ncnc2N)c12.Cl</chem>	C5H6ClN5	171.588	Adenine HCl
Selleck					
Chemicals	S1328	<chem>c1cc(CC)c2c(c3c([C@](CC)(CC(O)=O)OCC3)[nH]2)c1</chem>	C17H21NO3	287.354	Etodolac
Selleck					
Chemicals	S2046	<chem>c1(CC)cnc(CCOc2ccc(CC3SC(=O)NC3=O)cc2)cc1.Cl</chem>	C19H21ClN2O3S	392.9	Pioglitazone HCl
Selleck		<chem>C1(=O)N2[C@@]([H])([C@H](O)C(S[C@H]3C[C@H](CNS(=O)(=O)N)N</chem>			
Chemicals	S1374	<chem>C3)=C2C(O)=O)[C@]1([H])[C@H](O)C.O</chem>	C15H26N4O7S2	438.52	Doripenem Hydrate
Selleck					
Chemicals	S2085	<chem>c1(OC)cc(C(=O)OCC(N(C)C)(CC)c2ccccc2)cc(OC)c1OC</chem>	C22H29NO5	387.469	Trimebutine
Selleck		<chem>[C@H]1(N(C([C@H]2CC[C@H](C)CC2)=O)c3cc(C#CC(C)(C)C)sc3C(=O)O</chem>			VX-222 (VCH-222,
Chemicals	S1480	<chem>)CC[C@H](O)CC1</chem>	C25H35NO4S	445.615	Lomibuvir)
Selleck					
Chemicals	S2123	<chem>OC[C@H](O)[C@H](O)[C@H](O)[C@H](O)C=O</chem>	C6H12O6	180.156	Dextrose
Selleck					
Chemicals	S1619	<chem>c1c(C)c(NC(=O)C(C)NCCC)ccc1</chem>	C13H20N2O	220.311	Prilocaine
Selleck		<chem>c1(OC)c(OC)cc(Nc2ncc(F)c(Nc3ccc4c(NC(=O)C(C)(C)O4)n3)n2)cc1OC.c5</chem>			
Chemicals	S2194	<chem>cc(S(=O)(=O)O)ccc5</chem>	C28H29FN6O8S	628.629	R406
Selleck					
Chemicals	S1681	<chem>c1c(N)ccc(O)c1C(=O)O</chem>	C7H7NO3	153.135	Mesalamine
Selleck		<chem>C1[C@](O)(C(O)=O)C[C@H](OC(=O)C=Cc2ccc(O)c(O)c2)[C@H](O)[C</chem>			
Chemicals	S2280	<chem>@H]1O</chem>	C16H18O9	354.309	Chlorogenic Acid
Selleck		<chem>[Ca+2].c1cc2c(nc(C3CC3)c(C=C[C@H](C[C@H](O)CC(=O)[O-</chem>			
Chemicals	S1759	<chem>)O)c2c4ccc(F)cc4)cc1.c5cc6c(nc(C7CC7)c(C=C[C@H](C[C@H](O)CC(</chem>	C50H46CaF2N2O8	880.984	Pitavastatin Calcium
Selleck		<chem>=O)[O-])O)c6c8ccc(F)cc8)cc5</chem>			L-(+)-Rhamnose
Chemicals	S2317	<chem>[C@H]1(O)[C@@H](C)OC(O)[C@H](O)[C@@H]1O.O</chem>	C6H14O6	182.172	Monohydrate
Selleck					
Chemicals	S1808	<chem>c1ccc([N+](=O)[O-])c(C2C(C(OC)=O)=C(C)NC(C)=C2C(=O)OC)c1</chem>	C17H18N2O6	346.335	Nifedipine
Selleck					
Chemicals	S2354	<chem>C1CC2[C@](C)(CCCC2(C)C)[C@H](CCC(O)(C=C)C)[C@@]1(O)C</chem>	C20H36O2	308.499	Sclareol
Selleck					
Chemicals	S1880	<chem>C(N1CCCC1)c2cccc(OCNC(=O)COC(=O)C)c2.Cl</chem>	C19H29ClN2O4	384.898	Roxatidine Acetate HCl
Selleck		<chem>C1[C@@H](O)C[C@]2(C3[C@H]4[C@]5O)[C@@](O)([C@H](O)C)[C</chem>			
Chemicals	S2387	<chem>@]6([H])[C@H](OC)C5)[C@]2([H])C6)[C@]([H])(C4)[C@](OC(=O)c7c</chem>	C32H45BrN2O8	665.612	Lappaconite HBr
Selleck		<chem>cccc7NC(C=O)(CN3CC)C1.Br</chem>			
Chemicals	S2443	<chem>c1(S(NC(NCCCC)=O)(=O)=O)ccc(C)cc1</chem>	C12H18N2O3S	270.348	Tolbutamide
Selleck					
Chemicals	S2884	<chem>O1C(C)=CC(=O)NS1(=O)=O.[K]</chem>	C4H5KNO4S	202.25	Acesulfame Potassium
Selleck					
Chemicals	S2524	<chem>N1C([O-])=NC(=O)C1(c2cccc2)c3ccccc3.[Na+]</chem>	C15H11N2NaO2	274.25	Phenytoin sodium
Selleck					
Chemicals	S2897	<chem>c(c(Nc1ccc(Cl)cc1F)ncn2)(cc(OC)c(OC)c3)c23</chem>	C16H13ClFN3O2	333.745	ZM 306416
Selleck					
Chemicals	S2577	<chem>c1cc(NC(=O)C)ccc1OCC</chem>	C10H13NO2	179.216	Phenacetin
Selleck					
Chemicals	S2906	<chem>c1c(c2onc(C)c2NC(=O)OC(C)c3ccccc3C)ccc(CSCCC(=O)OC)c1</chem>	C24H25ClN2O5S	488.984	Ki16198
Selleck		<chem>c1ccc(CNc2nc(Nc3cc4c(NC(=O)C4)cc3)nc2C(F)(F)F)c(N(S(=O)(C)=O)C)</chem>			
Chemicals	S2672	<chem>n1.c5cc(S(=O)(=O)O)ccc5</chem>	C27H26F3N7O6S2	665.664	PF-00562271
Selleck					
Chemicals	S2916	<chem>c1cc(C(=O)Nc2cccc(NC(=O)CCC)c2)c(Br)cc1</chem>	C17H17BrN2O2	361.233	ML161
Selleck		<chem>c(ncc(c1cnn(C)c1)c2)(C=Cc3c(cc(NS(=O)(=O)N)C)C[C@H]4COCCO4)c</chem>			
Chemicals	S2774	<chem>c3)C5=O)c25</chem>	C24H25N5O5S	495.551	MK-2461

Selleck					
Chemicals	S2928	<chem>C(Nc1nccc(c2sc(Cc)nc2c3cccc(C)c3)c1)(=O)c4cccc4</chem>	C24H21N3OS	399.508	TAK-715
Selleck					
Chemicals	S2817	<chem>N1(c2cccc(C(F)(F)F)c2)c(c3C=CC1=O)c4c(ccc(c5ccc(N)nc5)c4)nc3</chem>	C24H15F3N4O	432.397	Torin 2
Selleck		<chem>C1[C@@H](O)C(=O)[C@H](CC)C[C@@]2([H])C(C=[C@H](C)[C@H]2C</chem>			
Chemicals	S3036	<chem>C[C@H](O)C[C@@H](O)CC([O-])=O=[C@H]1O.[Na+]</chem>	C23H35NaO7	446.51	Pravastatin sodium
Selleck		<chem>[C@H]1(O)[C@H](SC)O[C@H]([C@H](NC([C@H]2C[C@@H](CCC)C</chem>			
Chemicals	S2830	<chem>N2C)=O)C(C)C[C@H](O)[C@H]1O</chem>	C18H33ClN2O5S	424.983	Clindamycin
Selleck		<chem>[C@H]1(c2cccc2)c(c3CCN1C(O[C@]4([H])C(CCN5C4)CC5)=O)cccc3.C(O</chem>			
Chemicals	S3048	<chem>)(=O)CCC(O)=O</chem>	C27H32N2O6	480.553	Solifenacin succinate
Selleck					
Chemicals	S2852	<chem>[nH]1c(c2c(C3CCN(C)CC3)c1)ccc(O)c2</chem>	C14H18N2O	230.306	BRL-54443
Selleck					
Chemicals	S3064	<chem>[C@@H]1(O)CC[C@@H](NCc2cc(Br)cc(Br)c2N)CC1.Cl</chem>	C13H19Br2ClN2O	414.564	Ambroxol HCl
Selleck					
Chemicals	S2861	<chem>c1(C#Cc2c(C)n(c3ccc(OC(F)(F)F)cc3)c(C)n2)cc(Cl)nc1</chem>	C19H13ClF3N3O	391.774	CTEP (RO4956371)
Selleck					
Chemicals	S3079	<chem>C1(=C(O)C(=O)c2c(ccc2)C1=O)[C@H]3CC[C@H](c4ccc(Cl)cc4)CC3</chem>	C22H19ClO3	366.837	Atovaquone
Selleck					
Chemicals	S2870	<chem>c1(O)cccc(c2cnc(c3n2)nc(N)nc3N)c1</chem>	C12H10N6O	254.247	TG100713
Selleck					
Chemicals	S3113	<chem>c1nc(C)c(O)c(CO)c1CO.Cl</chem>	C8H12ClNO3	205.639	Pyridoxine HCl
Selleck					
Chemicals	S1195	<chem>c1cc2c(ccc(C3(O)CCn4c3cnc4)c2)cc1C(=O)NC</chem>	C18H17N3O2	307.346	TAK-700 (Orteronel)
Selleck		<chem>C1=C[C@@]2(C)C(C)C[C@]3([H])[C@@]2(F)[C@H](O)C[C@@]4(C)[C@</chem>			
Chemicals	S1933	<chem>@]3([H])C[C@@H](O)[C@@]4(O)C(=O)CO)=CC1=O</chem>	C21H27FO6	394.434	Triamcinolone
Selleck					
Chemicals	S1256	<chem>c1c(F)c(Cn2cc(C(N)=O)nn2)c(F)cc1</chem>	C10H8F2N4O	238.194	Rufinamide
Selleck		<chem>c1c(C2C(C(=O)OCC)=C(C)NC(C)=C2C(=O)OCC)c(C=CC(O)C(C)C(=O))</chem>			
Chemicals	S1994	<chem>ccc1</chem>	C26H33NO6	455.543	Lacidipine
Selleck					
Chemicals	S1334	<chem>c1(F)ccc(CNc2ccc(NC(OCC)=O)c(N)n2)cc1.O(C=O)C=CC(=O)O</chem>	C19H21FN4O6	420.392	Flupirtine maleate
Selleck					
Chemicals	S2051	<chem>C(O)=(O)[C@H]1CCCN1C(=O)[C@H](C)CS</chem>	C9H15NO3S	217.285	Captopril
Selleck		<chem>c1(Cl)cc(C(=O)NCC2CN(Cc3ccc(F)cc3)CCO2)c(OCC)cc1N.OC(=O)CC(O)(</chem>			
Chemicals	S1385	<chem>C(O)=O)CC(=O)O</chem>	C27H33ClFN3O10	614.016	Mosapride Citrate
Selleck					
Chemicals	S2092	<chem>c1(Cc2c[nH]cn2)c(C)c(C)ccc1.Cl</chem>	C12H15ClN2	222.714	Detomidine HCl
Selleck					
Chemicals	S1534	<chem>c1(Cl)cc2c([nH]c(C(NCCc3ccc(N4CCCCC4)cc3)=O)c2CC)cc1</chem>	C24H28ClN3O	409.952	Org 27569
Selleck					
Chemicals	S2124	<chem>OC[C@@H](O)[C@H](O)[C@@H](O)C=O</chem>	C5H10O5	150.13	Xylose
Selleck					
Chemicals	S1630	<chem>N(C(=O)C(=C1)C(NN1)=N2)=C2</chem>	C5H4N4O	136.111	Allopurinol
		<chem>C(=O)(O)C=CC(=O)O.O.c1(OC)ccc(C[C@H](C(C)C)[C@H](N)[C@@H](O)</chem>			
Selleck		<chem>C[C@@H](C(C)C)C(=O)NCC(C)(C)C(=O)N)cc1OCCCCO.c2(OC)ccc(C[C</chem>			
Chemicals	S2199	<chem>@H](C(C)C)[C@H](N)[C@@H](O)C[C@@H](C(C)C)C(=O)NCC(C)(C)C(</chem>	C64H110N6O16	1219.589	Aliskiren Hemifumarate
Selleck		<chem>=O)N)cc2OCCCC</chem>			
Chemicals	S1683	<chem>[Br-].C1(CC(O)C(=O)C(CO)c2ccccc2)C3([N+])(C(C)C)(C)C3CC1</chem>	C20H30BrNO3	412.361	Ipratropium Bromide
		<chem>N1(C)[C@H](CC(C)C)C(=O)N(C)[C@H](C(C)C)C(=O)N(C)[C@H]([C@@H]</chem>			
Selleck		<chem>([C@H](C)CC=CC)O)C(=O)N[C@@H](CC)C(=O)N(C)CC(=O)N(C)[C@@</chem>			
Chemicals	S2286	<chem>H](CC(C)C)C(=O)N[C@@H](C(C)C)C(=O)N(C)[C@@H](CC(C)C)C(=O)N[</chem>	C62H111N11O12	1202.611	Cyclosporin A
Selleck		<chem>C@@H](C)C(=O)N[C@H](C)C(=O)N(C)[C@@H](CC(C)C)C1=O</chem>			
Chemicals	S1761	<chem>c1(C(=O)c2cccs2)ccc(C(C)C(=O)O)cc1</chem>	C14H12O3S	260.308	Suprofen
Selleck					
Chemicals	S2321	<chem>c1c(CC=C)cc(c2c(O)ccc(CC=C)c2)c(O)c1</chem>	C18H18O2	266.334	Magnolol
Selleck		<chem>[Ca+2].O(c1ccccc1)c2cc(C(C(=O)O)[O-</chem>			
Chemicals	S1823	<chem>])Cccc2.O(c3ccccc3)c4cc(C(C(=O)[O-])C)ccc4</chem>	C30H26CaO6	522.602	Fenoprofen Calcium
Selleck		<chem>c1(OC)c(O)ccc(C2C(CO)O)c3c(ccc(C4OC5c(c(O)cc(O)c5)C(=O)C4O)c3)O</chem>			
Chemicals	S2358	<chem>2)c1</chem>	C25H22O10	482.436	Silymarin
Selleck					
Chemicals	S1885	<chem>C(C(=O)OCC)(C(c1c(Cl)c(Cl)ccc1)C(C(=O)O)C)=C(C)N2)=C2C</chem>	C18H19Cl2NO4	384.254	Felodipine
		<chem>c1(O[C@H]2[C@@H](O[C@]3([H])O[C@@H](C)[C@H](O)[C@@H](O)[C</chem>			
Selleck		<chem>@H]3O)[C@@H](O)[C@H](O)[C@@H](CO)O2)cc(O)c(C(=O)CCc4ccc(O</chem>			
Chemicals	S2389	<chem>)cc4)c(O)c1</chem>	C27H34O14	582.55	Naringin Dihydrochalcone

Selleck		<chem>C1[C@@H](O)[C@@]2(C)[C@@]([H])([C@H](O)[C@H](OC(=O)C)[C@]3(C)[C@@]2(O)C(=O)C[C@](C)(C=CO3)C(C)(C)C1</chem>	C22H34O7	410.501	Forskolin
Chemicals	S2449				
Selleck		<chem>c(sc(C(N)=O)c1)(cnc2Sc3ccc(C)cc3)c12</chem>	C15H12N2OS2	300.399	A-205804
Chemicals	S2885				
Selleck		<chem>c1cc2c(C(=O)c3c(c(O)c(O)cc3)C2=O)cc1</chem>	C14H8O4	240.211	Alizarin
Chemicals	S2526				
Selleck		<chem>c1cc(C(N)=O)cc(c2cc(Nc3ccc(OC(F)(F)F)cc3)ncn2)c1</chem>	C18H13F3N4O2	374.317	GNF-2
Chemicals	S2899				
Selleck		<chem>c1cc(C[C@@H](C(=O)OCC)N[C@H](C)C(=O)N2Cc3c(cccc3)C[C@H]2C(=O)O)ccc1.Cl</chem>	C25H31ClN2O5	474.977	Quinapril HCl
Chemicals	S2581				
Selleck		<chem>N1(C=C(C)C=CC1=O)c2ccccc2</chem>	C12H11NO	185.222	Pirfenidone
Chemicals	S2907				
Selleck		<chem>c1c(O)c2c(OC(c3ccccc3Cl)=CC2=O)c([C@@]4([H])CCN(C)C[C@H]4O)c1O.Cl</chem>	C21H21Cl2NO5	438.301	Flavopiridol HCl
Chemicals	S2679				
Selleck		<chem>c1(c2ncn1CC(=O)Nc3ccc(C(C)C)cc3)C(=O)N(C)C(=O)N2C</chem>	C18H21N5O3	355.391	HC-030031
Chemicals	S2918				
Selleck		<chem>c1c(C(O)=O)cc(C=Cc2ccc(OCc3c(C(C)C)onc3c4c(Cl)cccc4Cl)cc2Cl)cc1</chem>	C28H22Cl3NO4	542.838	GW4064
Chemicals	S2782				
Selleck		<chem>C1CC2=C(S(C(=N)N2CC(=O)c3ccc(C)cc3)CC1.Br</chem>	C16H19BrN2OS	367.304	Pifithrin-? (PFT?)
Chemicals	S2929				
Selleck		<chem>c1(NC(=O)C)ccc(C(Nc2ccccc2N)=O)cc1</chem>	C15H15N3O2	269.298	Cl994 (Tacedinaline)
Chemicals	S2818				
Selleck		<chem>N1(CCCC(O)=O)CCC(O[C@@H](c2ccc(Cl)cc2)c3ncccc3)CC1.c4ccc(S(=O)(=O)O)c4</chem>	C27H31ClN2O6S	547.063	Bepotastine Besilate
Chemicals	S3037				
Selleck		<chem>C1[C@@]2(C)[C@@]([H])(CC[C@]3([H])[C@@]2([H])CC[C@]4(C)[C@@]3([H])CCC4=O)C[C@H]1O</chem>	C19H30O2	290.44	Epiandrosterone
Chemicals	S2832				
Selleck		<chem>c1(S(Nc2c(OC3ccccc3OC)c(OCOC)nc(c4ncccc4)n2)(=O)=O)ccc(C(C)(C)C)cc1.O</chem>	C27H31N5O7S	569.629	Bosentan Hydrate
Chemicals	S3051				
Selleck		<chem>C(=O)(N1CCOCC1)Cc2c(c3n(C(=O)c4ccc(Cl)cc4)c2C)cc(OC)cc3</chem>	C23H23ClN2O4	426.893	BML-190
Chemicals	S2854				
Selleck		<chem>c(c1c(OCc2)(c2C3)[C@@](CCN4CC(=O)C[C@@]5([H])O1)[C@@](O)(CCC5=O)[C@@H]34.Cl</chem>	C19H22ClNO4	363.835	Naloxone HCl
Chemicals	S3066				
Selleck		<chem>c1(C(Nc2ccc(Cl)c2)=O)ncccc1</chem>	C12H9ClN2O	232.666	VU 0364770
Chemicals	S2862				
Selleck		<chem>c1(OC2c(C)cc(C#N)cc2C)c(Br)c(N)nc(Nc3ccc(C#N)cc3)n1</chem>	C20H15BrN6O	435.277	Etravirine (TMC125)
Chemicals	S3080				
Selleck		<chem>C(Nc1ccnc1)(=O)c2cc([N+])([O-])=O)ccc2Cl</chem>	C12H8ClN3O3	277.663	T0070907
Chemicals	S2871				
Selleck		<chem>OC1=C(O)C(=O)O[C@@H]1[C@H](CO)O</chem>	C6H8O6	176.124	Vitamin C
Chemicals	S3114				
Selleck		<chem>c1(S(Nc2nccs2)(=O)=O)ccc(N)cc1</chem>	C9H9N3O2S2	255.317	Sulfathiazole
Chemicals	S3116				
Selleck		<chem>c1cc(C(c2cccn2)CCN(C)C)ccc1.C(=O)(O)C=CC(=O)O</chem>	C20H24N2O4	356.416	Pheniramine Maleate
Chemicals	S4045				
Selleck		<chem>C1N(CN(CN2C3)CN13)C2</chem>	C6H12N4	140.186	Methenamine
Chemicals	S3139				
Selleck		<chem>C1[C@@]2(C)C[C@@H](SC(=O)C)[C@]3([H])[C@@]2([H])CC[C@@]4(C)[C@@]3([H])CC[C@]45CCC(=O)O5)=CC1=O</chem>	C24H32O4S	416.573	Spironolactone
Chemicals	S4054				
Selleck		<chem>c1(CN(Cc2ccc(C(C)(C)cc2)C)c(c3ccc1)cccc3.Cl</chem>	C23H28ClN	353.928	Butenafine HCl
Chemicals	S3154				
Selleck		<chem>c1c([N+])([O-])=O)n(CCS(=O)(=O)CC)c(C)n1</chem>	C8H13N3O4S	247.272	Tinidazole
Chemicals	S4068				
Selleck		<chem>c1cc2c(CN3C(=NC(=O)C3)N2)c(Cl)c1Cl.Cl</chem>	C10H8Cl3N3O	292.549	Anagrelide HCl
Chemicals	S3172				
Selleck		<chem>C(O)(=O)c1cccc1Nc2cccc(C)c2C</chem>	C15H15NO2	241.285	Mefenamic Acid
Chemicals	S4078				
Selleck		<chem>c(C(=C1CCN(C)CC1)c2c(cccc2)CC3)(nccc4)c34.C(O)(=O)C=CC(O)=O.C(O)(=O)C=CC(O)=O</chem>	C28H30N2O8	522.546	Azatadine dimaleate
Chemicals	S3186				
Selleck		<chem>C1=C[C@@]2(C)C[C@@H](F)C[C@]3([H])[C@@]2(F)[C@H](O)C[C@@]4(C)[C@@]3([H])C[C@@H](C)[C@@]4(C(=O)CO)O)=CC1=O</chem>	C22H28F2O5	410.452	Flumethasone
Chemicals	S4088				
Selleck		<chem>c1cc2c([nH]c3c2CCN(C[C@@]45[H])[C@]([H])(C(CC)=C4)[C@]3(C(OC)=O)C5)cc1</chem>	C21H24N2O2	336.427	Catharanthine
Chemicals	S3202				
Selleck		<chem>C1[C@@]2(C)C[C@]3([H])[C@@]2(F)[C@H](O)C[C@@]4(C)[C@@]3([H])C[C@@H]5[C@]4(C(Cl)=O)OC(C)(CO5)=CC1=O</chem>	C24H32ClFO5	454.959	Halcinonide
Chemicals	S4098				
Selleck		<chem>[C@]1([H])CC[C@H]2[C@H](C)CC(=O)O[C@]2(C)CC[C@@]3([H])[C@@]1([H])CC[C@]4([H])[C@]3(C)CC[C@@H](O)C4</chem>	C24H40O3	376.573	Lithocholic acid
Chemicals	S4003				
Selleck		<chem>N1(c2ccc(Cl)cc2)c3c(cccc3)N=C4C1=CC(=NC(C)C)C(Nc5ccc(Cl)cc5)=C4</chem>	C27H22Cl2N4	473.396	Clofazimine
Chemicals	S4107				

Selleck					
Chemicals	S4014	<chem>C1(OC(=O)[C@H](CO)c2ccccc2)CC3N(C)C(CC3)C1</chem>	C17H23NO3	289.369	Hyoscyamine
Selleck					
Chemicals	S4118	<chem>c1(nc[nH]c1)CCN.Cl.Cl</chem>	C5H11Cl2N3	184.067	Histamine 2HCl
Selleck					
Chemicals	S4023	<chem>c1(ccc(N)cc1)C(=O)OCCN(CC)CC.Cl</chem>	C13H21ClN2O2	272.771	Procaine HCl
Selleck					
Chemicals	S4132	<chem>c1cc(OC2OCCCC2)ccc1O</chem>	C11H14O3	194.227	Deoxyarbutin
Selleck					
Chemicals	S4037	<chem>C1(=O)N(CC)CC(CCN2CCOCC2)C1(c3ccccc3)c4ccccc4.Cl.O</chem> <chem>C([C@@H](N)C1=NCC(C(=O)N[C@@H](CC(C)C)C(N[C@@H](CCC(=O)O)C(=O)N[C@@H]([C@@H](CC(C)C)C(N[C@@H]2CCCCNC(=O)[C@H](C)C(N)=O)NC(=O)[C@H](CC(O)=O)NC(=O)[C@H](Cc3c[nH]cn3)NC(=O)[C@H](Cc4ccccc4)NC(=O)[C@H]([C@H](C)CC)NC(=O)[C@@H](CCCN)NC2=O)=O)=O)S1)(C)C</chem>	C24H33ClN2O3	432.983	Doxapram HCl
Selleck					
Chemicals	S4146		C65H101N17O16S	1408.667	Bacitracin
Selleck					
Chemicals	S4161	<chem>c1cc(C(=O)O)ccc1</chem>	C7H6O2	122.121	Benzoic Acid
Selleck					
Chemicals	S4257	<chem>c([nH]nn1)(cc(OC)c(C(=O)NCC2CCCN2CC=C)c3)c13.Cl</chem>	C16H22ClN5O2	351.831	Alizapride HCl
Selleck					
Chemicals	S4170	<chem>O1c(c2C=CC1=O)cccc2</chem>	C9H6O2	146.143	Coumarin
Selleck		<chem>c1cnc2c(c(Br)c(NC(NCC3=N3)cc2)n1.[C@H](C(=O)O)(O)[C@@H](O)C(=O)O</chem>	C15H16BrN5O6	442.221	Brimonidine Tartrate
Chemicals	S4266	<chem>N1(S(C(=O)=O)CCN(C(N[C@@H](c2ccccc2)C(N[C@H]3C(=O)N4[C@@]3([H])SC(C)(C)[C@@H]4C(=O)[O-])=O)=O)C1=O.[Na+]</chem>	C21H24N5NaO8S2	561.564	Mezlocillin Sodium
Selleck					
Chemicals	S4278	<chem>c1cc2c(CCC(=O)N2)c(OCC(O)CNC(C)(C)C)c1.Cl</chem>	C16H25ClN2O3	328.834	Carteolol HCl
Selleck					
Chemicals	S4189	<chem>C1C(OC(C(O)c2ccccc2)=O)CC(C)(C)CC1C</chem> <chem>[C@H]1(O)C[C@]([H])(O[C@@H]2[C@H](C)O[C@@]([H])(O[C@H]3CC[C@@]4(C)[C@]([H])(CC[C@]5([H])[C@@]4([H])C[C@@H](O)[C@@]6(C)[C@]5(O)CC[C@H]6C7=CC(=O)OC7C3)C[C@@H]2O)O[C@H](C)[C@H]1O[C@@]8([H])C[C@H](O)[C@H](O)[C@@H](C)O8</chem>	C17H24O3	276.371	Cyclandelate
Selleck					
Chemicals	S4290		C41H64O14	780.938	Digoxin
Selleck					
Chemicals	S4198	<chem>c1nc(N)sc1</chem>	C3H4N2S	100.142	Aminothiazole
Selleck		<chem>Cl.c1c(C(F)(F)F)c2c(c([C@@H]([C@@]3([H])CCCCN3)O)cc(C(F)(F)F)n2)cc1</chem>	C17H17ClF6N2O	414.773	Mefloquine HCl
Chemicals	S4420				
Selleck					
Chemicals	S4207	<chem>c1cc(OC(C)(C)C(O)=O)ccc1Cl</chem>	C10H11ClO3	214.646	Clofibric Acid
Selleck					
Chemicals	S4921	<chem>c(OCO1)(cc(C=C[N+](O-))=O)cc2)c12</chem>	C9H7NO4	193.156	MNS (3,4-Methylenedioxy- ?-nitrostyrene, MDBN)
Selleck					
Chemicals	S4217	<chem>c1(c(l)cc(C[C@H](N)C([O-])=O)cc1l)Oc2ccc(O)c(l)c2.[Na+]</chem>	C15H11Cl3NNaO4	672.955	Liothyronine Sodium
Selleck					
Chemicals	S7016	<chem>n1c(N)ncc(c2c3c(n(C(C)C)c(C)n3)nc(N4CCOCC4)n2)c1</chem> <chem>[C@@H]1(CC)[C@H](O[C@@]2([H])[C@H](O)[C@@H](O)[C@H](OC(=O)C(C)C(C)(C)O2)C(C)=CC(C)=CC[C@]([H])([C@H](O)C)OC(=O)C(CO)[C@@H]3O[C@H](C)[C@@H](OCc4c(O)c(C)c(C)c4CC=O)[C@H](O)[C@@H]3O)C=CC[C@H](O)C(C)=C1</chem>	C17H22N8O	354.41	VS-5584 (SB2343)
Selleck					
Chemicals	S4227		C52H74Cl2O18	1058.039	Fidaxomicin
Selleck					
Chemicals	S7036	<chem>c1c(NC(=O)[C@H]2NCCC2)ccc(c3nc(Nc4ccc(N5CCOCC5)cc4)ncc3)c1</chem>	C25H28N6O2	444.529	XL019
Selleck					
Chemicals	S4237	<chem>c1(OC)cc2c(nc2c2c(NC(C)CCCN)c1.OP(O)(=O)O.OP(O)(=O)O</chem> <chem>C(Nc1ccc(C(N2CCOCC2)=O)cc1)(C(=O)N(C)C=C3c4c(C)c(NC(=O)c5ccc(C(C)(C)C)cc5)ccc4)=N3</chem>	C15H27N3O9P2	455.337	Primaquine Diphosphate
Selleck					
Chemicals	S7051	<chem>C(O)(=O)CCC(O)=O.O1c2c(c(N)c(Cl)cc2C(NC3CCN(CCCOC)CC3)=O)CC1</chem>	C34H37N5O4	579.689	CGI1746
Selleck					
Chemicals	S4247		C22H32ClN3O7	485.958	Prucalopride Succinat
Selleck					
Chemicals	S7076	<chem>c1cc(S(=O)(N(CC(F)(F)F)c2ccc(C(F)(F)F)(O)C(F)(F)F)cc2)=O)ccc1</chem>	C17H12F9NO3S	481.333	T0901317
Selleck					
Chemicals	S3121	<chem>c1nc(C)n(CC(O)CC)c1[N+](O-)=O</chem>	C7H10ClN3O3	219.626	Ornidazole
Selleck		<chem>c1cc2c(C[C@]3([H])[C@@]2([H])CC[C@@]4(C)[C@@]3([H])CC[C@H]4OC(CCC5CC5)=O)cc1O</chem>	C26H36O3	396.562	Estradiol Cypionate
Selleck					
Chemicals	S3140	<chem>[C@H]1(CN)C[C@@]1(c2ccccc2)C(=O)N(CC)CC.Cl</chem>	C15H23ClN2O	282.809	Milnacipran HCl

Selleck		<chem>[C@@]1([H])(C[C@H](SCC(=O)O)[C@H]2[C@@]3(C)[C@@]4([H])[C@](CCC4=O)(C[C@H]3C)[C@@H](C)[C@H](O)[C@](C=C)(C)C2)C5)N(C)[C@]5([H])CC1</chem>	C30H47NO4S	517.763	Retapamulin
Chemicals	S4056				
Selleck					
Chemicals	S3155	<chem>N1(C)CCCCC1C(Nc2c(C)cccc2C)=O.Cl</chem>	C15H23ClN2O	282.809	Mepivacaine HCl
Selleck					
Chemicals	S4070	<chem>NC(=N)N.Cl</chem>	CH6ClN3	95.531	Guanidine HCl
Selleck					
Chemicals	S3173	<chem>N1(C)C(C)=CC(=O)N1c2ccccc2</chem>	C11H12N2O	188.226	Antipyrine
Selleck					
Chemicals	S4079	<chem>n1([C@@H]2[C@H](OCCO)[C@H](O)[C@H]2O)nnc3c1nc(SCCC)nc3N[C@@H]4C[C@@H]4c5ccc(F)c(F)c5</chem>	C23H28F2N6O4S	522.568	Ticagrelor
Selleck					
Chemicals	S3188	<chem>c1cc(C(O)CN)ccc1O.Cl</chem>	C8H12ClNO2	189.639	(+,-)-Octopamine HCl
Selleck					
Chemicals	S4089	<chem>C1=C[C@@]2(C)C([C@@H](F)C[C@]3([H])[C@@]2(F)[C@H](O)C[C@@]4(C)[C@]3([H])C[C@H](C)[C@@]4(O)C(C)C(=O)C(=O)CC1=O</chem>	C25H31ClF2O5	484.96	Halobetasol Propionate
Selleck					
Chemicals	S3204	<chem>c1(O)cccc(C2(CC)CCCCN(C)C2)c1.Cl</chem>	C15H24ClNO	269.81	Meptazinol HCl
Selleck					
Chemicals	S4099	<chem>c1(OCC(F)(F)F)c(C)c(C)[S@@](=O)c2[nH]c3c(cccc2)n2ncc1</chem>	C16H14F3N3O2S	369.361	Dexlansoprazole
Selleck					
Chemicals	S4004	<chem>[C@H](CO)(CC)NCCN[C@H](CO)CC.Cl.Cl</chem>	C10H26Cl2N2O2	277.232	Ethambutol HCl
Selleck					
Chemicals	S4109	<chem>C1Cc2c(cc(Cl)cc2)[C@@H](C)CN1.Cl</chem>	C11H15Cl2N	232.15	Lorcaserin HCl
Selleck					
Chemicals	S4015	<chem>C1(CCCCC1)NS(=O)(=O)O</chem>	C6H13NO3S	179.237	Cyclamic acid
Selleck					
Chemicals	S4120	<chem>c1n(CC(SCc2ccc(Cl)cc2)c3ccc(Cl)cc3Cl)ccn1.[N+](=[O-])(=O)O[Br-].[C@@]1([H])(C[C@@H](OC(=O)C(O)c2ccccc2)C3)[N+](C)(C)[C@]3([H])CC1</chem>	C18H16Cl3N3O3S	460.762	Sulconazole Nitrate
Selleck					Homatropine
Chemicals	S4024		C17H24BrNO3	370.281	Methylbromide
Selleck					
Chemicals	S4135	<chem>c1cc(Cl)c(C(O)CNC(C)C)cc1.Cl</chem>	C11H17Cl2NO	250.165	Clorprenaline HCl
Selleck					
Chemicals	S4038	<chem>c1(cccc2)c2nc(OCCCC)cc1C(=O)NCCN(CC)CC.Cl</chem>	C20H30ClN3O2	379.924	Dibucaine HCl
Selleck					
Chemicals	S4148	<chem>c1ccc([C@@H](N)C(=O)N[C@H]2[C@@]3([H])N([C@@H](C(=O)O)C(C)(C)S3)C2=O)cc1.O.O.O</chem>	C16H25N3O7S	403.451	Ampicillin Trihydrate
Selleck					
Chemicals	S4162	<chem>c1cc(OCCOCC[N+](C)(C)Cc2ccccc2)ccc1C(C)(C)CC(C)(C)C.[Cl-]</chem>	C27H42ClNO2	448.081	Benzethonium Chloride
Selleck					
Chemicals	S4258	<chem>c1(ccc(Cl)cc1Cl)[C@@H]2CSC(=C(C#N)n3cncc3)S2</chem>	C14H9Cl2N3S2	354.277	Luliconazole
Selleck					
Chemicals	S4171	<chem>C(CO)[N+](C)(C)C.[Cl-]</chem>	C5H14ClNO	139.624	Choline Chloride
Selleck					
Chemicals	S4267	<chem>c(C(=O)c1c(cccc1OC(C)=O)C2=O)(c(C(=O)C)cc(C(=O)O)c3)c23C(C(=O)OC)(C(c1cccc([N+](=[O-]))=O)c1)C(C(=O)OCCN(C)Cc2ccccc2)=C(C)N3)=C3C.Cl</chem>	C19H12O8	368.294	Diacerein
Selleck					
Chemicals	S4181	<chem>c1cc([C@@H](N)C(=O)N[C@H]2[C@@]3([H])N([C@@H](C(=O)O)C(C)(C)S3)C2=O)cc1.O.O.O</chem>	C26H30ClN3O6	515.986	Nicardipine HCl
Selleck					
Chemicals	S4279	<chem>c1c(Cl)c2c(C(=O)C(=C3O)[C@]([H])([C@]4([H])[C@@]3(O)C(=O)C(C(=O)N)=C(O)[C@@H]4N(C)C)[C@H]2O)c(O)c1.Cl</chem>	C21H22Cl2N2O8	501.314	Demeclocycline HCl
Selleck					
Chemicals	S4190	<chem>n1c(c2c(C(O)=O)cc1c3ccccc3)cccc2</chem>	C16H11NO2	249.264	Cinchophen
Selleck					
Chemicals	S4291	<chem>c1(C(=O)N)cc(C(O)CNC(C)CCc2ccccc2)ccc1O.Cl</chem>	C19H25ClN2O3	364.866	Labetalol HCl
Selleck					
Chemicals	S4199	<chem>c1ccc(CN(c2ccccc2)CC3=NCCN3)cc1.Cl</chem>	C17H20ClN3	301.814	Antazoline HCl
Selleck					
Chemicals	S4627	<chem>c(C(C)(C)CCC1(C)C)(cc(C(C)=Cc2ccc(C(=O)O)cc2)cc3)c13</chem>	C24H28O2	348.478	TTNPB (Arotinoid Acid)
Selleck					
Chemicals	S4208	<chem>c1cc2c(OC(C(=O)O)=CC2=O)cc1</chem>	C10H6O4	190.152	Chromocarb
Selleck					
Chemicals	S4926	<chem>c1(F)cc2c(CC[C@@H](N3C(=S)NC=C3CN)C2)c(F)c1.Cl</chem>	C14H16ClF2N3S	331.812	(R)-Nepicastat HCl
Selleck					
Chemicals	S4219	<chem>N1(CCN(CCCC(=O)c2ccc(F)cc2)CC1)c3ncccc3</chem>	C19H22FN3O	327.396	Azaperone
Selleck					
Chemicals	S7018	<chem>c1(S(NC(C)C)C)(=O)=O)cc(c2cn(c3c(F)c2)nc(N)n3)cnc1</chem>	C15H17FN6O2S	364.398	CZC24832
Selleck					
Chemicals	S4228	<chem>[C@](F)([C@]1(C)C(=CC(=O)C=C1)[C@@]([H])(C)C2)[C@](O)([H])C[C@@]3(C)[C@@]4([H])CC[C@@]3(C(=O)C)OC(=O)C[C@@]24[H]</chem>	C24H31FO5	418.498	Fluorometholone Acetate
Selleck					
Chemicals	S7037	<chem>n1ccc(c2ccc(CC(=O)Nc3ccc(c4cnccc4)cc3)cc2)cc1C</chem>	C25H21N3O	379.454	Wnt-C59 (C59)

Selleck		<chem>c1(OC)cc2c([C@@]3([H])N(C)CC2)cc1Oc(c45)[C@]([H])(N(C)CC4)Cc(cc</chem>			
Chemicals	S4238	<chem>c6Oc7cc(ccc7OC)C3)cc6)c8c(OCO8)c5</chem>	C37H38N2O6	606.707	Cepharanthine
Selleck		<chem>c1(OC(F)(F)O2)c2cc(C3(CC3)C(Nc4cc5c(n(C[C@@H](O)CO)c(C(C)(C)CO</chem>			
Chemicals	S7059	<chem>)c5)cc4F)=O)cc1</chem>	C26H27F3N2O6	520.498	VX-661
Selleck					
Chemicals	S4248	<chem>[Na+].[C]([O-])=O)Cc1cccc(C(=O)c2ccc(Br)cc2)c1N</chem>	C15H11BrNNaO3	356.147	Bromfenac Sodium
Selleck		<chem>N1(C)[C@@H](C(C)C)C(=O)N[C@@H](CCCC(N)=N)C(=O)NCC(=O)N[C</chem>			
Chemicals	S7077	<chem>@@H](CC(O)=O)C(=O)N[C@H](Cc2ccccc2)C1=O</chem>	C27H40N8O7	588.656	Cilengitide
Selleck					
Chemicals	S3129	<chem>c1(N)ccc(Cc2cc(OC)c(OC)c(OC)c2)c(N)n1</chem>	C14H18N4O3	290.318	Trimethoprim
Selleck					
Chemicals	S4047	<chem>c1(C(c2ccc(OC(C)=O)cc2)c3ncccc3)ccc(OC(C)=O)cc1</chem>	C22H19NO4	361.391	Bisacodyl
Selleck					
Chemicals	S3144	<chem>c1(CCN2C[C@H](C(c3ccccc3))(c4ccccc4)C(N)=O)CC2)cc5c(OCC5)cc1.Br</chem>	C28H31BrN2O2	507.462	Darifenacin HBr
Selleck					
Chemicals	S4057	<chem>c1(S(N)(=O)=O)cc2c(NC(C)N(C)S2(=O)=O)cc1Cl</chem>	C9H11Cl2N3O4S2	360.237	Methyclothiazide
Selleck		<chem>C1C[C@@]2([H])C(C[C@]3([H])[C@@]2([H])CC[C@@]4(C)[C@@]3([H]</chem>			
Chemicals	S3160	<chem>)CC[C@]4(O)C(C)=O)C#C)=C[C@H]1O(C(C)=O</chem>	C24H32O4	384.508	Ethynodiol diacetate
Selleck					
Chemicals	S4071	<chem>c1c(OC)c2c(O[C@]3(C(OC)=CC(=O)C[C@H]3C)C2=O)c(Cl)c1OC</chem>	C17H17ClO6	352.766	Griseofulvin
Selleck					
Chemicals	S3176	<chem>c1(CCNC)ncccc1.Cl.Cl</chem>	C8H14Cl2N2	209.116	Bethahistine 2HCl
Selleck					
Chemicals	S4080	<chem>c1(N)nc(N)c2c(nc(N)c(c3ccccc3)n2)n1</chem>	C12H11N7	253.263	Triamterene
Selleck					
Chemicals	S3190	<chem>OC[C@H]1O[C@@H](n2c(c3nc2)ncnc3NC)[C@H](O)[C@@H]1O</chem>	C11H15N5O4	281.268	N6-methyladenosine (m6A)
Selleck					
Chemicals	S4090	<chem>c1c(CCN2CCC3(OC(=O)NC3)CC2)cccc1.Cl</chem>	C15H21ClN2O2	296.792	Fenspiride HCl
Selleck		<chem>C1(C(O)(c2ccccc2)c3ccccc3)CCN(CCC(C)O)c4ccc(C(C)(C)C(=O)O)cc4)CC</chem>			
Chemicals	S3208	<chem>1.Cl</chem>	C32H40ClNO4	538.117	Fexofenadine HCl
Selleck					
Chemicals	S4100	<chem>c1cc(OCC(O)CNC(C)C)ccc1CCC(=O)OC.Cl</chem>	C16H26ClNO4	331.835	Esmolol HCl
Selleck		<chem>Cl.c1cc2c(C(=O)C(=C3O)[C@]([H])([C@@H](O)[C@]4([H])[C@@]3(O)C(</chem>			
Chemicals	S4005	<chem>=O)C(C(=O)N)=C(O)[C@@H]4N(C)C)[C@@H]2C)c(O)c1</chem>	C22H25ClN2O8	480.895	Doxycycline HCl
Selleck		<chem>c1cc2c(CC[C@]3([H])[C@@]2([H])CC[C@@]4(C)[C@@]3([H])CC[C@H]4</chem>			
Chemicals	S4110	<chem>O)cc1OC(=O)c5ccccc5</chem>	C25H28O3	376.488	Estradiol Benzoate
Selleck		<chem>[C@@]1(CO)[C@@H](O)C[C@@H](O)[C@@H]2O[C@H](C)[C@H](O)[C</chem>			
Chemicals	S4016	<chem>@@H](O)[C@@H]2O)C3)[C@]3(O)CC[C@]4([H])[C@@]1([C@H](O)C[C</chem>			
		<chem>@@]5(C)[C@]4(O)CC[C@H]5C6=CC(=O)OC6)[H].O.O.O.O.O.O.O</chem>	C29H60O20	728.775	Ouabain
		<chem>[C@@H]1(O)[C@@H]2O[C@@H](C)[C@@H](O)[C@H](N(C)O)[C@H]2O)</chem>			
		<chem>[C@@H](C)[C@H](O)CC(=O)O[C@H](CC)[C@H](CO[C@@H]3O[C@@</chem>			
Selleck		<chem>H](C)[C@@H](O)[C@@H](O)C[C@H]3OC)C=C(C)C=CC(=O)[C@H](C)C</chem>			
Chemicals	S4122	<chem>C@@H]1CCN4C[C@H](C)C[C@@H](C)C4</chem>	C46H80N2O13	869.133	Tilmicosin
Selleck					
Chemicals	S4025	<chem>[C@@H]1(O(C(=O)C(O)c2ccccc2)C[C@]3([H])N(C)[C@]([H])(CC3)C1.Br</chem>	C16H22BrNO3	356.255	Homatropine Bromide
Selleck					
Chemicals	S4136	<chem>OC(=O)C(C)c1cc2c(c3c(ccc(Cl)c3)[nH]2)cc1</chem>	C15H12ClNO2	273.714	Carprofen
Selleck					
Chemicals	S4039	<chem>C1(=NC(=O)C)N(C)N=C(S(=O)(=O)N)S1</chem>	C5H8N4O3S2	236.272	Methazolamide
Selleck					
Chemicals	S4149	<chem>c1(cccc(C([O-])=O)c1N)C(=O)c2ccccc2.O.[Na+]</chem>	C15H14NNaO4	295.266	Amfenac Sodium Monohydrate
		<chem>c1c(O)c2c([C@H](C)[C@]3([H])C(=C(O)[C@@]4(O)[C@]([H])([C@H](N(C</chem>			
Selleck		<chem>)C(C)O)=C(C(N)=O)C4=O)[C@H]3O)C2=O)cc1.c5c(O)c6c([C@H](C)[C@</chem>			
Chemicals	S4163	<chem>]7([H])C(=C(O)[C@@]8(O)[C@]([H])([C@H](N(C)C)C(O)=C(C(N)=O)C8=</chem>			
Selleck		<chem>O)[C@H]7O)C6=O)cc5.Cl.O.CCO.Cl</chem>	C46H58Cl2N4O18	1025.875	Doxycycline Hyclate
Chemicals	S4259	<chem>c(cc(C#N)cc1)c(CCCCN2CCN(c3ccc4c(cc(C(=O)N)O4)c3)CC2)c[nH]5)c15.</chem>			
Selleck		<chem>Cl</chem>	C26H28ClN5O2	477.986	Vilazodone HCl
Selleck					
Chemicals	S4172	<chem>[n+].[1](CCCCCCCCCCCCCCCC)cccc1.[Cl-]</chem>	C21H38ClN	339.986	Cetylpyridinium Chloride
Selleck					
Chemicals	S4268	<chem>C(O)(=O)c1cccc1Nc2ccc(C(F)(F)F)c2</chem>	C14H10F3NO2	281.23	Flufenamic acid
Selleck					
Chemicals	S4182	<chem>c1cc(C=NCC(=O)c2ccc(O)cc2)oc1[N+](=O)[O-]</chem>	C12H9N3O5	275.217	Nifuroxazide
Selleck					
Chemicals	S4280	<chem>c1cc(OCC(=O)OCCN(C)C)ccc1Cl.Cl</chem>	C12H17Cl2NO3	294.174	Meclofenoxate (Centrophenoxine) HCl
Selleck					
Chemicals	S4191	<chem>c1ccccc1C(=O)NCCC(=O)O</chem>	C10H11NO3	193.199	Betamipron

Selleck					
Chemicals	S4292	<chem>c1cc(C(O)(c2ccccc2)CCCN3CCCCC3)ccc1.Cl</chem>	C21H28ClNO	345.906	Diphenidol HCl
Selleck					
Chemicals	S4200	<chem>c1cc(C(=O)C(C)CN2CCCCC2)ccc1C.Cl</chem>	C16H24ClNO	281.821	Tolperisone HCl
Selleck					
Chemicals	S4900	<chem>CC(c1ccc(C(NC(Nc2ccc(NC(CCCCN(C)C)=O)cc2)=S)=O)cc1)(C)C</chem>	C25H34N4O2S	454.628	Tenovin-6
Selleck					
Chemicals	S4209	<chem>c1(C)cc(O)ccc1Cl</chem>	C7H7ClO	142.583	Chlorocresol
Selleck		<chem>n1c(N([C@@H]2[C@@H](C)CCN(C(CCN)=O)C2)c3c([nH]cc3)nc1.C(C(=O)O)C(C)(CC(O)=O)C(=O)O</chem>	C22H28N6O8	504.493	Tofacitinib (CP-690550) Citrate
Chemicals	S5001	<chem>n1c(NS(=O)(=O)c2ccc(C(C)(C)C)cc2)c(Oc3c(O)cccc3)c(OCCO)nc1c4ncc</chem>			
Selleck		<chem>cn4</chem>	C27H29N5O6S	551.614	Bosentan
Chemicals	S4220	<chem>C(C)(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](C)C(N[C@H](C)CF)=O)CC(=O)OC(=O)</chem>	C22H30FN3O7	467.488	Z-VAD-FMK
Selleck					
Chemicals	S7023	<chem>c1(C(=O)OCCN(CC)CC)ccc(N)c(OCCCC)c1.Cl</chem>	C17H29ClN2O3	344.877	Oxybuprocaine HCl
Selleck					
Chemicals	S4229	<chem>c1(C(=O)OCCN(CC)CC)ccc(N)c(OCCCC)c1.Cl</chem>	C17H29ClN2O3	344.877	Oxybuprocaine HCl
Selleck					
Chemicals	S7039	<chem>c1cc2c(c(Nc3cc(Br)ccc3)ncn2)cc1NC(=O)C=C</chem>	C17H13BrN4O	369.215	PD168393
Selleck					
Chemicals	S4239	<chem>C1=Cc2c(cc3c(ccc3)c2OC)OC1=O</chem>	C12H8O4	216.19	Bergapten
Selleck					
Chemicals	S7060	<chem>n1c(N)c2c(n(C(C)C)nc2c3ccc(C)cc3)nc1</chem>	C16H19N5	281.356	PP1
Selleck					
Chemicals	S4249	<chem>c1(C(=O)CC)c(O)cc(O)cc1O</chem>	C9H10O4	182.173	Flopropione
Selleck		<chem>c1(C(C)C)ccc(NC(NCCCN(C(C)C)C@H)2O[C@@H](n3cc(Br)c4c3ncnc4N)[C@H](O)[C@@H]2O)C(C)C(=O)O)cc1</chem>	C28H40BrN7O4	618.566	SGC 0946
Chemicals	S7079				
Selleck					
Chemicals	S3130	<chem>C1(=O)N[C@@H]2[C@H](C)[C@@H](CS[C@@H]2CCCCC(=O)O)N1</chem>	C10H16N2O3S	244.311	Biotin (Vitamin B7)
Selleck					
Chemicals	S4048	<chem>C1=CN(C)C(=S)N1C(OCC)=O</chem>	C7H10N2O2S	186.232	Carbimazole
Selleck					
Chemicals	S3146	<chem>C(N(C)C)CN(Cc1ccccc1)c2ncccc2.Cl</chem>	C16H22ClN3	291.819	Tripelennamine HCl
Selleck					
Chemicals	S4059	<chem>[Fe](N=O)(C#N)(C#N)(C#N)(C#N)C#N.[Na+].[Na+].[R]</chem>	C5FeN6Na2OR	261.918	Sodium Nitroprusside
Selleck					
Chemicals	S3161	<chem>c1n(CC(OCC2csc3c2cccc3Cl)c4ccc(Cl)cc4Cl)ccn1.[R]</chem>	C20H15Cl3N2ORS	437.77	Sertaconazole nitrate
Selleck					
Chemicals	S4072	<chem>[N+](C)(C)CCCCCCCC[N+](C)(C)C.[Br-].[Br-]</chem>	C16H38Br2N2	418.294	Decamethonium Bromide
Selleck					
Chemicals	S3178	<chem>S1(=O)(=O)c2c(cc(S(N)=O)=O)s2[C@@H](NCC)CN1CCCC</chem>	C12H21N3O5S3	383.507	Brinzolamide
Selleck					
Chemicals	S4081	<chem>c1cc(S(=O)(=O)[N-]C(=O)C)ccc1N.[Na+]</chem>	C8H9N2NaO3S	236.223	Sulfacetamide Sodium
Selleck		<chem>N1(C2SC(C)C1C(O)=O)C(=O)C2NC([C@H](C(O)=O)c3ccsc3)=O.[Na].[Na]</chem>			
Chemicals	S3193	<chem>c1(O)ccc(C(O)C(C)N2CCC(Cc3ccccc3)CC2)cc1.c4(O)ccc(C(O)C(C)N5CCC(Cc6ccccc6)CC5)cc4.C(=O)O[C@H](O)[C@@H](O)C(=O)O</chem>	C15H16N2Na2O6S2	430.407	Ticarcillin sodium
Selleck					
Chemicals	S4091	<chem>(Cc6ccccc6)CC5)cc4.C(=O)O[C@H](O)[C@@H](O)C(=O)O</chem>	C46H60N2O10	800.976	Ifenprodil Tartrate
Selleck					
Chemicals	S3209	<chem>N1(C)C(C)=C(N(C)C)C(=O)N1c2ccccc2</chem>	C13H17N3O	231.294	Amidopyrine
Selleck					
Chemicals	S4101	<chem>[C@@H]1(O)[C@@](CO)(CO)C[C@H](NC(CO)CO)[C@H](O)[C@H]1O</chem>	C10H21NO7	267.276	Voglibose
Selleck					
Chemicals	S4007	<chem>c1(C(=N)N)ccc(OCCCCO)c2ccc(C(=N)N)cc2)cc1.Cl.Cl</chem>	C19H26Cl2N4O2	413.341	Pentamidine
Selleck		<chem>c1(c2c(C(=O)N[C@H]3[C@H]4N([C@@H](C(O[Na])=O)C(C)(C)S4)C3=O)c(C)on2)c(Cl)cccc1Cl.O</chem>	C19H18Cl2N3NaO6S	510.323	Dicloxacillin Sodium
Chemicals	S4111				
Selleck					
Chemicals	S4017	<chem>N(CC=C)C(=S)N</chem>	C4H8N2S	116.185	Allylthiourea
Selleck					
Chemicals	S4123	<chem>c1(N2CCOCC2)nsnc1OC[C@@H](O)CNC(C)(C)C.C(C(=O)O)=CC(=O)O</chem>	C17H28N4O7S	432.492	Timolol Maleate
Selleck					
Chemicals	S4026	<chem>C(c1ccccc1)(c2ccc(Cl)cc2)N3CCN(CCOCCO)CC3.Cl.Cl</chem>	C21H29Cl3N2O2	447.826	Hydroxyzine 2HCl
Selleck					
Chemicals	S4138	<chem>N1(CCN(CC(O)CO)CC1)c2ccccc2</chem>	C13H20N2O2	236.31	Dropropizine
Selleck		<chem>[C@@]([H])([C@@]1([H])[C@]([H])([C@]2([H])C=CC(=O)CC2)CC1)CC3(C)[C@]([H])([H])C#C)[C@]34C</chem>	C20H26O2	298.419	Norethindrone
Chemicals	S4040				
Selleck					
Chemicals	S4151	<chem>c1(ccc(Cl)c(C(F)(F)F)c1)C2(O)CCN(CCCC(c3ccc(F)cc3)c4ccc(F)cc4)CC2</chem>	C28H27ClF5NO	523.965	Penfluridol
Selleck					
Chemicals	S4164	<chem>N1(C)C(=O)c2c(ncn2CC3OCCO3)N(C)C1=O</chem>	C11H14N4O4	266.253	Doxofylline

Selleck					
Chemicals	S4260	<chem>c(C(C)(C)CCC1(C)C)(ccc(NC(=O)c2ccc(C(=O)O)cc2)c3)c13</chem>	C22H25NO3	351.439	Tamibarotene
Selleck					
Chemicals	S4173	<chem>C(CCCCCCCC)CCCCCCCCO</chem>	C16H34O	242.441	1-Hexadecanol
		<chem>c1([C@]2(C(=O)O)C)c3c(c4c(cccc4)[nH]3)CN(CC5C2)CC(CC)=C5)cc6c(N(C)[C@]7([H])[C@]6(CC8)[C@]([H])(N89)[C@](CC)(C=CC9)[C@@H](OC(=O)C)[C@]7(O)C(=O)O)cc1OC.C(=O)O)[C@H](O)[C@@H](O)C(=O)O.C(=O)O)[C@H](O)[C@@H](O)C(=O)O</chem>	C53H66N4O20	1079.106	Vinorelbine Tartrate
Selleck	S4269				
Chemicals	S4184	<chem>N(C(=O)c1c(n(CCC(CO)CO)cn1)N2)=C2N</chem>	C10H15N5O3	253.258	Penciclovir
Selleck		<chem>C1C[C@]2([H])[C@@]([H])(CN(C[C@H](O)[C@H](CSc3ccccc3)NC(=O)c4ccccc(O)c4C)[C@H](C(=O)N(C)C)C2)CC1.OS(=O)(=O)C</chem>	C33H49N3O7S2	663.888	Nelfinavir Mesylate
Chemicals	S4282				
Selleck					
Chemicals	S4192	<chem>n1c(c2ccc1C)c(O)c(Cl)cc2Cl</chem>	C10H7Cl2NO	228.075	Chlorquinaldol
Selleck					
Chemicals	S4293	<chem>c1cc2c(N(CC(N(C)C)C)c3c(cccc3)S2)cc1.Cl</chem>	C17H21ClN2S	320.88	Promethazine HCl
Selleck					
Chemicals	S4201	<chem>c1(S(=O)(=O)C)ccc([C@@H](O)[C@@H](CF)NC(=O)C(Cl)Cl)cc1</chem>	C12H14Cl2FNO4S	358.213	Florfenicol
Selleck		<chem>C(Nc1ccc(Nc2nccc(c3ccccc3)n2)c(C)c1)=O)c4cccc(NC(=O)C=CCN(C)C)c4</chem>	C29H29N7O2	507.586	JNK-IN-8
Chemicals	S4901				
Selleck					
Chemicals	S4210	<chem>c1(N)ccc(C(OCC)=O)cc1</chem>	C9H11NO2	165.189	Benzocaine
Selleck					
Chemicals	S7000	<chem>c1(Nc2ccc(N3CC(C(N(C)C)CC3)cc2O)C)nc(Cl)c(Nc4ccccc4P(C)(C)=O)n1</chem>	C26H34ClN6O2P	529.014	AP26113
Selleck					
Chemicals	S4221	<chem>c1(C(=O)c2cc(Br)c(O)c(Br)c2)c(CC)oc3c1cccc3</chem>	C17H12Br2O3	424.083	Benzbromarone
Selleck					
Chemicals	S7024	<chem>c1([N+]([O-])=O)cc2c(C=CS2(=O)=O)cc1</chem>	C8H5NO4S	211.195	Stattic
Selleck					
Chemicals	S4230	<chem>c1(c2ccccc2)oc(CCC(O)=O)nc1c3ccccc3</chem>	C18H15NO3	293.317	Oxaprozin
Selleck		<chem>c1cc(OCCN2CCN(C(=O)C)CC2)ccc1C3CCN(C4=N5c(nnc5C(F)(F)F)CC4)CC3</chem>	C25H32F3N7O2	519.562	AZD3514
Chemicals	S7040				
Selleck					
Chemicals	S4240	<chem>c1cccc(C(OCCN(C)C)(C)c2ncccc2)c1.C(O)(=O)CCC(O)=O</chem>	C21H28N2O5	388.457	Doxylamine Succinate
Selleck		<chem>N([C@H]1C[C@@H](CCc2[nH]c3c(cc(C(C)(C)cc3)n2)C1)[C[C@H]4O[C@@H]([n5cnc6c5nnc6N])[C@H](O)[C@@H]4O)C(C)C</chem>	C30H42N8O3	562.706	EPZ5676
Chemicals	S7062				
Selleck					
Chemicals	S4250	<chem>c1(S(Nc2nnc(OC)cc2)(=O)=O)ccc(N)cc1</chem>	C11H12N4O3S	280.303	Sulfamethoxypyridazine
Selleck		<chem>c1ccc(Nc2nc(Nc3cc(C)c(C4CCNCCC4)cc3OC(C)C)ncc2Cl)c(S(=O)(=O)C(C)C)c1</chem>	C28H36ClN5O3S	558.135	LDK378
Chemicals	S7083				
Selleck					
Chemicals	S3132	<chem>c1(S(Nc2nccc(C)n2)(=O)=O)ccc(N)cc1</chem>	C11H12N4O2S	264.304	Sulfamerazine
Selleck					
Chemicals	S4049	<chem>c1cc(c2c(c3ccc(S(=O)(=O)N)cc3)c(C)on2)ccc1</chem>	C16H14N2O3S	314.359	Valdecoxib
Selleck					
Chemicals	S3147	<chem>C(N(CC)CC)(C(=O)C(C#N)=Cc1cc([N+]([O-])=O)c(O)c(O)c1</chem>	C14H15N3O5	305.286	Entacapone
Selleck					
Chemicals	S4062	<chem>c1([N+]([O-])=O)cncc(COC(=O)N)n1C</chem>	C6H8N4O4	200.152	Ronidazole
		<chem>[C@H]1[CO][C@@H]2O[C@H](C)[C@@H](O)[C@@H](OC)[C@H]2OC)C=C(C)C=CC(=O)[C@H](C)C[C@H](CC=O)[C@H](O)[C@@]3([H])O[C@H](C)[C@@H](O)[C@@]4([H])C[C@]([O])(C)[C@@H](O)[C@H](C)O4)[C@H](N(C)C)[C@H]3O)[C@@H](C)[C@H](O)CC(=O)O[C@@H]1CC.C(O)(=O)[C@H](O)[C@@H](O)C(O)=O</chem>	C50H83NO23	1066.187	Tylosin tartrate
Selleck	S3162				
Selleck					
Chemicals	S4073	<chem>[O-]C(=O)c1ccc(N)cc1O.[Na+]</chem>	C7H6NNaO3	175.117	Sodium 4-Aminosalicylate
Selleck		<chem>N1([C@]2([H])SC(C)(C)[C@@H]1C([O-])=O)C(=O)[C@H]2NC(C(C([O-])=O)c3ccccc3)=O.[Na+].[Na+]</chem>	C17H16N2Na2O6S	422.363	Carbenicillin disodium
Chemicals	S3179				
		<chem>C1C=CC=C[C@H](O)[C@H]2CC[C@H](N(C)C)[C@H](C)O2)[C@H](C)C[C@@H](CC=O)[C@H](O)[C@H]3O[C@@H](C)[C@H](O)[C@H]4O[C@H](C)[C@@H](O)[C@@]([C](O)C4)[C@@H](N(C)C)[C@@H]3O)[C@H](OC)[C@H](O)CC(=O)O[C@@H]1C</chem>	C43H74N2O14	843.053	Spiramycin
Selleck	S4082				
Selleck		<chem>N1(C2SC(C)(C)C1C(O)=O)C(=O)C2NC([C@H](NC(N3C(=O)NCC3)=O)c4cccc4)=O.[Na]</chem>	C20H23N5NaO6S	484.481	Azlocillin sodium salt
Chemicals	S3195				
Selleck					
Chemicals	S4092	<chem>Cl.c1cc(OCCCN2CCOCC2)ccc1OCCCC</chem>	C17H28ClNO3	329.862	Pramoxine HCl
Selleck		<chem>c1(c(OC)c2c(OCO2)c3)c3[C@H](C)[C@H](C)Cc4c1c(OC)c(OC)c(OC)c4</chem>	C23H28O6	400.465	Schisandrin B (Sch B)
Chemicals	S3600				

Selleck		<chem>c1cc(Cn2c(CCCC)nc2C=C(Cc3cccs3)C(=O)O)ccc1C(O)=O.CS(O)(=O)=O</chem>	<chem>C24H28N2O7S2</chem>	520.618	Eprosartan Mesylate
Chemicals	S4102				
Selleck		<chem>s1cc(Cc(Nc2ccc(CCN[C@H](O)c3ccccc3)cc2)=O)nc1N</chem>	<chem>C21H24N4O2S</chem>	396.506	Mirabegron
Chemicals	S4009				
Selleck		<chem>C1CCCC1(O)C(c2ccc(O)cc2)CN(C)C.C(=O)(O)CCC(=O)O</chem>	<chem>C20H31NO6</chem>	381.463	Desvenlafaxine Succinate
Chemicals	S4112				
Selleck		<chem>C(c1cnc(N2CCC[C@H]2CO)nc1NCc3ccc(O)c(Cl)c3)(=O)NCc4ncccn4</chem>	<chem>C23H26ClN7O3</chem>	483.951	Avanafil
Chemicals	S4019				
Selleck		<chem>c1(ccccc1)CC2=NCCN2.Cl</chem>	<chem>C10H13ClN2</chem>	196.677	Tolazoline HCl
Chemicals	S4124				
Selleck		<chem>c(c(C(=O)OCCN1CCCCC1)ccc2)(O(Cc3ccccc3)=C(C)C4=O)c24.Cl</chem>	<chem>C24H26ClNO4</chem>	427.921	Flavoxate HCl
Chemicals	S4027				
Selleck		<chem>C1N(C)CCN(Cc2ccccc2)c3ccccc3)C1.Cl.Cl</chem>	<chem>C18H24Cl2N2</chem>	339.303	Cyclizine 2HCl
Chemicals	S4139				
Selleck		<chem>c1(C([O-])=O)c(O)ccc(N=Nc2cc(C(=O)[O-])cc2)c1.[Na+].[Na+]</chem>	<chem>C14H8N2Na2O6</chem>	346.203	Olsalazine Sodium
Chemicals	S4041				
Selleck		<chem>c1(S(=O)(=O)O)cc(O)ccc1O.N(CC)CC</chem>	<chem>C10H17NO5S</chem>	263.311	Ethamsylate
Chemicals	S4152				
Selleck		<chem>c1cc2c(c(OCCCN(C)C)nn2Cc3ccccc3)cc1.Cl</chem>	<chem>C19H24ClN3O</chem>	345.866	Benzydamine HCl
Chemicals	S4165				
Selleck		<chem>c1(c2c(O)ccc1)C=[N+]3[Mn+3]([Cl-])([N](=C4)CC3([O-]c5c4cccc5OC)[O-]2</chem>	<chem>C18H18ClMnN2O4</chem>	416.738	EUK 134
Chemicals	S4261				
Selleck		<chem>c1(ccc(N)cc1)S(NC(N)=N)(=O)=O</chem>	<chem>C7H10N4O2S</chem>	214.245	Sulfaguandine
Chemicals	S4175				
Selleck		<chem>N1(CC(=O)N)C(=O)CC(O)C1</chem>	<chem>C6H10N2O3</chem>	158.155	Oxiracetam
Chemicals	S4270				
Selleck		<chem>c1(O)c(Cl)cc(Oc2c(Cl)cc(CC(=O)O)cc2)cc1</chem>	<chem>C14H9Cl3O4</chem>	621.932	Tiratricol
Chemicals	s4185				
Selleck		<chem>Nc1cc(Cl)c(C(=O)OCCN(CC)CC)cc1.Cl</chem>	<chem>C13H20Cl2N2O2</chem>	307.216	Chloroprocaine HCl
Chemicals	S4284				
Selleck		<chem>C1(N)=Nc2c(nn[nH]2)C(=O)N1</chem>	<chem>C4H4N6O</chem>	152.114	Azaguanine-8
Chemicals	S4194				
Selleck		<chem>c1cc(C(=O)NCCN(CC)CC)ccc1N.Cl</chem>	<chem>C13H22ClN3O</chem>	271.786	Procainamide HCl
Chemicals	S4294				
Selleck		<chem>C1OCCN(CC2CN(N=Cc3ccc([N+])([O-])=O)c3)C(=O)O2)C1.Cl</chem>	<chem>C13H17ClN4O6</chem>	360.75	Furaltadone HCl
Chemicals	S4203				
Selleck		<chem>n1c(c2c(NCCc3ccc(Oc4ccccc4)cc3)nc1)ccc(N)c2</chem>	<chem>C22H20N4O</chem>	356.42	QNZ (EVP4593)
Chemicals	S4902				
Selleck		<chem>n1c(C=Cc2ccc([C@H](CCc3ccccc3C(C)C)O)SCC4(CC([O-])=O)CC4)c2)ccc(c15)ccc(Cl)c5.[Na+]</chem>	<chem>C35H35ClNNaO3S</chem>	608.165	Montelukast Sodium MEK162 (ARRY-162, ARRY-438162)
Chemicals	S4211				
Selleck		<chem>c(ncn1C)(c(F)c(Nc2ccc(Br)cc2F)c(C(=O)NOCCO)c3)c13</chem>	<chem>C17H15BrF2N4O3</chem>	441.227	
Chemicals	S7007				
Selleck		<chem>[C@H]([C@@H](NC(=O)[C@H](NC(=O)N1CCN(CC)C(=O)C1=O)c2ccccc2)C3=O)SC(C)(C)[C@H]4C([O-])=O)N34.[Na+]</chem>	<chem>C23H26N5NaO7S</chem>	539.537	Piperacillin Sodium
Chemicals	S4222				
Selleck		<chem>C1(CCCCCCCCCC)=C(O)C(=O)C=C(O)C1=O</chem>	<chem>C17H26O4</chem>	294.386	Embelin
Chemicals	S7025				
Selleck		<chem>[C@H]1(Cc2cncn2C)COC(=O)[C@H]1CC.Cl</chem>	<chem>C11H17ClN2O2</chem>	244.718	Pilocarpine HCl
Chemicals	S4231				
Selleck		<chem>c1(C(=O)N2CCN(C)CCC2)cc(c3cc(C=C4c5c(ccc(Cl)c5)NC4=O)cc3)ccc1.Cl</chem>	<chem>C26H25Cl2N3O3</chem>	498.401	CX-6258 HCl
Chemicals	S7041				
Selleck		<chem>CCCCCCCCCCCCCCC[N+](C)(C)C.[Br-]</chem>	<chem>C19H42BrN</chem>	364.447	Cetrimonium Bromide (CTAB)
Chemicals	S4242				
Selleck		<chem>c1(Cl)c(F)c(C(=O)N2CCN(Cc3nc(Nc4scnn4)ccc3)CC2)ccc1</chem>	<chem>C20H19ClFN5OS</chem>	431.914	MK-8745
Chemicals	S7065				
Selleck		<chem>c(cccc1)(Nc2c(cccc2)S3)c13</chem>	<chem>C12H9NS</chem>	199.272	Phenothiazine
Chemicals	S4251				
Selleck		<chem>C(CCS1)(N=C(C(SCC(=O)Nc2sc3c(ccc(C)c3)n2)N(c4ccccc4)C5=O)=C15</chem>	<chem>C22H18N4O2S3</chem>	466.599	IWP-2
Chemicals	S7085				
Selleck		<chem>c1cc(S(=O)(=O)Nc2nc(C)cc(C)n2)ccc1N</chem>	<chem>C12H14N4O2S</chem>	278.33	Sulfamethazine
Chemicals	S3133				
Selleck		<chem>C([C@H](N)C(=O)OCC(OCCN1C2C(C(=O)NC(N)=N2)=C1)CO)(C)C.Cl</chem>	<chem>C14H25ClN6O5</chem>	392.838	Valganciclovir HCl
Chemicals	S4050				
Selleck		<chem>c1cc2c(CC[C@]3([H])[C@@]2([H])CC[C@]4(C)[C@@]3([H])CC[C@H]4OC(=O)CCCC)cc1O</chem>	<chem>C23H32O3</chem>	356.498	Estradiol valerate
Chemicals	S3149				
Selleck		<chem>C1C(=CC=C2CC[C@]3(C)[C@@]2([H])CC[C@H]3[C@H](C)CCCC(C)C)C(=C)CC[C@H]1O</chem>	<chem>C27H44O</chem>	384.638	Vitamin D3
Chemicals	S4063				
Selleck		<chem>C1[C@@H](N(C)[C@@H]2C1)C[C@@H](OCc3ccccc3)c4ccccc4)C2.CS(O)(=O)=O</chem>	<chem>C22H29NO4S</chem>	403.535	Benztrapine mesylate
Chemicals	S3163				

Selleck					
Chemicals	S4074	[O-]N=O.[Na+]	NNaO2	68.995	Sodium Nitrite
Selleck					
Chemicals	S3181	c1(cc(F)c2)c(N3C=C(C(O)=O)C1=O)c2CCC3C	C14H12FNO3	261.248	Flumequine
Selleck					
Chemicals	S4084	C(c1ccc(F)cc1)(c2ccc(F)cc2)N3CCN(Cc4ccc(OC)c(OC)c4OC)CC3.Cl.Cl	C27H32Cl2F2N2O3	541.457	Lomerizine HCl
Selleck					
Chemicals	S3196	N1CCC(C(c2ccccc2)(c3ccccc3)O)CC1	C18H21NO	267.365	Azacyclonol
Selleck					
Chemicals	S4095	C1(=O)C=C[C@@]2(C)C([C@@H](F)C[C@]3([H])([C@@]2(F)[C@H](O)C[C@@]4(C)[C@@]3([H])CC[C@@]4(O)C(CCC)=O)C(=O)CO C(=O)C)=C1	C27H34F2O7	508.551	Difluprednate
Selleck					
Chemicals	S3603	[C@]([C@H](C(C)=C)CC1)([C@]2([H])[C@](C)([C@@]3(C)[C@@]([H])([C@]4(C)[C@]([H])(C(C)C)[C@H](O)CC4)CC3)CC2)CC5)([C@]15C(=O)O)[H]	C30H48O3	456.7	Betulinic acid
Selleck					
Chemicals	S4104	c1cc(N=NNc2ccc(C(N)=N)cc2)ccc1C(=N)N.O.C(=O)CNC(C)=O.O.C(=O)CN C(C)=O	C22H29N9O6	515.522	Diminazene Aceturate
Selleck					
Chemicals	S4010	c1(OCC(O)CNC(C)C)ccc(NC(=O)CCC)cc1C(=O)C.Cl	C18H29ClN2O4	372.887	Acebutolol HCl
Selleck					
Chemicals	S4113	C1CCCCC1(O)C(c2ccc(O)cc2)CN(C)C	C16H25NO2	263.375	Desvenlafaxine
Selleck					
Chemicals	S4020	C(c1ncccc1)(c2ccc(OS([O-])(=O)=O)cc2)c3ccc(OS([O-])(=O)=O)cc3.[Na+].[Na+]	C18H13NNa2O8S2	481.407	Sodium Picosulfate
Selleck					
Chemicals	S4125	C(O[Na])(=O)CCCc1ccccc1	C10H11NaO2	186.183	Sodium Phenylbutyrate
Selleck					
Chemicals	S4031	C(O)(c1cccs1)(c2cccs2)C(=O)O[C@@H]3C([H])(CC[N+](CCCCc5ccccc5)C3)CC4.[Br-]	C26H30BrNO4S2	564.555	Acridinium Bromide
Selleck					
Chemicals	S4141	c1(C(N)=O)cc([N+](=O)[O-])cc([N+](O)=O)c1C	C8H7N3O5	225.158	Dinitolmide
Selleck					
Chemicals	S4042	c(cccc1)(c(C(=O)N[C@H]2[C@]3([H])N([C@H](C(O[Na])=O)C(C)S3)C2=O)c(C(C)CC)cc4)c14.O	C21H23N2NaO6S	454.472	Nafcillin Sodium
Selleck					
Chemicals	S4155	c(ccc(Cl)c1)(OC(=O)N2)c12	C7H4ClNO2	169.565	Chlorzoxazone
Selleck					
Chemicals	S4166	c1cc(S(=O)(=O)NC(NCCC)=O)ccc1Cl	C10H13ClN2O3S	276.74	Chlorpropamide
Selleck					
Chemicals	S4263	c1(C)cc(NC(=O)Cc2ccc(OC(C)C(C(=O)[O-])cc2)cc(C)c1.[Na+]	C20H22NNaO4	363.383	Efaproxiral Sodium
Selleck					
Chemicals	S4176	C(N)(CO)(CO)CO	C4H11NO3	121.135	Trometamol
Selleck					
Chemicals	S4274	C1c2c(cccc2O)C[C@@H](N(CCC)CCc3cccs3)C1	C19H25NOS	315.473	Rotigotine
Selleck					
Chemicals	S4186	C(C)CCCCCCCC[N+](C)(C)CCOc1ccccc1.[Br-]	C22H40BrNO	414.463	Domiphen Bromide
Selleck					
Chemicals	S4285	c1cc(C(c2ccccc2)=C(c3ccccc3)CCCl)ccc1OCCO	C24H23ClO2	378.891	Ospemifene
Selleck					
Chemicals	S4195	c1c(Br)c2c(nccc2)c(O)c1Br	C9H5Br2NO	302.95	Broxyquinoline
Selleck					
Chemicals	S4295	c1c(Cl)c(Nc2c(C(O[Na])=O)ccccc2)c(Cl)c(Cl)c1	C14H10Cl2NNaO2	318.13	Meclofenamate Sodium
Selleck					
Chemicals	S4204	[C@@H]1(O)[C@@]2([H])[C@@]([H])([C@H](O)CO2)OC1	C6H10O4	146.141	Isosorbide
Selleck					
Chemicals	S4904	N1(C(OC2ccc([N+](O-)=O)cc2)=O)CCC(C(c3ccc(c4c3)OCO4)(c5ccc(c6c5)OCO6)O)CC1	C27H24N2O9	520.487	JZL184
Selleck					
Chemicals	S4213	C1[C@H](C)O[C@@H](O[C@@H]2[C@H](C)[C@H](O[C@H]3C[C@@](C)(OC)[C@@H](O)[C@H](C)O3)[C@H](C)C(=O)O[C@@H](CC)[C@@](C)(O)C([H])([C@H](C)[C@]4([H])[C@H](C)C[C@@]2(O)C)O[C@H](COC COC)N4)[C@H](O)[C@H]1N(C)C	C42H78N2O14	835.074	Dirithromycin
Selleck					
Chemicals	S7008	n1c(N)c2c(n(C(C)C)C)nc2c3ccc(Cl)cc3)nc1	C15H16ClN5	301.774	PP2
Selleck					
Chemicals	S4223	C1(=O)C[C@H](O)C[C@H](CC[C@H]2[C@@H](C)C=CC([C@@]23[H])=CC[C@@H]3O)C([C@@H](C)CC)=O)O1	C23H34O5	390.513	Mevastatin
Selleck					
Chemicals	S7028	c1c(Cl)c2c(C=C([C@@H](Nc3c4c([nH]cn4)ncn3)C)N(c5ccccc5)C2=O)cc1	C22H17ClN6O	416.863	IPI-145 (INK1197)
Selleck					
Chemicals	S4232	c1(NC(=O)C)nc([N+](O-)=O)s1	C5H5N3O3S	187.176	Nithiamide
Selleck					
Chemicals	S7048	c1c2c(C3=NNC2=O)c(N[C@H](c4ccc(F)cc4)[C@H]3c5n(C)ncn5)cc1F	C19H14F2N6O	380.351	BMN 673
Selleck					
Chemicals	S4244	c1(O)cc2c([nH]cc2CCN)cc1.Cl	C10H13ClN2O	212.676	Serotonin HCl

Selleck					
Chemicals	S7070	<chem>C1CN(c2cc(NCCC(=O)OCC)nc(c3cccc3)n2)CCc4c1cccc4.Cl</chem>	C24H28ClN5O2	453.964	GSK J4 HCl
Selleck					
Chemicals	S4252	<chem>ClCCN(CCC)C.Cl</chem>	C5H12Cl3N	192.514	Mechlorethamine HCl
Selleck		<chem>[C@@](C)([C@H](C[C@H]12)C=C1)(C(=O)N(c3ccc(C(Nc4c5c(cccn5)ccc4)=O)cc3)C6=O)[C@@]26[H]</chem>	C26H21N3O3	423.463	IWR-1-endo
Chemicals	S7086				
Selleck		<chem>C(O)(=O)c1cccc1O.[Na]</chem>	C7H6NaO3	161.111	Sodium salicylate
Chemicals	S3137				
Selleck		<chem>c1(OC)cc2c(cc(CCC(=O)C)cc2)cc1</chem>	C15H16O2	228.286	Nabumetone
Chemicals	S4051				
Selleck		<chem>c1(C(OC)=O)sc(C)C1NC(=O)C(NCCC)C.Cl</chem>	C13H21ClN2O3S	320.835	Articaine HCl
Chemicals	S3150				
Selleck		<chem>c1(C(c2ccc(F)cc2)(CCCN(C)C)OC3c3cc(C#N)cc1.O.C(C(=O)=O)=O</chem>	C22H23FN2O5	414.427	Escitalopram Oxalate
Chemicals	S4064	<chem>C1CC(=C(C=C[C@@]2(C)[C@@]3([H])CC[C@@]2(O)CC=C)[C@]34[H])C(C</chem>	C21H26O2	310.43	Altrenogest
Selleck		<chem>C4)=CC1=O</chem>			
Chemicals	S3167				
Selleck		<chem>c1cc2c(cccc2OCC(O)CNC(C)C)cc1.Cl</chem>	C16H22ClNO2	295.804	Propranolol HCl
Chemicals	S4076				
Selleck		<chem>C(N(C)C)CC=C1c2c(cccc2)CCc3c1cccc3.Cl</chem>	C20H24ClN	313.864	Amitriptyline HCl
Chemicals	S3183				
Selleck		<chem>c1(OC[C@@H](O)CNC(C)C)ccc(CCOCC2CC2)cc1.Cl</chem>	C18H30ClNO3	343.889	Levobetaxolol HCl
Chemicals	S4085				
Selleck		<chem>C(O)(=O)c1ccc(C(F)(F)F)cc1O.C(C)=O</chem>	C10H7F3O4	248.155	Triflusal
Chemicals	S3200				
Selleck		<chem>c1cc2c(N(C3=CCN(CCCC(c4ccc(F)cc4)=O)CC3)C(=O)N2)cc1</chem>	C22H22FN3O2	379.427	Droperidol
Chemicals	S4096	<chem>[C@](O1)([C@@H]1[C@@H]2[C@@]([C(C)C](O2)[C@H]3O)([C@]4(C)[C</chem>	C20H24O6	360.401	Triptolide (PG490)
Selleck		<chem>@@]([H])(C5=C(C(=O)OC5)CC4)C6)[C@@]3(O7)[C@@H]67</chem>			
Chemicals	S3604				
Selleck		<chem>c1(cc(C)C(NC(=O)c2cc(l)cc(l)c2[O-])cc1Cl)C(C#N)c3ccc(Cl)cc3.[Na+]</chem>	C22H13Cl2I2N2NaO2	685.056	Closantel Sodium
Chemicals	S4105				
Selleck		<chem>C1(OC(C)OC(=O)OCC)=C(C(=O)Nc2cccc2)N(C)S(=O)(=O)c3c1cccc3</chem>	C20H21N3O7S	447.462	Ampiroxicam
Chemicals	S4011				
Selleck		<chem>c1ccc(Oc2c(Cl)cc3c(nc(SC)[nH]3)c2)c(Cl)c1Cl</chem>	C14H9Cl3N2O5	359.658	Triclabendazole
Chemicals	S4114				
Selleck		<chem>c1(cc(O)c(O)c([N+])([O-])=O)c1C(=O)c2ccc(C)cc2</chem>	C14H11NO5	273.241	Tolcapone
Chemicals	S4021				
Selleck		<chem>c1(C(=O)NC2CNCC2)cc(OC)c(OC)c(OC)c1</chem>	C15H22N2O4	294.346	Troxipide
Chemicals	S4128				
Selleck		<chem>C(c1cccc1)(c2cccc2)=C3CC[N+](C)(C)CC3.S([O-])(=O)(=O)OC</chem>	C21H27NO4S	389.508	Diphenamil Methylsulfate
Chemicals	S4034				
Selleck		<chem>c1cnc(C(c2cccc2)(C(=O)N)CCN(C(C)C)C(C)C)cc1.P(O)(O)(O)=O</chem>	C21H32N3O5P	437.47	Pentoxifyverine Citrate
Chemicals	S4143				
Selleck		<chem>N(CCN1)=C1C2CCCc(c23)cccc3.Cl</chem>	C13H17ClN2	236.74	Tetrahydrozoline HCl
Chemicals	S4043				
Selleck		<chem>c1cc(C(NCCc2ccc(OC(C(=O)O)(C)C)cc2)=O)ccc1Cl</chem>	C19H20ClNO4	361.819	Bezafibrate
Chemicals	S4159				
Selleck		<chem>n1c(NC2CC2)nc(N)nc1N</chem>	C6H10N6	166.184	Cyromazine
Chemicals	S4167				
Selleck		<chem>c1cc(OC(C)(C)C(=O)OCCOC(=O)c2cccc2)ccc1Cl</chem>	C18H18ClNO5	363.792	Etofibrate
Chemicals	S4264				
Selleck		<chem>N1C(=O)NC=CC1=O</chem>	C4H4N2O2	112.087	Uracil
Chemicals	S4177				
Selleck		<chem>c(sc(CC)c1)(n2c(nnc2C)CN=C3c4c(Cl)cccc4)c13</chem>	C17H15ClN4S	342.846	Etizolam
Chemicals	S4276				
Selleck		<chem>C(Nc1cccc1)(=O)c2cccc2O</chem>	C13H11NO2	213.232	Salicylanilide
Chemicals	S4187	<chem>[C@H]1(O)NC(=O)[C@@H](N2C(=O)[C@H]([C@H](O)C)NC(=O)[C@H]([C@H](O)[C@@H](O)c3ccc(O)cc3)NC(=O)[C@@H](N4C(=O)[C@H]([C@H](O)C)NC(=O)[C@@H](c5ccc(c6ccc(c7ccc(OCCCCC)cc7)cc6)cc5)=O)[C@H]1O)[C@H](O)[C@@H](CC(C)=CC(=O)O)CCCCCCCCC(=O)O)OC[C@]1([H])C[C@H]2[C@@]([C@@H](C)[C@@H](O)C)[C@@H](C)C2</chem>	C58H73N7O17	1140.237	Anidulafungin (LY303366)
Selleck					Ethacridine lactate
Chemicals	S4286	<chem>c1cc2c(nc3c(cc(OC)cc3)c2N)cc1N.O.C(C)C(=O)O.O</chem>	C18H23N3O5	361.392	monohydrate
Chemicals	S4196	<chem>[C@H]1(O)[C@H](O)[C@H](CC(C)=CC(=O)O)CCCCCCCCC(=O)O)OC[C@]1([H])C[C@H]2[C@@]([C@@H](C)[C@@H](O)C)[C@@H](O)C2</chem>	C26H44O9	500.622	Mupirocin
Selleck					
Chemicals	S4297				
Selleck		<chem>c1cc2c(c3c(ccc3)s2)cc1</chem>	C12H8S	184.257	Dibenzothiophene
Chemicals	S4205				
Selleck		<chem>c1(c2ccsc2)sc(C(N)=O)c(N)c1</chem>	C9H8N2OS2	224.303	SC-514
Chemicals	S4907				

Selleck		[C@H]1(C)[C@H](CO)O[C@H](O[C@@@]2(C)[C@H](O)[C@H](O)[C@H](O)[C@H](CO)O2)[C@H](O)[C@H]1O	C12H19Cl3O8	397.633	Sucralose
Chemicals	S4214				
Selleck		s1c(NC(=O)[C@H]2CCCN2C(=O)[C@H](C3CCCCC3)NC(=O)[C@H](C)NC)c4cccc4)nn1	C25H34N6O3S	498.641	GDC-0152
Chemicals	S7010				
Selleck		[C@H](O)(CO)[C@@H](O)CO	C4H10O4	122.12	Erythritol
Chemicals	S4224				
Selleck		c1cc2c(C(Cc3cc(C(=O)N4CC(C(O)C)CC4)c(F)cc3)=NNC2=O)cc1	C22H22FN3O3	395.427	AZD2461
Chemicals	S7029				
Selleck		c(ccc(C)c1)(oc(N)n2)c12	C7H5ClN2O	168.58	Zoxazolamine
Chemicals	S4233				
Selleck		N(C(=O)c1sc(C)nc1)[C@@H](CO)C(=O)N[C@@H](CO)C(=O)N[C@@H](Cc2ccccc2)C(=O)C3(C)CO3	C25H32N4O7S	532.609	Oprozomib (ONX 0912)
Chemicals	S7049				
Selleck		[C@@]1([H])([C@@H](O)CO)OC(=O)C(O)C1O.[Na]	C6H10NaO6	201.13	Sodium ascorbate
Chemicals	S4245				
Selleck		[C@]1([H])([C@@]2([H])N(C)CCc3c2cc4c(OCO4)c3)OC(=O)c5c1ccc6c5O	C20H17NO6	367.352	(+)-Bicuculline
Chemicals	S7071				
Selleck		N(C(N)=NC1)(c2c(cccc2)Cc3c4cccc3)C14.[H]Cl	C16H16ClN3	285.771	Epinastine HCl
Chemicals	S4253				
Selleck		c1(N2C[C@@H](C)NC3CCCC3)=O)CC[C@H]2C)cc(c4ccc5c([nH]nc5N)c4)nc(NC)n1	C25H34N8O	462.59	GSK2334470
Chemicals	S7087				
Selleck		C1(=S)NC(C)=CC(=O)N1	C5H6N2OS	142.179	Methylthiouracil
Chemicals	S3138				
Selleck		c(cccc1)([C@H](NC)CC[C@H]2c3cc(C)c(C)cc3)c12.Cl	C17H18Cl3N	342.691	Sertraline HCl
Chemicals	S4053				
Selleck		c1(S(NC(NC2CCCC2)=O)(=O)=O)ccc(CCN3C(=O)C(C)(C)c(c4C3=O)ccc(O)c4)cc1	C27H33N3O6S	527.632	Gliquidone
Chemicals	S3151				
Selleck		c1c(C)c(C=C=NNC(=N)N)c(C)cc1.CC(=O)O	C10H12Cl2N4O2	291.134	Guanabenz Acetate
Chemicals	S4065				
Selleck		N1([C@]2([H])SC(C)(C)[C@@H]1C([O-])=O)C(=O)[C@H]2NC(=O)[C@H](N)c3ccccc3.[Na+]	C16H18N3NaO4S	371.387	Ampicillin sodium
Chemicals	S3170				
Selleck		c1c(O)ccc(OC)c1	C7H8O2	124.137	Mequinol
Chemicals	S4077				
Selleck		O=C(c1cc(O)c(O)cc1)CNC.Cl	C9H12ClNO3	217.649	Adrenalone HCl
Chemicals	S3185				
Selleck		C1(N2CCN(C)CC2)=Nc3c(cccc3)Oc4c1cc(Cl)cc4.C(C(=O)O)CC(=O)O	C22H24ClN3O5	445.896	Loxapine Succinate
Chemicals	S4086				
Selleck		c1c(c2ccc1C(F)(F)F)N(CCCN3CCN(C)CC3)c(c4S2)cccc4.Cl.Cl	C21H26Cl2F3N3S	480.417	Trifluoperazine 2HCl
Chemicals	S3201				
Selleck		C1C[C@]2(C)C(C=C[C@]3([H])([C@]2([H])CC[C@]4(C)[C@@]3([H])CC[C@]4(C)C(=O)[H])=CC1=O	C21H28O2	312.446	Dydrogesterone
Chemicals	S4097				
Selleck		c(c1[nH]c2)(c2C[C@]3([H])[C@]4([H])C[C@H](CSC)CN3CCC)c4ccc1.CS(=O)(=O)O	C20H30N2O3S2	410.594	Pergolide mesylate
Chemicals	S4000				
Selleck		c1(cc(C)c(NC(=O)c2cc(l)cc(l)c2O)cc1Cl)(C#N)c3ccc(Cl)cc3	C22H14Cl2I2N2O2	663.074	Closantel
Chemicals	S4106				
Selleck		C1NCCC(=C2c3c(cccn3)CCc4c2ccc(Cl)c4)C1	C19H19ClN2	310.821	Desloratadine
Chemicals	S4012				
Selleck		CC(C)CC(=O)N	C5H11NO	101.147	Isovaleramide
Chemicals	S4116				
Selleck		c1cc(C(O)=O)ccc1S(=O)(=O)N(CCC)CCC	C13H19NO4S	285.359	Probenecid
Chemicals	S4022				
Selleck		c1cc(N2CCN(C[C@@H](O)CO)CC2)ccc1	C13H20N2O2	236.31	Levodropropizine
Chemicals	S4131				
Selleck		[C@](C)([C@@H]([C@H](C)C=C[C@H](C)(C)C)CC1)(CCCC2=CC=C3C[C@H](O)CCC3=C)[C@@]12[H]	C28H44O	396.648	Vitamin D2
Chemicals	S4035				
Selleck		c1c(C)[n+](Cc2c(N)nc(CCC)nc2)ccc1.Cl.[Cl-]	C14H20Cl2N4	315.241	Amprolium HCl
Chemicals	S4144				
Selleck		c1cc(SC(F)(F)F)ccc1Oc2ccc(N3C(=O)NC(=O)N(C)C3=O)cc2C	C18H14F3N3O4S	425.382	Toltrazuril
Chemicals	S4044				
Selleck		N([C@@H](C([O-])=O)C(C)(C)S1)(C(=O)[C@H]2NC(=O)Cc3ccccc3)[C@]12[H].[Na+]	C16H17N2NaO4S	356.372	Penicillin G Sodium
Chemicals	S4160				
Selleck		c1(NC(=O)C(C#N)=C(O)C)ccc(C(F)(F)F)cc1	C12H9F3N2O2	270.207	Teriflunomide
Chemicals	S4169				
Selleck		c1(ncccc1)C(=O)NCC(C)NC(=O)c2ncccc2	C15H16N4O2	284.313	Nicaraven
Chemicals	S4265				
Selleck		C(C(=O)C(C)(C)C)(Oc1ccc(Cl)cc1)n2ncnc2	C15H17ClN2O2	292.761	Climbazole
Chemicals	S4178				
Selleck		c1(O(C(N(C)C)=O)cc(C(O)CNC(C)(C)C)cc(OC(=O)N(C)C)c1.Cl	C18H30ClN3O5	403.901	Bambuterol HCl
Chemicals	S4277				

Selleck					
Chemicals	S4188	<chem>C(Oc1ccccc1C(O)=O)(=O)c2ccccc2O</chem>	C14H10O5	258.226	Sasapyrine
Selleck					
Chemicals	S4288	<chem>c1(N(CCC)CCC)ccc(CCCC(=O)O)cc1</chem>	C14H19Cl2NO2	304.212	Chloroambucil
Selleck					
Chemicals	S4197	<chem>C1(=O)NC(=O)CC(C)(CC)C1</chem>	C8H13NO2	155.194	Bemegride
Selleck					
Chemicals	S4299	<chem>c1cc2c(C(O)=C(CC3=C(O)c4c(cccc4)OC3=O)C(=O)O2)cc1</chem>	C19H12O6	336.295	Dicoumarol
Selleck					
Chemicals	S4206	<chem>C(N)CS.Cl</chem>	C2H8CINS	113.61	Cysteamine HCl
Selleck					
Chemicals	S4908	<chem>c1(nc2c(cc(O)cc2)c3CC)c3CN4C1=CC5=C(CO C(=O)[C@]5(O)CC)C4=O</chem>	C22H20N2O5	392.405	SN-38
Selleck					
Chemicals	S4216	<chem>[C@]([H])(C(=O)CC1)[C@@]2(C)[C@H](O C(=O)CSC(C)(CNC(=O)[C@H](N)C(C)C)C[C@@](C)(C=C)[C@@H](O)[C@@H]3C)[C@@]13CC[C@H]2C.Cl</chem>	C31H53ClN2O5S	601.281	Valnemulin HCl
Selleck					
Chemicals	S7015	<chem>CN[C@@H](C)C(=O)N[C@H](C=O)N1C[C@H](O)C[C@H]1Cc2c3c(cc(F)cc3)[nH]c2c4c(C[C@H]5N(C(=O)[C@H](CC)NC(=O)[C@H](C)NC)C[C@H](O)C5)c6c(cc(F)cc6)[nH]4)CC</chem>	C42H56F2N8O6	806.941	Birinapant
Selleck					
Chemicals	S4225	<chem>c1(OCC(N)C)c(C)cccc1C.Cl</chem>	C11H18ClNO	215.72	Mexiletine HCl
Selleck					
Chemicals	S7033	<chem>n1c(N)c(c(c2ccc(N(C(Cc3nc(C)ccc3)=O)CC4)c4c2F)cn5C)c5nc1</chem>	C23H21FN6O	416.451	GSK2656157
Selleck					
Chemicals	S4235	<chem>c1ccc(N=Nc2ccc(N)nc2N)cc1.Cl</chem>	C11H12ClN5	249.699	Phenazopyridine HCl
Selleck					
Chemicals	S7050	<chem>c1c(N2CCOC[C@H]2C)nc(c3c4c([nH]cc4)ccc3)nc1C5(CC5)S(=O)(=O)C</chem>	C21H24N4O3S	412.505	AZ20
Selleck					
Chemicals	S4246	<chem>Cl.c1cc([C@H]2C[C@@H]2N)ccc1</chem>	C9H12ClN	169.651	Tranylcypromine (2-PCPA) HCl
Selleck					
Chemicals	S7072	<chem>[C@H](NC)(C(=O)O)CC(=O)O</chem>	C5H9NO4	147.129	NMDA (N-Methyl-D-aspartic acid)
Selleck					
Chemicals	S4255	<chem>c1(NC(C)CCN(CC)CC)c2c(cc(Cl)cc2)nc3c1cc(O)cc3.Cl.Cl</chem>	C23H32Cl3N3O	472.879	Quinacrine 2HCl
Selleck					
Chemicals	S7088	<chem>C1CN(C2CCN(C(c3ccc(C(N4CCC(N5CCCC5)CC4)=O)c(Nc6cccc6)c3)=O)CC2)CC1</chem>	C32H43N5O2	529.716	UNC1215
Selleck					
Chemicals	S7090	<chem>C(N[C@@H](Cc1ccc(c2cn(c3n2)cccc3[C@@H](O)C)cc1)CNC(=O)CN(C)C(=O)c4ccc(O C(C)C)c(C)c4</chem>	C32H38ClN5O4	592.128	GSK923295
Selleck					
Chemicals	S7251	<chem>c1(C(F)(F)F)cc(c2nn(C=CC(=O)N3CC(F)(F)C3)cn2)cc(C(F)(F)F)c1</chem>	C16H10F8N4O	426.264	KPT-276
Selleck					
Chemicals	S7099	<chem>c1(N2CC[C@]3(O)C2=Nc4c(cc(C)cc4)C3=O)ccccc1</chem>	C18H16N2O2	292.332	(-)-Blebbistatin
Selleck					
Chemicals	S7263	<chem>c1cc2c(c(Sc3ccc(Cl)cc3)c(C)n2CC(O)=O)c(NC(=O)C)c1</chem>	C19H17ClN2O3S	388.868	AZD1981
Selleck					
Chemicals	S7114	<chem>C1CC(CO c2c(N=O)c(N)nc(N)n2)CCC1</chem>	C11H17N5O2	251.285	NU6027
Selleck					
Chemicals	S7279	<chem>c1cc2c(nc(N3CCN(C(=O)c4c(n5ncn5)ccc(C)c4)[C@H](C)CC3)o2)cc1Cl</chem>	C23H23ClN6O2	450.921	Suvorexant (MK-4305)
Selleck					
Chemicals	S7129	<chem>N1C(=O)C(=Cc2ccc([N+])([O-])=O)o2)C(=O)N1c3ccc(C(OCC)=O)cc3</chem>	C17H13N3O7	371.301	PYR-41
Selleck					
Chemicals	S7293	<chem>c1c(C)nc(NS(=O)(=O)c2ccc(NC(=S)NC(=O)COc3ccc(Br)cc3Cl)cc2)nc1C</chem>	C21H19BrClN5O4S2	584.894	ZCL278
Selleck					
Chemicals	S7139	<chem>c1cc(C=C2SC(=S)N(c3cc(C(F)(F)F)ccc3)C2=O)ccc1C(=O)O</chem>	C18H10F3NO3S2	409.402	CFT RinH-172
Selleck					
Chemicals	S7310	<chem>c(cccc1)(c2c(cc(NC(=O)C(C)(C)C)cc2)C(=O)C3=O)c13</chem>	C19H17NO3	307.343	SF1670
Selleck					
Chemicals	S7149	<chem>c1nc(C(C)=NNC(=S)N2CCC2)ccc1</chem>	C11H14N4S	234.321	NSC 319726
Selleck					
Chemicals	S7327	<chem>n1(c2ccc(OC)cc2)c(c3c([N+])([O-])=O)c1C)cc(O)cc3</chem>	C16H14N2O4	298.293	ID-8
Selleck					
Chemicals	S7167	<chem>c1ccn2c(c(OC)c(C)c2C(c3cc(C(=O)O[Na])c(N)cc3)=O)c1</chem>	C18H15N2NaO4	346.312	SSR128129E
Selleck					
Chemicals	S7340	<chem>c1c(Cl)c(c2nc(N)nc(SCCCC(=O)N)n2)c3c(c4ccc3)c1COC4</chem>	C19H18ClN5O2S	415.897	CH5138303
Selleck					
Chemicals	S7193	<chem>C1C(=O)Nc2c(nc2)c3c1c4c(ccc(Br)c4)[nH]3</chem>	C15H10BrN3O	328.163	1-Azakenpaulone
Selleck					
Chemicals	S7364	<chem>CN(c1ccc(c2cccc(NC(N(C)C)=O)c2)cc1)C</chem>	C17H21N3O	283.368	Atglistatin
Selleck					
Chemicals	S7209	<chem>c1(c2cccc2)cc3c([nH]cc3c4ccc(C(O)=O)c(C5CCCC5)c4)nc1</chem>	C25H22N2O2	382.454	GSK650394

Selleck					
Chemicals	S7378	<chem>c1c(S(=O)(=O)F)ccc(CCN)c1.Cl</chem>	C8H11ClFNO2S	239.695	AEBSF HCl
Selleck					
Chemicals	S7229	<chem>c1(NC(=O)C=Cc2cn(CC=Cc3ccccc3)nc2)c(N)cc(F)cc1</chem>	C21H19FN4O	362.4	RGFP966
Selleck					
Chemicals	S7399	<chem>CC(NC1=C(C(=O)CC(C)(C)C1)C2c3ccc([N+])([O-])=O)cc3)=C2C(OC4CCCCC4)=O</chem>	C25H30N2O5	438.516	FLI-06
Selleck					
Chemicals	S7430	<chem>c1cc(Oc2ccc(S(=O)(=O)CC3CS3)cc2)ccc1</chem>	C15H14O3S2	306.4	SB-3CT
Selleck					PRT062607 (P505-15,
Chemicals	S8032	<chem>n1cc(C(=O)N)c(Nc2cccc(n3ncnc3)c2)nc1N[C@H]4[C@H](N)CCCC4.Cl</chem>	C19H24ClN9O	429.907	BIIB057) HCl
Selleck					
Chemicals	S7448	<chem>[Ru]1(Cl)(OC(=O)CN1)(C=O)(C=O)C=O.[R]</chem>	C5H6ClNO5RRu	296.628	CORM-3
Selleck					
Chemicals	S8042	<chem>n1c(N)c(Cc2cc(OC)c(OCc3ccc(OC)cc3)cc2)cnc1N</chem>	C20H22N4O3	366.414	GW2580
Selleck					
Chemicals	S7461	<chem>c1ccc(Nc2ncnc(c3c(OC)ccc3)c2)cc1CS(=O)(=O)N</chem>	C18H18N4O3S	370.426	LDC000067
Selleck					
Chemicals	S8057	<chem>c1c2nc(Nc3cc(c(OCN4CCCC4)cc3)COCC=CCOCc5cc2ccc5)nc1</chem>	C28H32N4O3	472.579	Pacritinib (SB1518)
Selleck					
Chemicals	S7489	<chem>c1cc(Cl)ccc1CN(C=O)C(c2c3c(cc(Cl)cc3)[nH]c2C(=O)OCC)C(NC(C)(C)C)=O</chem>	C25H27Cl2N3O4	504.406	YH239-EE
Selleck					
Chemicals	S8077	<chem>c1(Cl)c(Cl)ccc(N2C(=O)C(Cl)=C(N3CCOCC3)C2=O)c1</chem>	C14H11Cl3N2O3	361.608	RI-1
Selleck					
Chemicals	S7505	<chem>CC(OCc1cc(c2cnn(C3CCNCC3)c2)cnc1N)c4c(Cl)c(F)ccc4Cl</chem>	C21H22Cl2FN5O	450.337	(S)-crizotinib
Selleck					
Chemicals	S7520	<chem>C1(=O)C2=C(C(CCC2)N(CC(=O)N(CCN(CC)CC)Cc3ccc(c4ccc(C(F)(F)F)cc4)cc3)C(SCc5ccc(F)cc5)=N1</chem>	C36H38F4N4O2S	666.771	Darapladib (SB-480848)
Selleck					
Chemicals	S7546	<chem>c1ccc(c2ccc(CC(=O)N(C)c3nc(C)c(S(N)(=O)=O)s3)cc2)nc1</chem>	C18H18N4O3S2	402.491	Pritelivir (BAY 57-1293)
Selleck					
Chemicals	S7635	<chem>N1(CCCCC2(C(NCC(F)(F)F)=O)c3c(cccc3)c4c2cccc4)CCC(NC(=O)c5ccccc5c6ccc(C(F)(F)F)cc6)CC1</chem>	C39H37F6N3O2	693.72	Lomitapide
Selleck					
Chemicals	S8007	<chem>c1(C(Nc2cccc2)=O)nc(c3ccc(S(C)(=O)=O)cc3)cnc1N</chem>	C18H16N4O3S	368.41	VE-821
Selleck					Vortioxetine (Lu
Chemicals	S8021	<chem>c1(C)cc(C)c(Sc2c(N3CCNCC3)cccc2)cc1.Br</chem>	C18H23BrN2S	379.358	AA21004) HBr
Selleck					
Chemicals	S7091	<chem>[C@H]1(C)[C@]2(O)O[C@H](C[C@H](OC)C(C)=CC=CC[C@H](C)C[C@H](C)C(=O)[C@H](OC)[C@H](O)C(C)=C[C@H](C)C(=O)C[C@H](C)[C@H]3C[C@H](OC)[C@H](n4cnnn4)CC3)OC(=O)[C@]5([H])N(CCCC5)C(=O)C2=O)CC1</chem>	C52H79N5O12	966.21	Zotatarlimus (ABT-578)
Selleck					
Chemicals	S7252	<chem>c1(C(F)(F)F)cc(c2nn(C=CC(NNc3ncnc3)=O)cn2)cc(C(F)(F)F)c1</chem>	C17H11F6N7O	443.306	KPT-330
Selleck					
Chemicals	S7102	<chem>n1c(N)c(c2onc(c3ccc(CNC)cc3)c2)nc(c4ccc(S(C(C)C)(=O)=O)cc4)c1</chem>	C24H25N5O3S	463.552	VE-822
Selleck					
Chemicals	S7265	<chem>C1CCC(C(NC(c2ccc(F)cc2)c3ccc(F)cc3)=O)(NC(=O)[C@H](CCCNC(=N)N)NC(C(C)C)C)C(=O)=O)C1</chem>	C35H49F2N7O4	669.805	MM-102
Selleck					
Chemicals	S7115	<chem>c1(C(F)(F)F)ccc(c2cc(OCc3c4c(sc(NC(=O)C)n4)ccc3)ncn2)cc1</chem>	C20H13F3N4O2S	430.403	AMG-517
Selleck					
Chemicals	S7280	<chem>C(=O)C(=O)Nc1ncc(Cl)cc1N[C@H]2CC[C@H](C(=O)N(C)C)C[C@H]2NC(=O)c3sc4c(CCN(C)C4)n3</chem>	C24H30ClN7O4S	548.058	Edoxaban
Selleck					
Chemicals	S7130	<chem>c1(SC#N)cc(SC#N)c(N)nc1N</chem>	C7H5N5S2	223.278	PR-619
Selleck					
Chemicals	S7295	<chem>c1(OC)cc2c(C(=O)NCC(c3cc(C)c(OCOC)c(C)c3)=N2)c(OC)c1</chem>	C20H22N2O5	370.399	RVX-208
Selleck					
Chemicals	S7140	<chem>c1(Cl)c(Cl)c2c(C(=O)CC2=O)c(Cl)c1Cl</chem>	C9H2Cl4O2	283.923	TCID
Selleck					
Chemicals	S7316	<chem>c1ccc(CNC(=O)c2ccc(c3nc(CS(=O)(=O)c4ccc(C)cc4)c(C)cc3)cc2)cn1</chem>	C25H23N3O4S	461.533	STF-118804
Selleck					
Chemicals	S7152	<chem>Cc1cc(c2cc(C=C3C(=O)N(c4ccc(C(O)=O)cc4)N=C3C)cc2)c([N+])([O-])=O)cc1C</chem>	C24H19N3O6	445.424	C646
Selleck					
Chemicals	S7329	<chem>c1ccc(OC2ccc(CNC(=O)c3nc(c4cc(Br)c(O)c(Br)c4)nc3)cc2)cc1</chem>	C22H15Br2N3O4	545.18	IOWH032
Selleck					
Chemicals	S7172	<chem>N(C(=O)CN1CCOCC1)[C@H](C)C(=O)N[C@H](Cc2ccc(OC)cc2)C(=O)N[C@H](Cc3ccccc3)C(=O)[C@]4(C)CO4</chem>	C31H40N4O7	580.672	ONX-0914 (PR-957)
Selleck					
Chemicals	S7351	<chem>c1(NCCCc2ccccc2)ccc(C)cc1N</chem>	C16H20N2	240.343	JSH-23
Selleck					
Chemicals	S7194	<chem>c1c(C)c(C#Cc2cnc3c(c[nH]3)c2)cc(C(=O)Nc4ccc(CN5CCN(C)CC5)c(C(F)(F)F)c4)c1.CS(O)(=O)=O.CS(O)(=O)=O</chem>	C31H35F3N6O7S2	724.771	GZD824
Selleck					
Chemicals	S7365	<chem>c1cc(C(=O)c2ccc(OC(CN3CCN(Cc4ccccc4)CC3)=O)cc2)ccc1</chem>	C27H28N2O3	428.523	AdipoRon

Selleck Chemicals	S7213	<chem>[C@H]1(CO)O[C@@]2([H])[C@]([H])(N=C(NCC)S2)[C@@H](O)[C@@H]1O</chem>	C9H16N2O4S	248.299	Thiamet G
Selleck Chemicals	S7379	<chem>c1c(O)c2c([C@H](C)[C@]3([H])C=C(O)[C@@]4(O)[C@]([H])([C@H](N(C)C)C(O)=C(C(N)=O)C4=O)[C@H]3O)C2=O)cc1.c5c(O)c6c([C@H](C)[C@]7([H])C=C(O)[C@@]8(O)[C@]([H])([C@H](N(C)C)C(O)=C(C(N)=O)C8=O)[C@H]7O)C6=O)cc5.Cl.O.CCO.Cl</chem>	C46H58Cl2N4O18	1025.875	E-64
Selleck Chemicals	S7233	<chem>c1c(c2cc(NC(OCC)=O)c3n(c(C)nn3)n2)cc(NS(=O)(=O)C)c(C)c1</chem>	C17H20N6O4S	404.443	Bromosporine Caffeic Acid Phenethyl
Selleck Chemicals	S7414	<chem>C(OCCc1cccc1)(=O)C=Cc2ccc(O)c(O)c2</chem>	C17H16O4	284.307	Ester
Selleck Chemicals	S7434	<chem>c1cc2c(cc(C[C@H](NC(=O)C(CC(=O)NO)CC(C)C)C(=O)N[C@@H](C)C(=O)NCCN)cc2)cc1</chem>	C26H37N5O5	499.602	TAPI-1
Selleck Chemicals	S8034	<chem>c1cc(NC(=O)C)c2c(C(=O)N[C@H](CS(=O)C(=O)c3ccc(OC)c(OCC)c3)C2=O)c1</chem>	C22H24N2O7S	460.5	Apremilast (CC-10004)
Selleck Chemicals	S7449	<chem>c1cc([N+])([O-])=O)c2c(cc(C(O)=O)[nH]2)c1</chem>	C9H6N2O4	206.155	CRT0044876
Selleck Chemicals	S8043	<chem>c1c2c(c3C(=O)N(CCCCCC(=O)NO)C2=O)c(ccc3)cc1</chem>	C18H18N2O4	326.347	Scriptaid
Selleck Chemicals	S7462	<chem>c1cc(OCC(=O)N(C(C)C)Cc2onc(c3cnccc3)n2)ccc1CCC</chem>	C22H26N4O3	394.467	PI-1840
Selleck Chemicals	S8058	<chem>c1ccc(C(Oc2c(c(O)cc(O)c2[C@H]3CCN(C)[C@H]3CO)C4=O)=C4)c(Cl)c1.Cl</chem>	C21H21Cl2NO5	438.301	P276-00
Selleck Chemicals	S7490	<chem>c1cc2c(c3C(=O)N(CCCSc4nnc(c5cncnc5)n4c6ccc(OC)cc6)C2=O)c(ccc3)c1</chem>	C29H23N5O3S	521.59	WIKI4
Selleck Chemicals	S8078	<chem>C1[C@@]([H])([C@]2(C(O)C)CCC1(C)C)[C@@]([H])([C@]3(C)CC2)C(=O)C=C([C@]34C)[C@@]([C@]5([H])CC4)C=C(C#N)C(=O)C5(C)</chem>	C32H43NO4	505.688	Bardoxolone Methyl
Selleck Chemicals	S7508	<chem>C1Cc2c(sc(NC(=O)c3c4c(cccc4)ccc3)c2C#N)OC1</chem>	C20H16N2OS	332.419	JNK Inhibitor IX
Selleck Chemicals	S7523	<chem>C1N(c2ccc(Nc3c4n(ccn4)cc(c5ccc6c([nH]nc6)c5)n3)cc2)CCOC1</chem>	C23H21N7O	411.459	GS-9973
Selleck Chemicals	S7565	<chem>c1(O)c(N(c2nc(Nc3ccc(N4CCN(C)CC4)cc3)nc2)C(Oc5c(C)cccc5C)=O)cc(c(OC)c1</chem>	C32H36N6O4	568.666	WH-4-023
Selleck Chemicals	S8000	<chem>c1cc(C(=O)NC(=S)Nc2ccc(NC(=O)C)cc2)ccc1C(C)C</chem>	C20H23N3O2S	369.481	Tenovin-1
Selleck Chemicals	S8009	<chem>c1(ccc(O)c(O)c1)C=C(C#N)C#N</chem>	C10H6N2O2	186.167	AG-18
Selleck Chemicals	S8022	<chem>[C@H]1(CO)O[C@@H](c2ccc(Cl)c(Cc3ccc(O[C@H]4COCC4)cc3)c2)[C@H](O)[C@@H](O)[C@H]1O</chem>	C23H27ClO7	450.909	Empagliflozin (BI 10773)
Selleck Chemicals	S7092	<chem>c1c(n2(C)c(C(=NN3CCN(Cc4ccccc4)CC3)c(C)n2)cccc1</chem>	C23H27N5	373.494	SANT-1
Selleck Chemicals	S7253	<chem>c1nc(N)c(C(Nc2ccnc2)=O)nc1c3ccc(S(N4CCN(C)CC4)(=O)=O)cc3</chem>	C21H23N7O3S	453.517	AZD2858
Selleck Chemicals	S7104	<chem>c1c(C=C2SC(=O)NC2=O)c(N3CCC[C@@H](N)C3)c(c4ccccc4)cc1</chem>	C21H21N3O2S	379.475	AZD1208
Selleck Chemicals	S7266	<chem>n1cc(C2[C@]3([H])[C@]([H])(C=CC3)c4c(c(F)cc(F)c4)N2)ccc1</chem>	C17H14F2N2	284.303	Golgicide A 3-Deazaneplanocin A
Selleck Chemicals	S7120	<chem>c1cc2c(ncn2[C@H]3[C@@H](O)[C@H](O)C(CO)=C3)c(N)n1</chem>	C12H14N4O3	262.265	(DZNeP)
Selleck Chemicals	S7282	<chem>CN1CCC(NC(C(NO)C2=C3C(Oc4ccc([N+])([O-])=O)cc4)=CC(=O)C=C3O)=C2)O)CC1</chem>	C22H22N4O7	454.433	NMS-E973
Selleck Chemicals	S7132	<chem>c1c([N+])([O-])=O)c(Sc2c(Cl)c(Cl)ccc2)sc1C(C)=O</chem>	C12H7Cl2NO3S2	348.225	P5091 (P005091)
Selleck Chemicals	S7297	<chem>c1c(c2c3c(cccc3)n(C)c2)nc(Nc4cc(NC(=O)C=C)c(N(C)CCN(C)C)cc4O)nc1</chem>	C28H33N7O2	499.607	AZD9291
Selleck Chemicals	S7142	<chem>Cc1ccc(S(c2cc([N+])([O-])=O)cc2)(=O)=O)cc1</chem>	C11H9NO5S	267.258	NSC697923
Selleck Chemicals	S7317	<chem>n1cc(Cl)c(Oc2cccc(NC(=O)CC)c2)nc1Nc3ccc(N4CCN(C)CC4)cc3OC</chem>	C25H29ClN6O3	496.989	WZ4003
Selleck Chemicals	S7153	<chem>c1cc(C=C2SC(=S)NC2=O)ccc1CC</chem>	C12H11NOS2	249.352	10058-F4
Selleck Chemicals	S7330	<chem>c1(Cl)ccc(SCC(=O)N2CCC(C(=O)NCCSSCCN(C)C)CC2)cc1.C(C(O)=O)(F)(F)F</chem>	C22H31ClF3N3O4S3	590.142	6H05
Selleck Chemicals	S7173	<chem>c1(F)c(Nc2cccc(NC(=O)C=C)c2)nc(Nc3ccc(OCCOC)cc3)nc1</chem>	C22H22FN5O3	423.44	AVL-292
Selleck Chemicals	S7353	<chem>C(CN(C(C)C)C[C@H]1O[C@@H](n2ccc3c2ncn3N)[C@H](O)[C@@H]1O)CNC(=O)Nc4ccc(C(C)C)cc4</chem>	C28H41N7O4	539.67	EPZ004777
Selleck Chemicals	S7195	<chem>c1cc(c2csc(NC(=O)NCCc3cc(O)ccc3)n2)ccn1</chem>	C16H14N4O2S	326.373	RKI-1447

Selleck					
Chemicals	S7367	<chem>n1cc(C(F)(F)F)c(NC)nc1Nc2c(C)nn(C(C)(C)C#N)c2</chem>	C14H16F3N7	339.319	GNE-0877
Selleck					
Chemicals	S7214	<chem>c(cc(Nc1ccc(F)cc1F)cc2)(CCc3c(cc(OC[C@H](O)CO)cc3)C4=O)c24</chem>	C24H21F2NO4	425.425	Skepinone-L
Selleck					
Chemicals	S7380	<chem>C(C[C@@H](C(=O)N)[C@H](C(=O)N)[C@H](C([H])=O)CCCNC(=N)N)CC(C)C)NC(=O)C(C)C.[R]</chem>	C20H38N6O4R	426.554	Leupeptin Hemisulfate
Selleck					
Chemicals	S7234	<chem>c1nc2c(c(C(=O)O)ccc2O)cc1</chem>	C10H7NO3	189.167	IOX1
Selleck					
Chemicals	S7417	<chem>Cl.Cl.n1c(N(C)C)c2c(n([C@@H]3O[C@@H](CO)[C@H](NC(=O)[C@@H](N)Cc4ccc(OC)cc4)[C@@H]3O)cn2)nc1</chem>	C22H31Cl2N7O5	544.431	Puromycin 2HCl
Selleck					
Chemicals	S7435	<chem>c1nc(NC(=O)NCc2ccc(OC)cc2)sc1[N+][I-](O-)=O</chem>	C12H12N4O4S	308.313	AR-A014418
Selleck					
Chemicals	S8035	<chem>c1nc(C(=O)Nc2ccc(S(Nc3ccccc3Cl))(=O)=O)c(Cl)c2)ccc1</chem>	C18H13Cl2N3O3S	422.285	VU 0364439
Selleck					
Chemicals	S7450	<chem>CC(Nc1ccc(Cc2ccc(NC(C)=O)cc2)cc1)=O</chem>	C17H18N2O2	282.337	FH1(BRD-K4477)
Selleck					
Chemicals	S8044	<chem>c1(C)cc2c(nc(NCCN)c3n2c(C)cn3)cc1</chem>	C14H17N5	255.318	BMS-345541
Selleck					
Chemicals	S7467	<chem>C1N(Cc2c(c3c(c4ccc3)cccc4)cn(Cc5n(Cc6ccc(Br)cc6)cnc5)c2)=O)COC1N1(C(=O)N2CCNC(=O)C2)[C@@H](c3ccc(Cl)cc3)[C@H](c4ccc(Cl)cc4)N=C1c5c(OC(C)C)cc(OC)cc5</chem>	C30H27BrN4O2	555.465	LB42708
Selleck					
Chemicals	S8059	<chem>C1c5c(OC(C)C)cc(OC)cc5</chem>	C30H30Cl2N4O4	581.49	Nutlin-3a
Selleck					
Chemicals	S7493	<chem>C(=O)(c1cccc1)Nc2nc(c3ccc(C)cc3C)cs2</chem>	C18H16N2OS	308.397	INH1
Selleck					
Chemicals	S7509	<chem>Cc1oc(CNc2c3c(ccc(c4oc(CO)cc4)c3)ncn2)cc1</chem>	C19H17N3O3	335.357	ML167
Selleck					
Chemicals	S7525	<chem>C1N(c2cc(OCC)c(Nc3ncc4c(N(C)C)c5c(cccc5)C(=O)N4C)n3)cc2)CCC(O)C1</chem>	C26H30N6O3	474.555	XMD8-92
Selleck					
Chemicals	S7566	<chem>C1(=O)N(C)C(=O)C(NCCc2ccc(F)cc2)=C1c3c(C)[nH]c4c3cccc4</chem>	C22H20FN3O2	377.412	IM-12
Selleck					
Chemicals	S8001	<chem>c1cc(Nc2ncc(C(NCCCCC(=O)NO)=O)cn2)c3cccc3)ccc1</chem>	C24H27N5O3	433.503	Rocilinostat (ACY-1215)
Selleck					
Chemicals	S8010	<chem>C(O)(=O)C=CC(O)=O.C(#N)c1cc(CN2CCC(Nc3ncc4c3cc(Cl)s4)CC2)ccc1F</chem>	C23H21ClFN5O4S	517.96	PRX-08066 Maleic acid
Selleck					
Chemicals	S8023	<chem>c(CCCC1)(sc(NC(=O)c2ccc(OC)c(OC)c2)c3C(N)=O)c13</chem>	C18H20N2O4S	360.427	TCS 359
Selleck					
Chemicals	S7093	<chem>S(c1c(c2ccc1O)cccc2)Sc3c(c4ccc3O)cccc4</chem>	C20H14O2S2	350.454	IPA-3
Selleck					
Chemicals	S7255	<chem>c1(OC(F)(F)F)c(Nc2ncc3c(c4c(c(C(=O)N)nn4CCO)CC3)n2)cc(N5CCN(C)CC5)cc1</chem>	C24H27F3N8O3	532.518	NMS-P937 (NMS1286937)
Selleck					
Chemicals	S7106	<chem>c([nH]cc1c2nc(Nc3ccc(N4CCC(N)CC4)cc3OC)ncc2Cl)(cccc5)c15</chem>	C24H25ClN6O	448.948	AZD3463
Selleck					
Chemicals	S7269	<chem>C1(=O)N(C)C2C(C=NC(Nc3cc(SC)ccc3)=N2)C=C1c4c(Cl)cccc4Cl</chem>	C21H18Cl2N4OS	445.365	PD173955
Selleck					
Chemicals	S7122	<chem>c1(N(C2CC3)C3CC(NC(c4c(C)cc(C(=O)N)c(N[C@H](C)CC)c4)=O)C2)ccc(C(C5CC5)=O)cn1</chem>	C29H37N5O3	503.636	XL888
Selleck					
Chemicals	S7284	<chem>c1(C(F)(F)F)c(Nc2cc(NC(C=O)O)ccc2)nc(Nc3ccc(N4CCN(C(=O)C)CC4)c3OC)nc1</chem>	C27H28F3N7O3	555.552	CO-1686 (AVL-301)
Selleck					
Chemicals	S7133	<chem>c1c([N+][O-])=O)c(Sc2c(F)cc(F)cc2)sc1C(C)=O</chem>	C12H7F2NO3S2	315.316	P22077
Selleck					
Chemicals	S7300	<chem>c1(cc(NC(=O)CN(C)C)cc2)c2NC(=O)c3c1cccc3.Cl</chem>	C17H18ClN3O2	331.797	PJ34 HCl
Selleck					
Chemicals	S7143	<chem>c1(c2cc(C)nc2)nc(C(C(=O)Nc3ncc(c4nccnc4)cc3)cc1C</chem>	C23H20N6O	396.444	LGK-974
Selleck					
Chemicals	S7319	<chem>c1(NCCCN2CCOCC2)nccc(Nc3cc(c4cc3)c(c5n4CC)cccc5)n1</chem>	C25H30N6O	430.545	EHop-016
Selleck					
Chemicals	S7155	<chem>ONC(=O)[C@@H](CS)c1cccs1)[C@H](CC(C)C)C(=O)N[C@H](Cc2ccccc2)C(NC)=O</chem>	C23H31N3O4S2	477.64	Batimastat (BB-94)
Selleck					
Chemicals	S7332	<chem>c1(Cl)cc(OC)c(NCC(=O)N2CCC(NS(=O)(=O)C=C)CC2)cc11</chem>	C16H21ClIN3O4S	513.778	K-Ras(G12C) inhibitor 9
Selleck					
Chemicals	S7176	<chem>c1(csc(Nc2ccc(O)cc2)n1)c3ccc(Cl)cc3</chem>	C15H11ClN2OS	302.779	SKI II
Selleck					
Chemicals	S7355	<chem>c(ccc(Cl)c1)(C(=O)N(Nc2ccccc2)C([C@@H](CC#C)N(CCCN)C(c3c(F)c(Cl)cc3)=O)=N4)c14</chem>	C28H24Cl2FN5O2	552.427	ARQ 621
Selleck					
Chemicals	S7198	<chem>c1cc2c(NC(=C3c4c(cc(Br)cc4)NC3=O)C2=NO)cc1</chem>	C16H10BrN3O2	356.173	BIO
Selleck					
Chemicals	S7368	<chem>n1cc(C(F)(F)F)c(NC)nc1Nc2cnn([C@@H]3[C@H](F)CN(C4COC4)CC3)c2Cl</chem>	C17H20ClF4N7O	449.834	GNE-9605

Selleck					Losmapimod
Chemicals	S7215	<chem>c1(C(=O)NC2CC2)cc(c3ncc(C(=O)NCC(C)(C)C)cc3)c(C)C(F)c1</chem>	C22H26FN3O2	383.459	(GW856553X)
Selleck		<chem>c1cc2c(c(C[C@H](NC(=O)[C@H](CC(C)C)NP(=O)(O)O)[C@@H]3O[C@@H](C)[C@H](O)[C@@H](O)[C@H]3O)C(O)=O)c[nH]2)cc1.[Na][Na]</chem>	C23H34N3Na2O10P	589.483	Phosphoramidon Disodium Salt
Chemicals	S7237	<chem>C1C(N)C1c2ccc(c3ccccc(O)c3)cc2</chem>	C15H15NO	225.286	OG-L002
Selleck					
Chemicals	S7421	<chem>c1c(Nc2[nH]nc(c23)ncnc3N)ccc(F)c1</chem>	C11H9FN6	244.228	CGP 57380
Selleck					
Chemicals	S7436	<chem>CCCCCCCCCCCCCCCCn1c(C)[n+](Cc2ccccc2)cc1.[I-]</chem>	C27H45IN2	524.564	NH125
Selleck					
Chemicals	S8036	<chem>c1(C(=O)C=Cc2ccc(O)c(O)c2)ccc(O)cc1O</chem>	C15H12O5	272.253	Butein
Selleck					
Chemicals	S7451	<chem>Cc1ccc(Cl)cc1N(S(C)(=O)=O)CC(Nc2c(F)cccc2F)=O</chem>	C16H15ClF2N2O3S	388.817	FPH1 (BRD-6125)
Selleck					
Chemicals	S8047	<chem>c1(O)ccc(C=NNC(c2cc3c(cccc3)cc2O)=O)cc1O</chem>	C18H14N2O4	322.315	Dynasore
Selleck					
Chemicals	S7470	<chem>c1cnc(C=NNC(N)=S)c(N)c1</chem>	C7H9N5S	195.245	Triapine
Selleck		<chem>c1(O)cc2c(cc(C)c(c3c(C)cc4c(cc(O)c(O)c4C(NC[C@@H](c5ccccc5)C)=O)c3O)c2O)c(C(NC[C@@H](c6ccccc6)C)=O)c1O</chem>	C42H40N2O8	700.776	Sabutoclox
Chemicals	S8061				
Selleck					
Chemicals	S7494	<chem>c1(C)cc(C)c(c2nc(NC(=O)c3ccccc3)sc2)c(C)c1</chem>	C19H18N2OS	322.424	INH6
Selleck					
Chemicals	S7513	<chem>CN1C(=O)N(Cc2cc(F)ccc2C#N)C(N3CC(N)CCC3)=CC1=O</chem>	C18H20FN5O2	357.382	Trelagliptin
Selleck					
Chemicals	S7526	<chem>C(NCCO)(=O)c1cccc(c2cc(Nc3ccc(OC(F)(F)F)cc3)ncn2)c1</chem>	C20H17F3N4O3	418.369	GNF-5
Selleck					
Chemicals	S7587	<chem>c1(NC(c2nnc2N)=NO)cc(Cl)c(F)cc1</chem>	C9H7ClFN5O2	271.636	INCB024360
Selleck					
Chemicals	S8002	<chem>c1c(C(O)=O)c2c(n(Cc3c(C)c(C(F)F)cc3)c(C)n2)cc1N4CCOCC4</chem>	C22H22F3N3O3	433.424	GSK2636771
Selleck					
Chemicals	S8014	<chem>C(O)(CCc1ccc(NCc2cccc(Oc3ccccc3)c2)cc1)=O</chem>	C22H21NO3	347.407	GW9508
Selleck					
Chemicals	S8024	<chem>n1c(c2ncc1c3ccccc3)cc(OC)c(OC)c2</chem>	C16H14N2O2	266.295	Tyrphostin AG 1296
Selleck		<chem>c(scc1)(c(Nc2n[nH]c3c2CN(C(N[C@@H](c4ccccc4)CN(C)C)=O)C3(C)C)nc(C)n5)c15</chem>	C25H30N8OS	490.624	PF-3758309
Chemicals	S7094				
Selleck		<chem>c1cc2c(nc(CCc3ccc(OC)c(Cl)c3)n2C[C@@H](N4CCOCC4)C)cc1c5c(C)onc5</chem>	C28H33ClN4O3	509.04	SGC-CBP30
Chemicals	S7256	<chem>C</chem>			
Selleck		<chem>CC(n1nc(c2c(F)c(NS(C)(=O)=O)cc(Cl)c2)c3ccnc(NCC(NC(OC)=O)C)n3)c1)C</chem>	C22H27ClFN7O4S	540.011	LGX818
Chemicals	S7108				
Selleck					
Chemicals	S7270	<chem>c1c(C(F)F)F)cc(NC(=O)c2ccncc2)c(N3CCCC3)c1</chem>	C18H18F3N3O	349.35	SRPIN340
Selleck					
Chemicals	S7124	<chem>c1n2c(c(NNC(c3nccnc3)=O)nc4c2ccc(F)c4)cc1</chem>	C16H11FN6O	322.297	SC144
Selleck					
Chemicals	S7285	<chem>c1c(n2c(COc3cc(C)c(c4ccc(S(C)(=O)=O)cc4)cc3)nnc2SC5CCCC5)cncc1</chem>	C27H28N4O3S2	520.666	NMS-873
Selleck					
Chemicals	S7134	<chem>c1cc(n2c(C)cc(C(=O)CN3CCCC3)c2)ccc1F</chem>	C18H21FN2O	300.371	IU1
Selleck					
Chemicals	S7301	<chem>C(CCS1)(N=C(SCC(=O)Nc2ccc(c3ccccc3)cn2)N(c4ccccc4)C5=O)=C15</chem>	C25H20N4O2S2	472.582	IWP-L6
Selleck					
Chemicals	S7145	<chem>c1cc2c(c(c3ncc(CN4CCOCC4)cc3)c(O)[nH]2)cc1C#N</chem>	C19H18N4O2	334.372	AZD1080
Selleck					
Chemicals	S7320	<chem>c1(cc(OC)cc2)c2SC(=CC(=O)C)N1CC</chem>	C13H15NO2S	249.329	TG003
Selleck					Ilomastat (GM6001,
Chemicals	S7157	<chem>c1cc2c([nH]cc2C[C@H](NC([C@H](CC(C)C)CC(NO)=O)=O)C(NC)=O)cc1</chem>	C20H28N4O4	388.461	Galaridin)
Selleck					
Chemicals	S7333	<chem>c1cc(OC(C)=O)N2CCC(NC(=O)CCCS)CC2c(Cl)cc1Cl</chem>	C17H22Cl2N2O3S	405.339	K-Ras(G12C) inhibitor 6
Selleck					
Chemicals	S7177	<chem>c1cc(S(=O)(=O)Cc2cc(C)cc(OCc3ccc(CN4CCC[C@@H]4CO)cc3)c2)ccc1</chem>	C27H31NO4S	465.604	PF-543
Selleck					
Chemicals	S7356	<chem>c1c(NS(c2ccccc2)(=O)=O)cc(c3ccc4n(C(C(OC)=O)cn4)c3)cn1</chem>	C21H18N4O4S	422.457	HS-173
Selleck					
Chemicals	S7199	<chem>c1cc2c(c(NCc3ccccc3)nc(NCc4ccccc4)n2)cc1</chem>	C22H20N4	340.421	DBeQ
Selleck					
Chemicals	S7369	<chem>C1SC(NN=C(C(O)=O)Cc2c(N(O)O)cccc2)=NC1c3ccc(Cl)c(Cl)c3</chem>	C18H16Cl2N4O4S	455.315	4EGI-1
Selleck					
Chemicals	S7217	<chem>c1cc(C(=O)Nc2ncc3c(cc[nH]3)c2)ccc1</chem>	C14H11N3O	237.257	OAC1

Selleck							(-)-p-Bromotetramisole
Chemicals	S7383	<chem>OC(=O)C(=O)O.C1SC(=N2)N(C[C@@H]2c3ccc(Br)cc3)C1</chem>	C13H13BrN2O4S	373.222			Oxalate
Selleck							
Chemicals	S7241	<chem>C1C(NS(c2ccc(c3ccsc3)c(NC(Nc4cc(C(F)(F)F)ccc4)=O)c2)(=O)=O)C1</chem>	C21H18F3N3O3S2	481.511			AGI-6780
Selleck		<chem>c1(ccnc2c2cccc1S(=O)(=O)N(C)[C@@H](Cc3ccc(OS(=O)(=O)c4cccc5c4ccnc5)cc3)C(=O)N6CCN(c7ccccc7)CC6</chem>	C38H35N5O6S2	721.844			KN-62
Chemicals	S7422						
Selleck							
Chemicals	S7437	<chem>c1ccc(C=CC(NC(NC(Nc2ccc(Cl)cc2)=S)C(Cl)(Cl)Cl)=O)cc1</chem>	C18H15Cl4N3OS	463.208			Sal003
Selleck							
Chemicals	S8037	<chem>c1cc2c([nH]cc2CC3C(=O)N(C)C(=S)N3)cc1</chem>	C13H13N3OS	259.327			Necrostatin-1
Selleck							
Chemicals	S7452	<chem>c1cc(OC)c(NC(=S)Nc2cn(CC)nc2C(=O)N)cc1Cl</chem>	C14H16ClN5O2S	353.827			FPH2 (BRD-9424)
Selleck		<chem>c1cc(C2=C(C)N3CCN(c4ccc(C(NS(=O)(=O)c5cc([N+][[O-]])=O)c(NCC6CCOCC6)cc5)=O)c(Oc7cc8c([nH]cc8)nc7)c4)CC3)CCC(C)(C)C2)ccc1Cl</chem>	C45H50ClN7O7S	868.439			ABT-199 (GDC-0199)
Chemicals	S8048						
Selleck							
Chemicals	S7473	<chem>CCCCN(C(Nc1ccccc1)=O)Cc2ccc(C(NO)=O)cc2</chem>	C19H23N3O3	341.404			Nexturastat A
Selleck		<chem>N1(C(=O)N2CCNC(=O)C2)[C@H](c3ccc(Cl)cc3)[C@@H](c4ccc(Cl)cc4)N=C1c5c(OC(C)C)cc(OC)cc5</chem>	C30H30Cl2N4O4	581.49			Nutlin-3b
Chemicals	S8065						
Selleck							
Chemicals	S7497	<chem>Cc1[nH]c(c2c1CCNC(c3scccc3)=O)cccc2</chem>	C16H16N2OS	284.376			CK-636
Selleck							
Chemicals	S7515	<chem>C1C(c2ccccc2)=NOC1CC(O)=O</chem>	C11H11NO3	205.21			VGX-1027
Selleck							
Chemicals	S7528	<chem>c1(C(F)(F)F)c(NCC)nc(Nc2c(OC)cc(C(=O)N3CCOCC3)c(F)c2)nc1</chem>	C19H21F4N5O3	443.395			GNE-7915
Selleck							
Chemicals	S7589	<chem>c1c(n2c(c3ccc(n4ccnc4)cc3)ccc2CCC(=O)O)c(C)cc(C(=O)N)c1</chem>	C24H22N4O3	414.456			N6022
Selleck							
Chemicals	S8003	<chem>N(c1cc(Cl)ccc1OC)C(Nc2c(c3nc(C)c2)cccc3)=O</chem>	C18H16ClN3O2	341.792			PQ 401
Selleck		<chem>N(c1cccc(Oc2c(c3ncn2)cc(OC)c(OC)c3)c1)C(Nc4cc(C(C)(C)C(F)(F)F)on4)=O</chem>	C24H22F3N5O5	517.457			CEP-32496
Chemicals	S8015						
Selleck							
Chemicals	S8025	<chem>c1c(C(F)(F)F)ccc(S(=O)(CCNC(=O)c2ccc(Cl)cc2)=O)n1</chem>	C15H12ClF3N2O3S	392.781			GSK3787
Selleck							
Chemicals	S7096	<chem>c1(CCC(Nc2nc3c(cc(Cl)cc3)s2)=O)ccc(OC)c(O)C)c1</chem>	C18H17ClN2O3S	376.857			KY02111
Selleck							
Chemicals	S7257	<chem>c1ccc(NC(=O)C=C)cc1Nc2nc(Nc3ccc(Oc4cc(C(=O)N)C)ccc4)cc3)nc2F</chem>	C26H22FN7O3	499.496			CNX-774
Selleck		<chem>n1nc2n(c3c(c(C)c(C)s3)C4ccc(Cl)cc4)=N[C@@H]2CC(=O)OC(C)(C)C)c1C</chem>	C23H25ClN4O2S	456.988			(+)-JQ1
Chemicals	S7110						
Selleck							
Chemicals	S7272	<chem>c1(O)c(C=O)c2c(C(C)=CC(=O)O2)cc1</chem>	C11H8O4	204.179			478C
Selleck							
Chemicals	S7125	<chem>c1(C(F)(F)F)cc(c2nn(C=CC(OC(C)C)=O)cn2)cc(OC)c1</chem>	C16H16F3N3O3	355.312			KPT-185
Selleck							
Chemicals	S7289	<chem>c1cc(C(=O)C=Cc2nc3c(ccccc3)cc2)ccn1</chem>	C17H12N2O	260.29			PFK15
Selleck							
Chemicals	S7135	<chem>c1(Cl)cc2c(N(Cc3c(Cl)ccc(Cl)c3)C(=O)C2=NOC(C)=O)cc1</chem>	C17H11Cl3N2O3	397.64			LDN-57444
Selleck							
Chemicals	S7303	<chem>n1c(Nc2c(C)cc(C=CC#N)cc2C)ccnc1Nc3ccc(C#N)cc3</chem>	C22H18N6	366.419			Rilpivirine
Selleck							
Chemicals	S7146	<chem>CC(OCc1ccc(c2cnc3n(ncc3c4c(c5ncc4)ccccc5)c2)cc1)C</chem>	C24H20N4O	380.442			DMH1
Selleck							
Chemicals	S7324	<chem>c1(c2nc(C(F)(F)F)on2)cc(C(=O)NCC3(c4sc(c5ccccc5)n4)CCOCC3)ccc1</chem>	C25H21F3N4O3S	514.519			TMP269
Selleck		<chem>c1(CN2CCN(CC)CC2)cn(C(Nc3ncc(F)c(c4cc5c(nc(C)n5C(C)C)c(F)c4)n3)cc1.CS(O)(=O)=O</chem>	C28H36F2N8O3S	602.699			LY2835219
Chemicals	S7158						
Selleck							
Chemicals	S7336	<chem>c1(l)cc(C(O)=O)c(NC(=O)[C@@H](NCc2ccccc2)Cc3ccccc3)cc1</chem>	C23H21N2O3	500.329			CW069
Selleck							
Chemicals	S7185	<chem>C1CCC(NC(=O)C(C2ccccc2C)N(c3ccccc(F)c3)C(=O)Cn4c(C)ccc4)CC1</chem>	C27H31FN4O2	462.559			AGI-5198
Selleck		<chem>c1ccc(CNc2nc(Nc3cc(CC(=O)N4)c4cc3)ccc2C(F)(F)F)c(N(S(C)(=O)=O)C)n1.Cl</chem>	C21H21ClF3N7O3S	543.95			PF-562271 HCl
Chemicals	S7357						
Selleck		<chem>c1(C(F)(F)F)c(Nc2cc(NC(=O)C=C)ccc2)nc(Nc3ccc(NC4CN(CCF)C4)cc3OC)nc1</chem>	C26H27F4N7O2	545.532			CNX-2006
Chemicals	S7206						
Selleck		<chem>c1ccc(C(N(c2ccc(C(O)=O)cc2)C(=O)C3=Cc4cc(c5ccc([N+][[O-]])=O)cc5)cc4)=C3)cc1</chem>	C28H18N2O6	478.452			4E1RCat
Chemicals	S7370						
Selleck		<chem>C(N(c1cc(C(F)(F)F)ccc1)C(=O)C(C(=O)Nc2ccc(S(=O)(=O)C)cn2)=C3)=C3c4n(C)ccc4</chem>	C24H20F3N5O4S	531.507			Alvelestat (AZD9668)
Chemicals	S7218						

Selleck					
Chemicals	S7391	[C@@H](NC(=O)OCc1ccccc1)(C(=O)NC(C)C(=O)CF)Cc2ccccc2	C21H23FN2O4	386.417	Z-FA-FMK
Selleck					
Chemicals	S7242	c1c2c(C(=O)N(c3ccccc3OCC)C(C)(N4CCN(C(=O)COc5ccc(Cl)cc5)CC4)C)=N2)ccc1	C30H31ClN4O4	547.045	Erastin
Selleck					
Chemicals	S7423	c1(ccccc1CN(C)C)C=Cc2ccc(Cl)cc2N(CCO)S(=O)(=O)c3ccc(OC)cc3.P(O)(O)(=O)=O.[H]	C26H32ClN2O8PS	599.033	KN-93 Phosphate
Selleck					
Chemicals	S7438	CC(NC(CCC(Nc(c1C2=O)cccc1)=N2)=O)c3ccccc3	C19H19N3O2	321.373	ME0328
Selleck					
Chemicals	S8038	c1cc2c(C=CNC2=O)c(OCC(=O)c3ccccc3)c1	C17H13NO3	279.29	UPF 1069
Selleck					
Chemicals	S7458	CCNC(C)(NNC1=C2C(=O)C=C(O)C(CI)=C2)C1c3ccc(OC)cc3=O	C19H18ClN3O4	387.817	VER-49009
Selleck					
Chemicals	S8050	c1c2c(c3c(CO C(=O)N3c4ccc(C(C)(C)C#N)cc4)cn2)cc(c5cc6c(cccc6)nc5)c1O1C=C(OCCCCCSc2c3c(cc(C(F)(F)F)cc3)nc2)C(=O)C=C1CN4CCOCC4.Cl.Cl	C30H22N4O2	470.521	ETP-46464
Selleck					
Chemicals	S7482		C25H29Cl2F3N2O4S	581.475	EHT 1864
Selleck					
Chemicals	S8072	c1cc(C(=O)NC(C)CCC)cc(Cl)c1Cl	C12H15Cl2NO	260.16	NSC 405020
Selleck					
Chemicals	S7499	c1c(NN=C(C#N)C(=O)c2noc(C(C)(C)C)c2)cccc1Cl	C16H15ClN4O2	330.769	ESI-09
Selleck					
Chemicals	S7516	Cc1n(c2ccc(Cl)cc2)nc1C(Nc3ccc(N4CCC(N5CCOCC5)CC4)c(C#N)c3)=O	C27H29ClN6O2	505.011	Y-320
Selleck					
Chemicals	S7529	c1(c2ncc(C)c(NCc3ccc(n4ccnn4)cc3)n2)cccc1C(C)C	C23H24N6	384.477	ML323
Selleck					Santacruzamate A
Chemicals	S7595	c1ccccc1CCNC(=O)CCNC(=O)OCC	C15H22N2O3	278.347	(CAY10683)
Selleck					
Chemicals	S8004	C(c1ccc(c2c1)cccc2)(=O)CCN(Cc3ccccc3)C(C)C.Cl	C23H26ClNO	367.912	ZM 39923 HCl
Selleck					
Chemicals	S8016	N(C)Cc1cc(c2ccccc2F)n(S(c3ccccc3)(=O)=O)c1.C(O)(=O)C=CC(O)=O	C21H20FN3O6S	461.463	TAK-438
Selleck					
Chemicals	S8028	c1cc2c(ncc(C(=O)Nc3cc(O)C(O)C)cc3C(=O)Nc4ccc(CCN5CCc6c(cc(O)C)c(O)C)c6)C5)cc4)c2)cc1	C38H38N4O6	646.732	Tariquidar
Selleck					
Chemicals	S7097	n1c(c2cc(F)ccc2[C@H]3Cc4c(C(C)nc(N)n4)C(=O)N3)cccc1OC	C20H18FN5O2	379.388	HSP990 (NVP-HSP990)
Selleck					
Chemicals	S7258	Cc1sc(Sc2c(c3ncn2)cc(O)C(O)C)c3nn1	C13H12N4O2S2	320.39	SKLB1002
Selleck					
Chemicals	S7111	c1ccc2c(c3n(cnc3)C2CC(O)C4CCCCC4)c1	C18H22N2O	282.38	NLG919
Selleck					
Chemicals	S7273	n1c(N2CCC(c3nc(C(=O)Nc4[nH]c5c(ccc(C(=O)c6ccccc6)c5)n4)cs3)CC2)c7c(ccs7)nc1	C29H23N7O2S2	565.669	SC75741
Selleck					
Chemicals	S7127	c1cc(CN2CC3=C(N(Cc4ccccc4C)C(=N5)N(CC5)C3=O)CC2)ccc1	C24H26N4O	386.489	TIC10
Selleck					
Chemicals	S7291	c(nc(NC(=O)C1CC1)s2)(ccc(Oc3ccc(F)c(NC(=O)Cc4cc(C(F)(F)F)ccc4)c3)c5C#N)c25	C27H18F4N4O3S	554.515	TAK-632
Selleck					
Chemicals	S7136	c1cc(NC(=S)NC(NC(=O)C(c2ccccc2)c3ccccc3)C(Cl)(Cl)Cl)cc([N+])([O-])=O)c1F	C23H18Cl3FN4O3S	555.836	CGK 733
Selleck					
Chemicals	S7304	c1(C)sc2c(C(c3ccc(Cl)cc3)=N[C@@H](CC(N)=O)c4n2c(C)nn4)c1C	C19H18ClN5OS	399.897	CPI-203
Selleck					
Chemicals	S7147	C1NCCN(c2ccc(c3cnc4n(ncc4c5ccccc56)nc6)c3)cc2)C1	C25H22N6	406.482	LDN-212854
Selleck					
Chemicals	S7325	n1c(N[C@H]2CC[C@H](O)CC2)c(C(=O)NCc3ccc(n4ccnc4)cc3)cnc1NCCCC	C25H33N7O2	463.575	UNC2881
Selleck					
Chemicals	S7162	N(c(c1C(=O)N2c3cc(O)C(Cl)cc3Cl)cccc1)=C2S	C15H10Cl2N2O2S	353.223	Mdivi-1
Selleck					
Chemicals	S7337	C1CC(c2ccc(CN(c3ccc(C(=O)O)cc3)C(CN(C)S(=O)(=O)c4c(F)c(F)c(F)c(F)c4F)=O)cc2)CCC1	C29H27F5N2O5S	610.592	SH-4-54
Selleck					
Chemicals	S7189	n(c(C)nn1)(c2c(cc(O)C)cc2)C(c3ccc(Cl)cc3)=N[C@H]4CC(=O)NCC)c14	C22H22ClN5O2	423.895	I-BET-762
Selleck					
Chemicals	S7359	n1c(N)c(c2cc(O)C)c(O)C(O)C2cc(c3cc(O)ccc3)c1	C20H20N2O4	352.384	K02288
Selleck					
Chemicals	S7207	c1cccc2c1n(CCCSC(N)=N)cc2C3=C(c4c(c5n(C4)cccc5)C(=O)NC3=O.CS(O)(=O)=O	C26H27N5O5S2	553.653	Ro 31-8220 Mesylate
Selleck					
Chemicals	S7372	Cc1nc(n2c1c3nc(Nc4c(Br)cc(OC)cc4Br)sc3)nc2	C17H13Br2N5OS	495.191	PTC-209
Selleck					
Chemicals	S7223	n1c(c2ccc1c3c[nH]nc3c4nc(C)ccc4)ccn2	C17H13N5	287.319	RepSox
Selleck					
Chemicals	S7392	CC(CCN(C)C(NC(C1OC1C(O)=O)=O)CC(C)C)=O)C	C15H26N2O5	314.377	Loxistatin Acid (E-64C)

Selleck					
Chemicals	S7243	<chem>c1(NC2CCCC2)c(N)cc(C(=O)OCC)cc1</chem>	C15H22N2O2	262.347	Ferrostatin-1 (Fer-1)
Selleck					
Chemicals	S7424	<chem>c1cc2c(c(C=C(C(=O)O)S)c[nH]2)cc1F</chem>	C11H8FNO2S	237.25	PD 151746
Selleck					
Chemicals	S7440	<chem>CN(C(c1n(C2CCCC2)c(c3c1)nc(Nc4ccc(N5CCNCC5)cn4)nc3)=O)C</chem>	C23H30N8O	434.537	LEE011
Selleck					
Chemicals	S8039	<chem>n1c(N)c2c(n(CCCNC(C)C)c(Sc3c(l)cc4c(OCCO4)c3)n2)nc1</chem>	C18H21N6O2S	512.368	PU-H71
Selleck					
Chemicals	S7459	<chem>n1cc(c2c(C)cc(O)c(Cl)c2)c(c3ccc(OC)c3)c1C(=O)NCC</chem>	C19H17ClN2O5	388.802	VER-50589
Selleck					
Chemicals	S8051	<chem>c1(Br)cnc(OCOc2ncnc(NS(=O)(NCCC)=O)c2c3ccc(Br)cc3)nc1</chem>	C19H20Br2N6O4S	588.273	Macitentan
Selleck					
Chemicals	S7484	<chem>c1c(Cl)cc(S(=O)(=O)Nc2ccc([N+](=O)[O-])=O)cc2C)c(Cl)c1</chem>	C13H10Cl2N2O4S	361.2	FH535
Selleck					
Chemicals	S8073	<chem>c1ncc(n2c(C)cc(C=C3C(=O)NC(=S)S3)c2C)cc1</chem>	C15H13N3OS2	315.413	Optovin
Selleck					
Chemicals	S7500	<chem>c1c(C)cc(C)c(S(n2c(C)cc(C)c2)(=O)=O)c1C</chem>	C15H19NO2S	277.382	HJC0350
Selleck					
Chemicals	S7517	<chem>CC(O)(C(F)F)C(Nc1ccc(S(c2ccc(C(N(C)C)=O)cc2)(=O)=O)cc1Cl)=O</chem>	C19H18ClF3N2O5S	478.87	AZD7545
Selleck		<chem>c1(ccccc1OCCOc2ccccc2N(CC(=O)O)COC(=O)C)CC(=O)OCCO(C(=O)C)N(C</chem>			
Chemicals	S7534	<chem>CC(=O)OCCO(C(=O)C)CC(=O)OCOC(=O)C</chem>	C34H40N2O18	764.684	BAPTA-AM
		<chem>CN[C@@H](C)C(=O)N[C@@H](C1CCCC1)C(=O)N2CCC[C@H]2C(N[C@@H](C(c3ccccc3)c4ccccc4)C(=O)NCCCCCN(C([C@H](C5ccccc5)c6ccc6)NC(=O)[C@@H]7CCCN7C(=O)[C@H](C8CCCCC8)NC(=O)[C@H](C)NC)=O)=O</chem>			
Selleck			C70H96N10O8	1205.573	BV-6
Chemicals	S7597				
Selleck					
Chemicals	S8005	<chem>S1C(=Cc2cccc(C(F)F)c2)C(=O)NC1=O</chem>	C11H6F3NO2S	273.231	SMI-4a
Selleck					
Chemicals	S8019	<chem>N1(c2ncnc3cc[nH]3)CCC(N)(C(N[C@H](c4ccc(Cl)cc4)CCO)=O)CC1</chem>	C21H25ClN6O2	428.915	AZD5363
Selleck					
Chemicals	S8029	<chem>c1(cc(Cl)nc(SCC(=O)O)n1)Nc2ccc(C)c2C</chem>	C14H14ClN3O2S	323.798	WY-14643 (Pirinixic Acid)
Selleck		<chem>N1(C(C(c2ccccc2)c3ccccc3)=O)Cc4c(n(C5ccc(N(C)C)c(C)c5)cn4)C[C@H]1C(=O)O</chem>			
Chemicals	S7098		C31H32N4O3	508.611	PD123319
Selleck					
Chemicals	S7261	<chem>c1cc2c(C(=O)C(=O)C3=C2OC(C)C3)cc1</chem>	C15H14O3	242.27	Beta-Lapachone
Selleck					
Chemicals	S7113	<chem>[C@@H]1(CO)[C@H](O)[C@H](O)[C@H](N2C=CC=NC2=O)O1</chem>	C9H12N2O5	228.202	Zebularine
Selleck					
Chemicals	S7276	<chem>n1c2c(cccc2)c(Nc3ccc(C(=O)Nc4ccc(Nc5cc(C)nc(N)n5)cc4)cc3)cc1</chem>	C27H23N7O	461.518	SGI-1027
Selleck		<chem>C1OCCC(N(c2cc(c3ccc(CN4CCOCC4)cc3)cc(C(=O)NCC5=C(C)C=C(C)NC5=O)c2C)CC)C1</chem>			
Chemicals	S7128		C34H44N4O4	572.738	EPZ-6438
Selleck					
Chemicals	S7292	<chem>c1(C)ccc(C(NCCCCC(=O)Nc2c(N)cccc2)=O)cc1</chem>	C20H25N3O2	339.431	RG2833 (RGFP109)
Selleck					
Chemicals	S7138	<chem>c1cc2c(c(c3ccccc3)nc(Nc4ccc(C(=O)Nc5cc(CNC)ccc5C)cc4)n2)cc1</chem>	C30H27N5O	473.568	BMS-833923
Selleck					
Chemicals	S7307	<chem>c1cc2c(CCN2C(Cc3cc(C(F)F)ccc3)=O)cc1c4cn(C)c5c4c(N)ncn5</chem>	C24H20F3N5O	451.444	GSK2606414
Selleck					
Chemicals	S7148	<chem>COc1ccc(c2cnc3n(ncc3c4cccc(c45)nccc5)c2)cc1</chem>	C22H16N4O	352.389	ML347
Selleck					
Chemicals	S7326	<chem>C(NS(=O)(c1ccc(Br)s1)=O)(=O)c2ccc(Cl)cc2Cl</chem>	C11H6BrCl2NO3S2	415.11	Tasisulam
Selleck		<chem>c1cc(c2cc(C(NCC(C(=O)NC(C)=C3=C3CCC(=O)C4c(n(C(C)C)nc4)c2)enc1N5CCN(C(C)C)CC5</chem>			
Chemicals	S7165		C33H43N7O2	569.74	UNC1999
Selleck					
Chemicals	S7338	<chem>c1cc2c(n(C)cc2c3ccnc(Nc4c(OC)cc(N5CCN(C)CC5)cc4)n3)cn1</chem>	C24H27N7O	429.517	AZ191
Selleck					
Chemicals	S7192	<chem>n1c(N)c2c(OCCN(c3ccc([C@H]4CC[C@H](CC(=O)O)CC4)cc3)C2=O)nc1</chem>	C21H24N4O4	396.44	PF-04620110
Selleck					
Chemicals	S7360	<chem>Cc1c2c(n(c3C(Cc(Nc4ccc(O)cc4)=O)N=C2c5ccc(Cl)cc5)c(C)nn3)sc1C</chem>	C25H22ClN5O2S	491.992	OTX015
Selleck					
Chemicals	S7208	<chem>c1cccc2c1n(CCCN(C)C)cc2C3=C(c4c(c5[nH]c4)cccc5)C(=O)NC3=O</chem>	C25H24N4O2	412.484	GF109203X
Selleck					
Chemicals	S7373	<chem>C1CN(C2CCN(C(c3cncc(Br)c3)=O)CC2)CC1</chem>	C15H20BrN3O	338.243	UNC669
Selleck		<chem>c1cc2c(n([C@H](COc3ccc(c4nc5c(cccc5)n4Cc6cccc6)cc3)C7CCNCC7)c(c8ccccc8)n2)cc1</chem>			
Chemicals	S7224		C40H37N5O	603.755	Deltarasin
Selleck					
Chemicals	S7393	<chem>CCOC(C1OC1C(NC(C(NCCC(C)C)=O)CC(C)C)=O)=O</chem>	C17H30N2O5	342.43	Aloxistatin

Selleck		<chem>c1(C(=O)NC2CCN(C)CC2)ccc(Nc3ncc4c(N(C5CCCC5)CC(F)(F)C(=O)N4C)n3)c(OC)c1</chem>	C27H35F2N7O3	543.609	Ro3280
Chemicals	S7248				
Selleck		<chem>n1n(c2ccc(NC(CCl)=O)cc2)c(c3ccc(Cl)c(Cl)c3)nc1OCCOC</chem>	C19H17Cl3N4O3	455.722	MI-2 (MALT1 inhibitor)
Chemicals	S7429				
Selleck		<chem>c1cc2c([nH]c(c3ccc(C(C)(C)C)cc3)n2)cc1N(CC)C(Nc1ccc(c2nc(N3CCOC[C@@H]3C)c4c(CN(C5COCC5)CC4)n2)cc1)=O</chem>	C17H18N2	250.338	ZLN005
Chemicals	S7447				
Selleck		<chem>c1ccc(S(c2ccc([N+][O-])=O)c(OC(c3ccc(Cl)cc3)=O)c2)(=O)=O)cc1</chem>	C24H32N6O3	452.549	GDC-0349
Chemicals	S8040				
Selleck		<chem>n1c(N)nc(OCc2scc(Br)c2)c3c1nc[nH]3</chem>	C19H12ClNO6S	417.82	BTB06584
Chemicals	S7460				
Selleck		<chem>Cc1cc(N2CCOCC2)ccc1Nc3nc(NC4CCCC4)c5c(nc[nH]5)n3</chem>	C10H8BrN5OS	326.172	Lomeguatrib
Chemicals	S8056				
Selleck		<chem>c1nccc(C(NNc2ccccc2)=O)c1C1(=Cc2ccc(F)cc2)C(=O)C(=Cc3ccc(F)cc3)CN(CC4=CC(C)(C)N(O[H])C4(C)C)C1</chem>	C22H29N7O	407.512	MPI-0479605
Chemicals	S7488				
Selleck		<chem>c(N(c1nccs1)C=C(C(O)=O)C2=O)(nc(N3C[C@@H](O[C][C@@H](NC)C3)cc4)c24</chem>	C12H11N3O	213.235	PluriSIn #1 (NSC 14613)
Chemicals	S8076				
Selleck		<chem>c1(OC)cc(Br)c(Nc2scc(c3c(C)nc4n3cccn4)n2)c(Br)c1.Br</chem>	C28H30F2N2O2	464.547	HO-3867
Chemicals	S7501				
Selleck		<chem>c1c(c2ccc(CN3CCS(=O)(=O)CC3)cc2)n4c(nc(NC(=O)C5CC5)n4)cc1n1c(c2c(NC3CCN(Cc4ccccc4)CC3)nc1N5CCCN(C)CC5)cc(OC)c(OC)c2.Cl.Cl</chem>	C18H19N5O4S	401.44	Voreloxin (SNS-595)
Chemicals	S7518				
Selleck		<chem>n1c(C)c(CSc2ccc(OC(CO)=O)c(C)c2)sc1c3ccc(C(F)(F)F)c(F)c3</chem>	C17H14Br3N5OS	576.103	PTC-209 HBr
Chemicals	S7539				
Selleck		<chem>n1c(c2c(N)cc1C)ccc(Nc3cc(C)nc(NC(C)CCCN(C)CC)cn3)c2.Cl.Cl.Cl</chem>	C21H23N5O3S	425.504	Filgotinib (GLPG0634)
Chemicals	S7605				
Selleck		<chem>c1([C@@H](O)C)C(=O)N2Cc3c([nH]nc3NC(c4ccc(N5CCN(C)CC5)cc4)=O)C2)ccccc1</chem>	C28H41Cl3N6O2	600.023	BIX 01294
Chemicals	S8006				
Selleck		<chem>c1cc2c(NC(=O)C2=C(Nc3ccc(N(C(=O)CN4CCN(C)CC4)C)cc3)c5ccccc5)cc1C(=O)OC</chem>	C21H17F4NO3S2	471.488	GW0742
Chemicals	S8020				
Selleck		<chem>c1cc(Nc2nc(N(C)c3cc4c(c(C)n(C)n4)cc3)ccn2)cc(S(=O)(=O)N)(N)=O)c1C.Cl</chem>	C24H38Cl3N7	530.964	NSC 23766
Chemicals	S8031				
Selleck		<chem>c1(C(CCC(C)(C)C2)=C2CN3CCN(c4ccc(C(=O)NS(=O)(=O)c5ccc(N[C@@H](CS66cccc6)CCN7CCOCC7)c(S(=O)(=O)C(F)(F)F)c5)cc4)CC3)ccc(Cl)c</chem>	C47H55ClF3N5O6S3	974.613	ABT-263 (Navitoclax)
Chemicals	S1001				
Selleck		<chem>c1ccccc1</chem>	C26H30N6O3	474.555	Danuserib (PHA-739358)
Chemicals	S1107				
Selleck		<chem>c1cc2c(NC(=O)C2=C(Nc3ccc(N(C(=O)CN4CCN(C)CC4)C)cc3)c5ccccc5)cc1C(=O)OC</chem>	C31H33N5O4	539.625	Nintedanib (BIBF 1120)
Chemicals	S1010				
Selleck		<chem>n1cc2c(N(C3CCCC3)C(=O)C(C(=O)C)=C2C)nc1Nc4ccc(N5CCNCC5)cn4.Cl</chem>	C24H30ClN7O2	483.994	Palbociclib (PD-0332991)
Chemicals	S1116				
Selleck		<chem>c1(OC)cc2c(c(Nc3cc(Cl)c(F)cc3)ncn2)cc1OCCCN4CCOCC4</chem>	C22H24ClF4N4O3	446.902	Gefitinib (ZD1839)
Chemicals	S1025				
Selleck		<chem>c1cc2c(C(=O)C3=C([N](Cc4cncn4)=C(C)N3CCOC)C2=O)cc1.[Br-]</chem>	C20H19BrN4O3	443.294	YM155 (Sepantronium Bromide)
Chemicals	S1130				
Selleck		<chem>c1cc(Nc2nc(N(C)c3cc4c(c(C)n(C)n4)cc3)ccn2)cc(S(=O)(=O)N)(N)=O)c1C.Cl</chem>	C21H24ClN7O2S	473.979	Pazopanib HCl
Chemicals	S1035				
Selleck		<chem>C=C(C)[C@H](O)C(N)=O)[C@@H](O)C=C(C)C(=O)N2(C(=O)C2=C(C)[C@H]1(O)C)[C@@H](O)C(CO)CO)CC[C@@H](C)[C@@H]2O)C(=O)[C@@]3([H])N(CCC3C)C(=O)C(=O)[C@](O)(O)[C@@]4([H])C(C)[C@H](O)C(C)=CC=CC=C[C@@H](C)C[C@@H](C)C(=O)[C@H](O)C</chem>	C32H49ClN4O8	653.206	17-DMAG (Alvespimycin)
Chemicals	S1142				
Selleck		<chem>[C@H](O)C(C)=C[C@@H](C)C(=O)C2[C@H](C)CC4C1</chem>	C56H87NO16	1030.287	Temsirolimus (CCI-779, NSC 683864)
Chemicals	S1044				
Selleck		<chem>c(scc1)(c(NCCc2nc(NC(=O)Nc3cccc(Cl)c3)s2)ncn4)c14.CS(O)(=O)=O</chem>	C19H19ClN6O4S3	527.04	SNS-314 Mesylate
Chemicals	S1154				
Selleck		<chem>c1cc2c(n(C3CCN(Cc4ccccc4)CC3)cc2C5=C(c6cn(C)c7c6cccc7)C(=O)NC5=O)cc1</chem>	C32H29N5O2	515.605	Enzastaurin (LY317615)
Chemicals	S1055				
Selleck		<chem>c1(C(=O)N)cc2c(nccc2O)c3ccc(NC(NC4CC4)=O)c(Cl)c3)cc1OC</chem>	C21H19ClN4O4	426.853	Lenvatinib (E7080)
Chemicals	S1164				
Selleck		<chem>c1(c2cnn(C3CCNCC3)c2)cn(C)nc(O[C@H](C)c4c(Cl)c(F)ccc4Cl)c1</chem>	C21H22Cl2FN5O	450.337	Crizotinib (PF-02341066)
Chemicals	S1068				
Selleck		<chem>c1cccc2c1c(CNc3ccc(Nc4cncn4)cc3)c[nH]2</chem>	C21H20N4	328.41	JNJ-26854165 (Serdemetan)
Chemicals	S1172				
Selleck		<chem>c1(c2cc3c(C=CN4C3=NNC4=O)nc2c5ccc(C6(N)CCC6)cc5)ccccc1.Cl.Cl</chem>	C25H23Cl2N5O	480.389	MK-2206 2HCl
Chemicals	S1078				
Selleck		<chem>c1(C=Cc2ccccc2)nc(N3CCN(C)CC3)cc(Nc4cc(C)[nH]n4)n1</chem>	C21H25N7	375.47	ENMD-2076
Chemicals	S1181				
Selleck		<chem>c1cc2c(c(CN(C)C)c(C(NCCO)c3ccc(C(NO)=O)cc3)=O)cc1</chem>	C21H23N3O5	397.424	PCI-24781 (Abexinostat)
Chemicals	S1090				
Selleck		<chem>C1(=O)c(c2C(=O)N1C3CCC(=O)NC3=O)ccccc2</chem>	C13H10N2O4	258.23	Thalidomide
Chemicals	S1193				

Selleck					Rucaparib (AG-
Chemicals	S1098	<chem>c1([nH]c2c(c3cc(F)c2)c1CCNC3=O)c4ccc(CNC)cc4.P(O)(O)(O)=O</chem>	C19H21FN3O5P	421.359	014699,PF-01367338)
Selleck					
Chemicals	S1204	<chem>c1c2c(c(CCN(C)=O)c[nH]2)cc(O)c1</chem>	C13H16N2O2	232.278	Melatonin
Selleck					
Chemicals	S1213	<chem>n1c(OC)c2c(n([C@@H]3O[C@H](CO)[C@@H](O)[C@@H]3O)cn2)nc1N[C@@H]1(C)O[C@H](O[C@@H]2([H])C[C@](O)(C=O)CO)Cc3c2c(O)c4c(C(=O)c5c(c(O)c5)C4=O)c3O)C[C@H](N)[C@@H]1O[C@@H]6CCC</chem>	C11H15N5O5	297.267	Nelarabine
Selleck					
Chemicals	S1393	<chem>CO6</chem>	C32H37NO12	627.636	Pirarubicin
Selleck					
Chemicals	S1226	<chem>n1c(N2CCOCC2)c3c(nc(c4ccc(OC)c(CO)c4)cc3)nc1N5C[C@H](C)O[C@H](C)C5</chem>	C25H31N5O4	465.545	KU-0063794
Selleck					
Chemicals	S1407	<chem>c1ccc(CCC(C=C[C@H]2[C@H](O)C[C@H](O)[C@H]2CC=CCCC(NCC)=O)O)cc1</chem>	C25H37NO4	415.566	Bimatoprost
Selleck					
Chemicals	S1243	<chem>C(NCCc1c(c2ccc1)cc(OC)cc2)(=O)C</chem>	C15H17NO2	243.301	Agomelatine
Selleck					
Chemicals	S1431	<chem>c1(S(=O)(=O)N2CCN(C)CC2)cc(C(=O)N(C=O)c3c4c(CCC)nn3C)=N4)c(OCC)c1.C(C(C(=O)O)(O)CC(=O)O)C(=O)O</chem>	C28H38N6O11S	666.7	Sildenafil Citrate
Selleck					
Chemicals	S1257	<chem>c1(N2C=NN([C@@H](CC)[C@@H](O)C)C2=O)ccc(N3CCN(c4ccc(OC[C@H]5C[C@](Cn6cncn6)(c7c(F)cc(F)cc7)OC5)cc4)CC3)cc1</chem>	C37H42F2N8O4	700.777	Posaconazole
Selleck					
Chemicals	S1453	<chem>c1c([C@@](N)(c2ccc3c(C(c4ccc(Cl)c4)=CC(=O)N3C)c2)c5n(C)cnc5)ccc(Cl)c1</chem>	C27H22Cl2N4O	489.396	Tipifarnib
Selleck					
Chemicals	S1271	<chem>[C@@H]1(N[C@@H]2[C@@H](O)[C@@H](O)[C@H](O)C(CO)=C2)[C@H](C)O[C@H](O)[C@@H]3[C@H](CO)O[C@H](O)[C@@H]4[C@H](CO)O[C@@H](O)[C@H](O)[C@H]4O)[C@H](O)[C@H]3O)[C@H](O)[C@H]1O</chem>	C25H43NO18	645.605	Acarbose
Selleck					
Chemicals	S1462	<chem>C(O)=O)c1cccc1N[C@@H](C(C(N2C=C3C)=NC(N4CCOCC4)=CC2=O)=C3)C</chem>	C22H24N4O4	408.45	AZD6482
Selleck					
Chemicals	S1287	<chem>c1c(C(O)=O)cc(NCCCC)c(Oc2ccccc2)c1S(N)(=O)=O</chem>	C17H20N2O5S	364.416	Bumetanide
Selleck					
Chemicals	S1476	<chem>c1(c2c(c3nc(C)ccc3)nc(C(C)(C)C)[nH]2)cc4c(ncn4)cc1</chem>	C21H21N5	343.425	SB525334
Selleck					
Chemicals	S1302	<chem>C1CN(CCCl)P(=O)(NCCCl)OC1</chem>	C7H15Cl2N2O2P	261.086	Ifosfamide
Selleck					
Chemicals	S1487	<chem>[nH]1c2c(CN(C(=O)C3CCN(C)CC3)C2(C)C)c(NC(=O)CC(C)C)n1</chem>	C19H31N5O2	361.482	PHA-793887
Selleck					
Chemicals	S1336	<chem>c1(C(F)(F)F)ccc(C(=NOCCN)CCCCOC)cc1.C(=CC(O)=O)C(O)=O</chem>	C19H25F3N2O6	434.407	Fluvoxamine maleate
Selleck					
Chemicals	S1502	<chem>c1ccc([C@@H](N)C(=O)N[C@H]2[C@@]3([H])N(C(C(O)=O)=C(C)CS3)C2=O)cc1</chem>	C16H17N3O4S	347.389	Cephalexin
Selleck					
Chemicals	S1363	<chem>c1c(Oc2cc(F)c(NC(=O)Nc3c(F)cc(F)cc3)cc2)c4c(cc(OC)c(OC)c4)nc1</chem>	C24H18F3N3O4	469.413	Ki8751
Selleck					
Chemicals	S1519	<chem>c1(Cl)c(N2CCN(CC(=O)Nc3nccs3)CC2)c4c([nH]c(c5ccc(N(C)C)cc5)n4)nc1</chem>	C23H25ClN8OS	497.016	CCT129202
Selleck					
Chemicals	S1379	<chem>C(O)(=O)C=C(C(C)C)=CC=C(C(C)C)=CC(C(C)(C)CCC1)=C1C</chem>	C20H28O2	300.435	Isotretinoin
Selleck					
Chemicals	S1531	<chem>c1cc2c(NC(=O)C2=C(c3ccccc3)Nc4cccc(CN(C)C)c4)cc1C(=O)N(C)C</chem>	C27H28N4O2	440.537	BIX 02189
Selleck					
Chemicals	S1002	<chem>c1c(C(NS(=O)=O)=O)c2cc([N+])([O-])=O)c(N[C@H](CCN(C)C)CS c3ccccc3)cc2=O)ccc(N4CCN(Cc5ccccc5c6c</chem>	C42H45ClN6O5S2	813.427	ABT-737
Selleck					
Chemicals	S1109	<chem>c1(C(=O)NC2CCN(C)CC2)cc(OC)c(Nc3nc4c(N(C)C(=O)[C@@H](CC)N4C5CCCC5)cn3)cc1</chem>	C28H39N7O3	521.654	BI 2536
Selleck					
Chemicals	S1012	<chem>c1(N2CCOCC2)cc3c(nc(C(C(=O)NC=C4)=C4NC[C@@H](O)c5cc(Cl)ccc5)[nH]3)c(C)c1</chem>	C25H26ClN5O3	479.959	BMS-536924
Selleck					
Chemicals	S1117	<chem>[C@H]1(O)[C@@H](n2cc3c(c4N(C)N=C3N)c2ncn4)O[C@H](CO)[C@H]1O</chem>	C13H16N6O4	320.304	Triciribine
Selleck					
Chemicals	S1026	<chem>c1(NC(c2ccc(CN3CCN(C)CC3)cc2)=O)cc(Nc4nc(c5cnc5)ccn4)c(C)cc1.O</chem>	C30H35N7O4S	589.708	Imatinib Mesylate (ST1571)
Selleck					
Chemicals	S1132	<chem>c1c(C(N)=O)cc(N)cc1</chem>	C7H8N2O	136.151	INO-1001
Selleck					
Chemicals	S1036	<chem>c1c(C(NOC[C@@H](CO)O)=O)c(Nc2c(F)cc(1)cc2)c(F)c(F)c1</chem>	C16H14F3IN2O4	482.193	PD0325901
Selleck					
Chemicals	S1143	<chem>c1(O)cc(C=C(C#N)C(=O)NCc2ccccc2)ccc1O</chem>	C17H14N2O3	294.305	AG-490 (Tyrphostin B42)
Selleck					
Chemicals	S1045	<chem>c1cc(C(=O)[C@H](C)C=C(C)C=CC(=O)NO)ccc1N(C)C</chem>	C17H22N2O3	302.368	Trichostatin A (TSA)
Selleck					
Chemicals	S1155	<chem>c1(C)ccc(S(=O)(=O)OCC(=O)Nc2cc(O)c(C(=O)O)cc2)cc1</chem>	C16H15NO7S	365.358	S3I-201

Selleck		<chem>C1OC[C@@H](COC(=O)Nc2c(C)c3n(ncnc3Nc4ccc5c(cnn5Cc6cccc(F)c6)c4)c2)NC1.Cl</chem>	C27H28ClFN8O3	567.014	AC480 (BMS-599626)
Chemicals	S1056				
Selleck		<chem>c1cc(S(Nc2ccnc2Nc3ccc(O)cc3)(=O)=O)ccc1OC</chem>	C18H17N3O4S	371.41	ABT-751 (E7010)
Chemicals	S1165				
Selleck		<chem>c1(O)c(c2onc(C(NCC)=O)c2c3ccc(CN4CCOCC4)cc3)cc(C(C)C)c(O)c1</chem>	C26H31N3O5	465.541	AUY922 (NVP-AUY922)
Chemicals	S1069				
Selleck		<chem>c1(N2CCN(C)CC2)ccc(Nc3nc(Oc4cccc(NC(=O)C=C)c4)c(Cl)cn3)c(O)C)c1</chem>	C25H27ClN6O3	494.973	WZ4002
Chemicals	S1173				
Selleck		<chem>c1(Cl)cc(N(S(=O)(=O)c2ccc3c(C=Cc4c(C)c(C(=O)N5CCN(C)CC5)c(C)[nH]4)C(=O)N3)c2)C)ccc1</chem>	C28H30ClN5O4S	568.087	SU11274
Chemicals	S1080				
Selleck		<chem>[C@@H]1(O)C(=O)N2Cc3c(cccc3F)C2)C[C@@H]4N(C(=O)[C@@H](NC(=O)O)C(C)(C)CCCCC=C[C@@H]5[C@](C5)(C(=O)NS(C6CC6)(=O)=O)NC4=O)C1</chem>	C35H46FN5O9S	731.831	Danoprevir (ITMN-191)
Chemicals	S1183				
Selleck		<chem>c1cc2c(nc(c3ccccc3)cc2)cc1c4nc([C@@H]5C[C@@](O)(C)C5)n6c4c(N)ccc6</chem>	C26H23N5O	421.494	OSI-906 (Linsitinib)
Chemicals	S1091				
Selleck		<chem>c(cc(OCCCCCCC(=O)NO)c(OC)c1)c(Nc2cccc(C#C)c2)ncn3)c13</chem>	C24H26N4O4	434.488	CUDC-101
Chemicals	S1194				
Selleck		<chem>c1cc2c(C(c3c(F)cccc3F)=NCc4c2nc(Nc5ccc(C(O)=O)cc5)nc4)cc1Cl</chem>	C25H15ClF2N4O2	476.862	MLN8054
Chemicals	S1100				
Selleck		<chem>c1cc2n(C(C=NN(C)S(=O)(=O)c3cc([N+](=[O-])=O)ccc3C)cn2)cc1Br.Cl</chem>	C16H15BrClN5O4S	488.743	PIK-75
Chemicals	S1205				
Selleck		<chem>n1c(N)c2c(n([C@@H]3O[C@H](CO)[C@@H](O)[C@@H]3F)cn2)nc1Cl</chem>	C10H11ClFN5O3	303.677	Clofarabine
Chemicals	S1218				
Selleck		<chem>c1(O)ccc(C=Cc2cc(O)cc(O)c2)cc1</chem>	C14H12O3	228.243	Resveratrol
Chemicals	S1396				
Selleck		<chem>c1(O)cc2c(C(C(=O)c3ccc(OCCN4CCCC4)cc3)c(c5ccc(O)cc5)s2)cc1.Cl</chem>	C28H28ClNO4S	510.044	Raloxifene HCl
Chemicals	S1227				
Selleck		<chem>c1cc(N2C(=O)O[C@@H](CNC(=O)C)C2)cc(F)c1N3CCOCC3</chem>	C16H20FN3O4	337.346	Linezolid
Chemicals	S1408				
Selleck		<chem>c1cc2c(cc3c2ncnc3N4CCN(C(NCc5cc6c(OCO6)cc5)=S)CC4)cc1</chem>	C23H21N5O3S	447.51	Amuvatinib (MP-470)
Chemicals	S1244				
Selleck		<chem>c1(Cl)c(NC2=NCCN2)c3c(nsn3)cc1.Cl</chem>	C9H9Cl2N5S	290.172	Tizanidine HCl
Chemicals	S1437				
Selleck		<chem>C(=O)(C1CC1)C(N2Cc3c(sc(OC(C)=O)c3)CC2)c4cccc4F</chem>	C20H20FNO3S	373.441	Prasugrel
Chemicals	S1258				
Selleck		<chem>c1(N2CCN(C)CC2)ccc(C(Nc3n[nH]c4c3CN(C(Nc5c(CC)cccc5CC)=O)C4)=O)cc1</chem>	C28H35N7O2	501.623	PHA-680632
Chemicals	S1454				
Selleck		<chem>N1(C(Nc2cccc(Nc3ncc(Br)c(NCCc4[nH]cnc4)n3)c2)=O)CCCC1</chem>	C20H23BrN8O	471.354	BX-912
Chemicals	S1275				
Selleck		<chem>c1(F)cc2c(N(C3CC3)C=C(C(=O)O)C2=O)c(OC)c1N4C[C@@]5([H])[C@]([H])(NCCC5)C4.Cl</chem>	C21H25ClFN3O4	437.892	Moxifloxacin HCl
Chemicals	S1465				
Selleck		<chem>O1CC2=C(C=C3N(Cc4c3nc5c(cccc5)c4)C2=O)[C@@](O)(CC)C1=O</chem>	C20H16N2O4	348.352	Camptothecin
Chemicals	S1288				
Selleck		<chem>C1[C@@H](C)[C@@H](C[C@@H](O)C)O[C@]2(O[C@@H]3[C@@]([H])(C)[C@@H](O)C(=O)C=C[C@@H](C)[C@@H](O)[C@@H](C)C(=O)[C@@H](C)CC=CC[C@@H](CC)CC3)[C@@H]2C)C1</chem>	C45H74O11	791.062	Oligomycin A
Chemicals	S1478				
Selleck		<chem>C1C[C@@]2(C)C(C(C)=C[C@@]3([H])[C@@]2([H])CC[C@@]4(C)[C@@]3([H])OC[C@@]4(OC(C)=O)C(=O)C)=CC1=O</chem>	C24H32O4	384.508	Megestrol Acetate
Chemicals	S1304				
Selleck		<chem>c1(CCS(NC)(=O)=O)cc2c([nH]cc2C3CCN(C)CC3)cc1.Cl</chem>	C17H26ClN3O2S	371.925	Naratriptan
Chemicals	S1488				
Selleck		<chem>c1(O)cc(O)c2c(OC=C(c3ccc(O)cc3)C2=O)c1</chem>	C15H10O5	270.237	Genistein
Chemicals	S1342				
Selleck		<chem>N1(C)C(=O)c2c(ncn2CC(O)CO)N(C)C1=O</chem>	C10H14N4O4	254.243	Dyphylline
Chemicals	S1504				
Selleck		<chem>O1[C@@H]([C@]12C)C[C@H](C=Cc3cc(C)n3)OC(=O)C[C@@H](O)C(C)(C)C(=O)[C@@H](C)[C@@H](O)[C@@H](C)CCC2</chem>	C27H41NO6S	507.683	Epothilone B (EPO906, Patupilone)
Chemicals	S1364				
Selleck		<chem>c1(nc(Nc2cc(OC)cc(OC)c2)c(NS(=O)(=O)c3ccc(NC(c4cc(OC)c(C)cc4)=O)cc3)n5)c5cccc1</chem>	C31H29N5O6S	599.657	SAR245409 (XL765)
Chemicals	S1523				
Selleck		<chem>c1c(C)c(OC(C)=O)N[C@@H]([C@@H](O)C[C@@H](NC([C@@H](C(C)C)N2C(=O)NCCC2)=O)Cc3ccccc3)Cc4ccccc4)c(C)cc1</chem>	C37H48N4O5	628.801	Lopinavir
Chemicals	S1380				
Selleck		<chem>c1(F)cc(c2cc(NC(=O)N)c(C(=O)N[C@@H]3CCCCNC3)s2)ccc1</chem>	C17H19FN4O2S	362.422	AZD7762
Chemicals	S1532				
Selleck		<chem>c1([nH]nc2N)c2c(c3ccc(NC(Nc4cc(C)ccc4F)=O)cc3)ccc1</chem>	C21H18FN5O	375.399	Linifanib (ABT-869)
Chemicals	S1003				
Selleck		<chem>c1(CC)c(C(=O)O)C(=O)Nc2c(cccc2OCC(O)=O)n1c3ccccc3</chem>	C21H20N2O5	380.394	Varespladib (LY315920)
Chemicals	S1110				

Selleck						
Chemicals	S1013	c1nc(C(=O)N[C@@H](Cc2ccccc2)C(=O)N[C@@H](CC(C)C)B(O)O)cnc1	C19H25BN4O4	384.237	Bortezomib (PS-341)	
Selleck						
Chemicals	S1118	c1cc2c(nc(NS(c3ccc(C)cc3)(=O)=O)c(Nc4ccc5c(nsn5)c4)n2)cc1	C21H16N6O2S2	448.521	XL147	
Selleck		c1cc2c(c(Nc3cc(Cl)c(OCC4cc(F)ccc4)cc3)nccn2)cc1c5ccc(CNCCS(=O)(C)=			Lapatinib (GW-572016)	
Chemicals	S1028	O)o5.c6cc(S(=O)(=O)O)ccc6C.c7cc(S(=O)(=O)O)ccc7C	C43H42CIFN4O10S3	925.461	Ditosylate	
Selleck		c1c(OCC)c(Cc2c(ccc(Cl)c2)c3c(cnc(Nc4ccc(C(=O)O)c(OCC)c4)n3)C5=N5)c(F)	C27H20CIFN4O4	518.924	Alisertib (MLN8237)	
Chemicals	S1133	F)cc1				
Selleck						
Chemicals	S1038	c(cc1c2cccn1)(c(N3CCOCC3)nc(c4cc(O)ccc4)n5)c25	C19H16N4O3	348.355	PI-103	
Selleck						
Chemicals	S1144	c1c(C(C)(C)C)c(NC(=O)C2=CNc3c(cccc3)C2=O)cc(O)c1C(C)(C)C	C24H28N2O3	392.491	Ivacaftor (VX-770)	
Selleck						
Chemicals	S1046	c(cc(OCC1CCN(C)CC1)c(OC)c2)(nnc3Nc4ccc(Br)cc4F)c23	C22H24BrFN4O2	475.354	Vandetanib (ZD6474)	
Selleck		N(C(=O)N([C@H]1[C@@H](O)[C@H](O)[C@@H](CO)1)C=C2F)=C2NC(
Chemicals	S1156	=O)OCCCCC	C15H22FN3O6	359.35	Capecitabine	
Selleck					Obatoclox Mesylate	
Chemicals	S1057	c1cc2c([nH]c(C3=NC(=Cc4[nH]c(C)cc4C)C(OC)=C3)c2)cc1.CS(O)(=O)=O	C21H23N3O4S	413.49	(GX15-070)	
Selleck						
Chemicals	S1166	[Pt](N)(Cl)(Cl)N	Cl2H4N2Pt	298.029	Cisplatin	
Selleck		c1c(Cl)c(CS(=O)(=O)c2ccc3c(C(=Cc4[nH]c(C)C(C(=O)N5CCC[C@@H]5C				
Chemicals	S1070	N6CCCC6)c4C)C(=O)N3)c2)c(Cl)cc1	C32H34Cl2N4O4S	641.608	PHA-665752	
Selleck						
Chemicals	S1174	C(Nc1ccc(C#N)c(C(F)(F)F)c1)(=O)[C@](O)(C)COc2ccc(C#N)cc2	C19H14F3N3O3	389.328	MK-2866 (GTx-024)	
Selleck						
Chemicals	S1082	c1(Cl)ccc(NC(=O)c2c(Cl)cc(S(=O)(=O)C)cc2)cc1c3ccccc3	C19H14Cl2N2O3S	421.297	Vismodegib (GDC-0449)	
Selleck		c1c(C[C@H](NC(=O)OCC2scnc2)[C@@H](O)[C@@H](NC(=O)[C@H](C				
Chemicals	S1185	(C)C)NC(=O)N(C)Cc3nc(C(C)C)sc3)Cc4ccccc4)ccccc1	C37H48N6O5S2	720.944	Ritonavir	
Selleck					KU-55933 (ATM Kinase	
Chemicals	S1092	c1cc2c(Sc3c(c(C(OC(N4CCOCC4)=CC5=O)=C5)ccc3)S2)cc1	C21H17NO3S2	395.495	Inhibitor)	
Selleck		C1(=O)C=C([C@]2(C)C=C1)C(=O)C[C@]([H])([C@]23[H])(C@@)([H])([C				
Chemicals	S1196	@@]4(C)CC3)CC4=O	C20H24O2	296.403	Exemestane	
Selleck						
Chemicals	S1101	c1cc2c(c(Cc3ccncc3)nnc2Nc4ccc(Cl)cc4)cc1.Cl.Cl	C20H17Cl3N4	419.735	Vatalanib (PTK787) 2HCl	
Selleck						
Chemicals	S1206	c1cc(OCC(CNC(C)C)O)ccc1COCCOC(C)C.OCC(=O)C=CC(=O)O	C22H35NO8	441.515	Bisoprolol fumarate	
Selleck						
Chemicals	S1219	c1nc(N)ccc1C(Nc2ccccc3c3nc(N4CCOCC4)c5c(c6c(ncoc6)o5)n3)c2=O	C25H21N7O3	467.479	YM201636	
Selleck		[C@H]1(N2CCOCC2)C[C@@]3(C)[C@@]([H])(CC[C@]4([H])(C@@]3([H])				
Chemicals	S1397	CC[C@@]5(C)[C@@]4([H])C[C@H]([N+](CC=C)CCCC6)[C@H]5OC(C)=				
Selleck		O)C[C@@H]1O.[Br-]	C32H53BrN2O4	609.678	Rocuronium Bromide	
Chemicals	S1229	n1c(N)c2c(n([C@@H]3O[C@H](COP(O)(O)=O)[C@@H](O)[C@@H]3O)c				
Selleck		n2)nc1F	C10H13FN5O7P	365.212	Fludarabine Phosphate	
Chemicals	S1409	c1(OC)cc2c(nc(N(C)CCCNC(=O)C3OCCC3)nc2N)cc1OC.Cl	C19H28ClN5O4	425.91	Alfuzosin HCl	
Selleck						
Chemicals	S1247	c1(NC(=O)c2c(C)onc2)ccc(C(F)(F)F)cc1	C12H9F3N2O2	270.207	Leflunomide	
Selleck						
Chemicals	S1439	c1(OC)cc(C=CC(=O)Nc2c(C(=O)O)cccc2)ccc1OC	C18H17NO5	327.331	Tranilast	
Selleck						
Chemicals	S1260	c1ccc(CCCN[C@]([H])(C)c2c3c(cccc3)ccc2)cc1C(F)(F)F.Cl	C22H23ClF3N	393.873	Cinacalcet HCl	
Selleck						
Chemicals	S1455	c1(OC2CCCC2)cc(C3(C#N)CCC([H])(C(O)=O)CC3)ccc1OC	C20H25NO4	343.417	Cilomilast	
Selleck						
Chemicals	S1276	c1(C2(CC(CC3C2)CC4C3)C4)cc(c5ccc6c(ccc(C(=O)O)c6)c5)ccc1OC	C28H28O3	412.52	Adapalene	
Selleck		[C@@H]1(O)CC(=CC=C2CCC[C@@]3(C)[C@@]2([H])CC[C@H]3[C@H](
Chemicals	S1466	C)CCCC(O)(C)C(C)=C)[C@@H](O)C1	C27H44O3	416.636	Calcitriol	
Selleck						
Chemicals	S1289	C1(F)=CN(C(=O)NCCCCC)C(=O)NC1=O	C11H16FN3O3	257.261	Carmofur	
Selleck		c(cccn1)(c(OCC[C@H](O)CN2CCN([C@H]3c4c(cccc4)[C@H]5[C@H](C5(F)			Zosuquidar (LY335979)	
Chemicals	S1481	F)c6c3cccc6)CC2)ccc7c17.Cl.Cl.Cl	C32H34Cl3F2N3O2	636.987	3HCl	
Selleck						
Chemicals	S1312	[C@H]1(O)O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1NC(=O)N(C)N=O	C8H15N3O7	265.221	Streptozotocin (STZ)	
Selleck						
Chemicals	S1489	c1(Cl)ccc(c2c(C)nc(NC(=O)C)s2)cc1S(NCCO)(=O)=O	C14H16ClN3O4S2	389.878	PIK-93	
Selleck		c1cc(S(=O)(=O)N(C(=O)N[C@H]2CC[C@H](C)CC2)ccc1CCNC(=O)N3C(=				
Chemicals	S1344	O)C(CC)=C(C)C3	C24H34N4O5S	490.616	Glimepiride	

Selleck Chemicals	S1505	<chem>[C@H]1N(C(=O)C(c2csc(N)n2)=NOC(C)(C)C(=O)O)[C@@H](C)N(S(=O)(=O)O)C1=O</chem>	C13H17N5O8S2	435.433	Aztreonam
Selleck Chemicals	S1366	<chem>c1(F)ccc(CNC(=O)C2=C(O)C(C)=O)N(C)C(N3CCCCS3(=O)=O)=N2)cc1</chem>	C17H19FN4O5S	410.42	BMS-707035
Selleck Chemicals	S1524	<chem>c1ccc(Cl)c(C(=O)Nc2c(C(=O)NC3CCNCC3)=O)n[nH]c2)c1Cl</chem>	C16H17Cl2N5O2	382.244	AT7519
Selleck Chemicals	S1381	<chem>N(C(C(=O)O)=C(SC1CNC(C(N(C)C)=O)C1)C2C)(C(=O)C3C(O)C)C23</chem>	C17H25N3O5S	383.463	Meropenem
Selleck Chemicals	S1533	<chem>c1(OC)c(O)cc(Nc2nc(F)c(Nc3ccc4c(NC(=O)C(C)C(O)4)n3)n2)cc1OC</chem>	C22H23FN6O5	470.454	R406 (free base)
Selleck Chemicals	S1004	<chem>c1c(C(=O)N)c2c([nH]c([C@]3(C)CCCN3)n2)cc1</chem>	C13H16N4O	244.292	Veliparib (ABT-888)
Selleck Chemicals	S1111	<chem>c1(NC(=O)C2(CC2)C(=O)Nc3ccc(Oc4ccnc5c4cc(OC)c(OCCCN6CCOCC6)c5)c(F)c3)ccc(F)cc1</chem>	C34H34F2N4O6	632.654	Foretinib (GSK1363089)
Selleck Chemicals	S1017	<chem>c1(OC)cc2c(ncnc2Oc3ccc4c(cc(C)[nH]4)c3F)cc1OCCCN5CCCC5</chem>	C25H27FN4O3	450.505	Cediranib (AZD2171)
Selleck Chemicals	S1119	<chem>c(cc(O)C)c(O)C1c1(ncccc2Oc3ccc(NC(=O)C4(CC4)C(=O)Nc5ccc(F)cc5)cc3)c12</chem>	C28H24FN3O5	501.506	Cabozantinib (XL184, BMS-907351)
Selleck Chemicals	S1029	<chem>c1cc2c(CN(C3CCC(=O)NC3=O)C2=O)c(N)c1</chem>	C13H13N3O3	259.261	Lenalidomide (CC-5013)
Selleck Chemicals	S1134	<chem>N(C1CC1)C(Nc2c([nH]nc2c3nc4c(ccc(CN5CCOCC5)c4)[nH]3)=O</chem> <chem>[C@@H]1(O)CC[C@@H](C[C@@H](C)[C@H]2OC(=O)[C@@H](N3C(=O)C(=O)[C@](O)(O)[C@@H]4C[C@@H](OC)C(C)=CC=CC=C[C@@H](C)C[C@@H](C)C(=O)[C@@H](OC)[C@H](O)C(C)=C[C@@H](C)C(=O)C2)[C@H](C)CC4)CCCC3)C[C@H]1OC</chem>	C19H23N7O2	381.432	AT9283
Selleck Chemicals	S1039		C51H79NO13	914.172	Rapamycin (Sirolimus)
Selleck Chemicals	S1145	<chem>c1(C(C)C(C)oc(CSc2sc(NC(C3CCNCC3)=O)nc2)nc1</chem>	C17H24N4O2S2	380.528	SNS-032 (BMS-387032)
Selleck Chemicals	S1047	<chem>c1cc(NC(CCCCCC(=O)NO)=O)ccc1</chem>	C14H20N2O3	264.32	Vorinostat (SAHA, MK0683)
Selleck Chemicals	S1157	<chem>C(NC(=O)[C@@H](NC(c1nc(c2ccccc2)ccc1)=O)[C@H](O)C)[C@H](B(O)O)C)C</chem>	C21H28BN3O5	413.275	CEP-18770 (Delanzomib)
Selleck Chemicals	S1060	<chem>c1c2c(C(=O)NN=C2Cc3ccc(F)c(C(=O)N4CCN(C(C5CC5)=O)CC4)c3)ccc1</chem>	C24H23FN4O3	434.463	Olaparib (AZD2281, KU-0059436)
Selleck Chemicals	S1167	<chem>c1(C=CCNC(=O)COC)cc2c(ncnc2Nc3cc(C)c(Oc4cnc(C)cc4)cc3)cc1</chem>	C27H27N5O3	469.535	CP-724714
Selleck Chemicals	S1071	<chem>c1cc2c([C@@]([H])([C@@H](C(=O)OCC(C#N)C(C(=O)O)CC)=C(N)O2)cc1Br</chem>	C17H17BrN2O5	409.231	HA14-1
Selleck Chemicals	S1175	<chem>n1c(Cl)c2c(n(Cc3ncc(C)c(O)C3C)cn2)nc1N</chem>	C14H15ClN6O	318.761	BIIB021
Selleck Chemicals	S1084	<chem>c([nH]c(C)c1)(ccc(Oc2c3n(cc(O[C@H](O)C)c3C)ncn2)c4F)c14</chem>	C19H19FN4O3	370.378	Brivanib (BMS-540215)
Selleck Chemicals	S1186	<chem>c1cc2c(ccc(C(C)=CC(=O)Nc3ccccc3C(O)=O)c2)cc1</chem>	C21H17NO3	331.365	BIBR 1532
Selleck Chemicals	S1093	<chem>c1ccc(F)c(NC(=O)c2cc(c3nc4n(ccc4)c3c5nc(Nc6cc(C)C)c(N7CCC(N8CCN(S(=O)(=O)C)CC8)CC7)cc6OC)nc5)ccc2OC)c1F</chem>	C44H47F2N9O5S	851.963	GSK1904529A
Selleck Chemicals	S1197	<chem>C1=C[C@@]2(C)[C@@]([H])(CC[C@]3([H])[C@@]2([H])CC[C@@]4(C)[C@@]3([H])CC[C@H]4C(=O)NC(C)C)NC1=O</chem>	C23H36N2O2	372.544	Finasteride
Selleck Chemicals	S1102	<chem>c1cc(SC(=C(C#N)C(C#N)=C(N)Sc2ccccc2N)N)c(N)cc1.CCO</chem>	C20H22N6OS2	426.558	U0126-EtOH
Selleck Chemicals	S1207	<chem>c1(Oc2c3c(cc(O)C)c(O)C3)nc2)cc(Cl)c(NC(Nc4ncc(C)c4)=O)cc1</chem>	C22H19ClN4O5	454.863	Tivozanib (AV-951)
Selleck Chemicals	S1220	<chem>c1cc2c(nccc2CNc3ccsc3C(=O)Nc4ccc(OC(F)(F)F)cc4)cc1</chem>	C22H16F3N3O2S	443.442	OSI-930
Selleck Chemicals	S1398	<chem>O1C(CO)C=CC1N2C=C(C)C(=O)NC2=O</chem>	C10H12N2O4	224.213	Stavudine (d4T)
Selleck Chemicals	S1231	<chem>c1(O)c(CN(C)C)c2c(nc3c(CN4C3=CC5=C(CO)C(=O)[C@]5(O)CC)C4=O)c2)cc1.Cl</chem>	C23H24ClN3O5	457.907	Topotecan HCl
Selleck Chemicals	S1415	<chem>c1c(Cl)c([C@@H](C(OC)=O)N2Cc3c(scc3)CC2)ccc1.OS(=O)(=O)O</chem> <chem>C(c1c(cc(O)C)[C@@]2(C(=O)O)C(C)[C@](CN3CC(c24)c(c5[nH]4)cccc5)([H])C[C@](CC)(O)C3)c1)N6C)([C@]6([H])[C@](C(OC)=O)(O)[C@H]7OC(C)=O)(CC8)[C@]([H])([C@@]7(CC)C=CC9)N89</chem>	C16H18ClNO6S2	419.9	Clopidogrel
Selleck Chemicals	S1248		C46H58N4O9	810.974	Vinblastine
Selleck Chemicals	S1442	<chem>c1cc(F)cc(F)c1[C@]([O])([C@@H](C)c2c(F)cn2)Cn3ncnc3</chem>	C16H14F3N5O	349.31	Voriconazole
Selleck Chemicals	S1261	<chem>c1(n2nc(C(F)F)F)cc2c3ccc(C)cc3)ccc(S(=O)(=O)N)cc1</chem>	C17H14F3N3O2S	381.372	Celecoxib

Selleck						
Chemicals	S1456	<chem>c1(c2ccc(c3nncoc3)cc2)ncccc1S(Nc4ncc(C)nc4OC)(=O)=O</chem>	C19H16N6O4S	424.433	Zibotentan (ZD4054)	
Selleck						
Chemicals	S1278	<chem>n1c(N(C)C)nc(N(C)C)nc1N(C)C</chem>	C9H18N6	210.279	Altretamine	
Selleck		<chem>C1[C@@H](O)CC(=CC=C2[C@]3([H])[C@@]([C@]([H])([C@H](C)C</chem>				
Chemicals	S1467	<chem>=C[C@@H](C)C(C)C)CC3)CCC2C(=C)[C@H]1O</chem>	C28H44O2	412.648	Doxercalciferol	
Selleck						
Chemicals	S1291	<chem>c1c(C(N2CCN(CCOCC(=O)O)CC2)c3ccc(Cl)cc3)cccc1.Cl.Cl</chem>	C21H27Cl3N2O3	461.81	Cetirizine DiHCl	
Selleck		<chem>c1c(c2[nH]c([C@@H]3CCCN3C(=O)[C@@H](NC(=O)OC)C(C)nc2)ccc(c</chem>				
Chemicals	S1482	<chem>4ccc(c5[nH]c([C@@H]6CCCN6C(=O)[C@@H](NC(=O)OC)C(C)nc5)cc4)</chem>	C40H50N8O6	738.875	Daclatasvir (BMS-790052)	
Selleck						
Chemicals	S1315	<chem>c1c(Cl)c(C(OC(Nc2c(c3ccc(CSCCC(=O)O)cc3)onc2C)=O)C)ccc1</chem>	C23H23ClN2O5S	474.957	Ki16425	
Selleck		<chem>c1cc2n(c(C#Cc3cc(C(Nc4ccc(CN5CCN(C)CC5)c(C(F)(F)F)c4)=O)ccc3C)cn</chem>				
Chemicals	S1490	<chem>2)nc1</chem>	C29H27F3N6O	532.559	Ponatinib (AP24534)	
Selleck						
Chemicals	S1352	<chem>c1(c2cccc(O)c2)nc3c(nc(N)nc3N)nc1c4cc(O)ccc4</chem>	C18H14N6O2	346.343	TG100-115	
Selleck		<chem>[C@@H]1(CCCCCC(=O)O)C(=O)C[C@H](O)[C@H]1C=C[C@@H](O)C</chem>				
Chemicals	S1508	<chem>CCCC</chem>	C20H34O5	354.481	Alprostadil	
Selleck						
Chemicals	S1367	<chem>c1(ccc2c(c23)c(C(=O)N(CCN(C)C)C3=O)cc(N)c1</chem>	C16H17N3O2	283.325	Amonafide	
Selleck		<chem>c1cc(C(C)(C)O)nc(N2c3c(cnc(Nc4ccc(N5CCN(C)CC5)cc4)n3)C(=O)N2CC=C</chem>				
Chemicals	S1525	<chem>C)c1</chem>	C27H32N8O2	500.595	MK-1775	
Selleck						
Chemicals	S1382	<chem>c1(cccc2c2Cc3c(cccc3)C4N1CCN(C)C4.Cl</chem>	C18H21ClN2	300.826	Mianserin HCl	
Selleck						
Chemicals	S1536	<chem>c1cc2c(nc(n3cnc(c34)cc(OCCOC)cc4)cc2)c(N5CCC(N)CC5)c1</chem>	C24H27N5O2	417.503	CP-673451	
Selleck						
Chemicals	S1005	<chem>c1(Sc2ccc3c([nH]nc3C=Cc4ncccc4)c2)c(C(NC)=O)cccc1</chem>	C22H18N4OS	386.47	Axitinib	
Selleck						
Chemicals	S1112	<chem>c1cc(Sc2nnc3n2nc(c4cn(C)nc4)cc3)cc5c1nccc5</chem>	C18H13N7S	359.408	SGX-523	
Selleck						
Chemicals	S1020	<chem>c1cc(C(=O)NOCC2CC2)c(Nc3c(Cl)cc(l)cc3)c(F)c1F</chem>	C17H14ClF2IN2O2	478.66	PD184352 (Cl-1040)	
		<chem>C(CO[C@@H]1CC[C@@H](C[C@H](C)[C@@H]2CC(=O)[C@H](C)C=C(C</chem>				
Selleck		<chem>C)[C@H](O)[C@@H](OC)C(=O)[C@H](C)C[C@H](C)C=CC=C(C)[C@@@H](OC)C[C@@H](O[C@@]3(O)C(=O)C(=O)N[C@@H]4C(=O)O2)C</chem>				
Chemicals	S1120	<chem>CCC)CC[C@H]3C)[C@H]1OC)O</chem>	C53H83NO14	958.224	Everolimus (RAD001)	
Selleck						
Chemicals	S1030	<chem>c1(CNCCc2c3c(cccc3)[nH]c2C)ccc(C=CC(NO)=O)cc1</chem>	C21H23N3O2	349.426	Panobinostat (LBH589)	
Selleck						
Chemicals	S1137	<chem>C(OC(C)C)(=O)C(=C1SC=CS1)C(OC(C)C)=O</chem>	C12H16O4S2	288.383	Malotilate	
Selleck		<chem>c1(Cl)c(C(F)(F)F)cc(NC(=O)Nc2ccc(OC3cc(C(=O)NC)ccc3)cc2)cc1.c4c(S(</chem>				
Chemicals	S1040	<chem>=O)(=O)O)ccc(C)c4</chem>	C28H24ClF3N4O6S	637.027	Sorafenib Tosylate	
Selleck						
Chemicals	S1147	<chem>c1(OCCCN(C)CCO)cc2c(c(Nc3cc(C(=O)Nc4cc(F)ccc4)n[nH]3)ncn2)cc1</chem>	C26H30FN7O3	507.56	Barasertib (AZD1152-HQPA)	
Selleck						
Chemicals	S1048	<chem>c1(Nc2n[nH]c(C)c2)nc(Sc3ccc(NC(C4CC4)=O)cc3)nc(N5CCN(C)CC5)c1</chem>	C23H28N8OS	464.586	VX-680 (Tozasertib, MK-0457)	
Selleck						
Chemicals	S1158	<chem>n1c(c2onc(N3CCC(OC4cc(F)ccc4Br)CC3)c2)nnn1CC(O)=O</chem>	C17H16BrFN6O4	467.249	MK-8245	
Selleck						
Chemicals	S1064	<chem>c1(C)ccc(NC(c2ccc(CN3CCN(C)CC3)cc2)=O)cc1Nc4sc(c5cnccc5)n4</chem>	C28H30N6OS	498.642	Masitinib (AB1010)	
Selleck						
Chemicals	S1168	<chem>CCCC(CCC)C(=O)[O-].[Na+]</chem>	C8H15NaO2	166.193	Valproic acid sodium salt (Sodium valproate)	
Selleck						
Chemicals	S1072	<chem>n1c(N2CCOCC2)nc(n3c(C(F)F)nc4c3cccc4)nc1N5CCOCC5</chem>	C19H21F2N7O2	417.413	ZSTK474	
Selleck						
Chemicals	S1177	<chem>c1cc2c(OC(c3c(N)c(OC)ccc3)=CC2=O)cc1</chem>	C16H13NO3	267.279	PD98059	
Selleck						
Chemicals	S1085	<chem>c1(S(=O)(=O)Nc2cccc2)cc(C=CC(=O)NO)ccc1</chem>	C15H14N2O4S	318.348	Belinostat (PXD101)	
Selleck						
Chemicals	S1188	<chem>c1c(Cn2ncnc2)cc(C(C#N)(C)C)cc1C(C#N)(C)C</chem>	C17H19N5	293.366	Anastrozole	
Selleck						
Chemicals	S1094	<chem>c1(cc(Cn2nnc3c2nc(c4cnn(CCO)c4)cn3)cc5)c5nccc1</chem>	C19H16N8O	372.383	PF-04217903	
Selleck						
Chemicals	S1199	<chem>n1c(Cl)nc2c(ncn2[C@@H]3O[C@H](CO)[C@@H](O)C3)c1N</chem>	C10H12ClN5O3	285.687	Cladribine	
Selleck						
Chemicals	S1103	<chem>O1CCN(CCCOC2cc3c(c(Nc4ccc(NC(c5cccc5)=O)cc4)ncn3)cc2OC)CC1</chem>	C29H31N5O4	513.588	ZM 447439	
Selleck		<chem>c1c(OC)c2c(C(=O)c3c(c(O)c4c(C[C@]([O])(C(=O)CO)C[C@H]4O[C@]5([</chem>				
Chemicals	S1208	<chem>[H])O)[C@@H](C)[C@@H](O)[C@@H](N)C5)c3O)C2=O)c1.Cl</chem>	C27H30ClNO11	579.98	Doxorubicin (Adriamycin)	

Selleck					
Chemicals	S1221	c1[nH]c(N=NN(C)C)c(C(N)=O)n1	C6H10N6O	182.183	Dacarbazine
Selleck		n1c(N)c2c(n(C[C@@H](C)OCP(=O)OCOC(O(C)C)=O)OCOC(=O)OC(C			Tenofovir Disoproxil
Chemicals	S1400)C)n2)nc1.C(C(O)=O)=CC(O)=O	C23H34N5O14P	635.515	Fumarate
Selleck		c1(O C)cc2c(C[C@]3([H])[C@@]2([H])CC[C@@]4(C)[C@@]3([H])CC[C			2-Methoxyestradiol (2-
Chemicals	S1233	@H]4O)cc1O	C19H26O3	302.408	MeOE2)
Selleck					
Chemicals	S1422	c1cc(OCCCC(=O)NO)c(C)cc1Cl	C11H14ClNO3	243.687	Droxinostat
Selleck					
Chemicals	S1249	c1(S(=O)(=O)N)ccc(Nc2nn(C(=O)c3c(F)cccc3F)c(N)n2)cc1	C15H12F2N6O3S	394.356	JNJ-7706621
Selleck					
Chemicals	S1443	c1cc2c(cc(C(C)N(C(=O)N)O)s2)cc1	C11H12N2O2S	236.29	Zileuton
Selleck		c1(CN(S(=O)(=O)c2ccc(Cl)cc2)[C@H](CCCF(F)F)C(=O)N)ccc(c3nocn3)c			Avagacestat (BMS-
Chemicals	S1262	c1F	C20H17ClF4N4O4S	520.885	708163)
Selleck		O(C)C(=O)N[C@@H](C(C)(C)C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)			
Chemicals	S1457	CN(Cc2ccc(c3cccn3)cc2)NC(=O)[C@H](C(C)(C)C)NC(=O)O.C.S(O)(O)(=	C38H54N6O11S	802.934	Atazanavir Sulfate
Selleck		O)=O			
Chemicals	S1282	[C@@](C)(O O1)(CC2)O[C@@]([H])(O C(=O)[C@H]3C)[C@]1([C@@]3([C15H22O5	282.332	Artemisinin
Selleck		H])CC[C@@H]4C)[C@@]24[H]			TSU-68 (SU6668,
Chemicals	S1470	c1cc2c(NC(=O)C2=Cc3c(C)c(CCC(=O)O)c(C)[nH]3)cc1	C18H18N2O3	310.347	Orantinib)
Selleck					
Chemicals	S1294	C1Cc2c(ccc(OCCCCc3nnnn3C4CCCCC4)c2)NC1=O	C20H27N5O2	369.461	Cilostazol
Selleck					
Chemicals	S1483	c1(O C)cc(C(=O)C)ccc1OCCCN2CCC(c3c4c(cc(F)cc4)n3)CC2	C24H27FN2O4	426.481	lloperidone
Selleck		c1(nc(N2CCN(C(=O)C3Oc4c(cccc4)OC3)CC2)nc5N)c5cc(O C)c(O C)c1.S(C)			
Chemicals	S1324	(=O)(O)=O	C24H29N5O8S	547.581	Doxazosin Mesylate
Selleck		CC(C)(C)c1[nH]c(c2ccc3c(n(CC(C)(C)C)c(N)n3)n2)c(c4ccc(F)cc4)n1.CS(O)(
Chemicals	S1494	=O)=O.CS(O)(=O)=O	C26H37FN6O6S2	612.737	LY2228820
Selleck					
Chemicals	S1354	c1cc2c([nH]c(S(=O)Cc3c(C)c(OCC(F)F)F)ccn3)n2)cc1	C16H14F3N3O2S	369.361	Lansoprazole
Selleck		N1(O)C(=O)[C@]2([H])N([C@H](c3cc4c(O CO4)cc3)c5c(c6c(cccc6)[nH]5)C			
Chemicals	S1512	2)C(=O)C1	C22H19N3O4	389.404	Tadalafil
Selleck					
Chemicals	S1368	c1c(C)c(C(=CC(C)=CC=CC(C)=CC(=O)O)c(C)c(C)c1O C	C21H26O3	326.429	Acitretin
Selleck		c1cc(c2cn3c(sc4c3ccc(OCCN5CCOCC5)c4)n2)ccc1NC(=O)Nc6noc(C(C)(C)			
Chemicals	S1526	C)c6	C29H32N6O4S	560.667	Quizartinib (AC220)
Selleck		c1(C(Oc2ccc3c(c(ccc(C(N)=N)c3)c2)=O)ccc(NC(N)=N)cc1.S(=O)(=O)(C)O.			
Chemicals	S1386	S(=O)(=O)(C)O	C21H25N5O8S2	539.582	Nafamostat Mesylate
Selleck					
Chemicals	S1537	c(C(=O)c1c(c(C)c(C)cc1)O2)(cccc3CC(=O)O)c23	C17H14O4	282.291	DMXAA (Vadimezan)
Selleck					
Chemicals	S1006	c1c(O C2CCOCC2)c3c(ncnc3Nc4c5c(O CO5)ccc4Cl)cc1OCCN6CCN(C)CC6	C27H32ClN5O5	542.026	Saracatinib (AZD0530)
Selleck					
Chemicals	S1113	c(nc1c1nonc1N)n2CC)(c(C#CC(C)(O)C)nc3O C[C@H]4CCNC4)c23	C21H27N7O3	425.484	GSK690693
Selleck					
Chemicals	S1021	n1c(Nc2sc(C(=O)Nc3c(C)cccc3Cl)n2)cc(N4CCN(CCO)CC4)nc1C	C22H26ClN7O2S	488.006	Dasatinib
Selleck					Mocetinostat
Chemicals	S1122	C(Nc1ccccc1N)(=O)c2ccc(CNc3nccc(c4ccnc4)n3)cc2	C23H20N6O	396.444	(MGCD0103)
Selleck		c1c(CNc2ncccc2C(Nc3cc4c(C(C)CN4)cc3)=O)ccnc1.P(O)(O)(=O)O.P(Motesanib Diphosphate
Chemicals	S1032	O)(O)(=O)O	C22H29N5O9P2	569.441	(AMG-706)
Selleck					
Chemicals	S1139	c1c(O)c2c(O C3(CCNCC3)C=C2c4ccc(C(N(CC)CC)=O)cc4)cc1.Cl	C24H29ClN2O3	428.952	ADL5859 HCl
Selleck					
Chemicals	S1041	n1ccc(c2nc(Nc3cc(C)ccc3)sc2)cc1	C15H13N3S	267.349	STF-62247
Selleck		c1cc(C(N[C@@H](c2ccccc2)[C@@H](O)C(=O)O)[C@@H]3C(C)=C4C(C)(
Chemicals	S1150	C)[C@](O)([C@@H](O C(=O)c5ccccc5)C6[C@@]([C@H](O)C[C@@H]	C47H51NO14	853.906	Paclitaxel
Selleck		7[C@@]6(O C(=O)C)CO7)C(=O)[C@@H]4O C(=O)C(C3)=O)ccc1			
Chemicals	S1049	[C@@H]1(C(Nc2ccnc2)=O)CC[C@@H]([C@H](N)C)CC1.Cl.Cl	C14H23Cl2N3O	320.258	Y-27632 2HCl
Selleck					
Chemicals	S1159	N1=C(c2cc(C(C)C)c(O)cc2O)N(c3ccc(c4c3)n(C)cc4)C(=O)N1	C20H20N4O3	364.398	Ganetespib (STA-9090)
Selleck		c1(c2nc3c(sc(CN4CCN(S(C)(=O)=O)CC4)c3)c(N5CCOCC5)n2)c6c([nH]nc6)			
Chemicals	S1065	ccc1	C23H27N7O3S2	513.636	GDC-0941
Selleck					
Chemicals	S1169	C(N1C(=NC(N2CCOCC2)=CC1=O)C(C(Nc3ccccc3)C)=C4)=C4C	C21H24N4O2	364.441	TGX-221
Selleck					
Chemicals	S1075	c1c2c(c(C(C(=O)NC3=O)=C3c4c(Cl)cc(Cl)cc4)cn2C)ccc1	C19H12Cl2N2O2	371.217	SB216763

Selleck					Regorafenib (BAY 73-
Chemicals	S1178	<chem>c1cc(Oc2ccc(NC(=O)Nc3cc(C(F)(F)F)c(Cl)cc3)c(F)c2)cc(C(NC)=O)n1</chem>	C21H15ClF4N4O3	482.815	4506)
Selleck					
Chemicals	S1087	<chem>c1c(C(=O)N)cc([N+][I-])=O)c(1)c1</chem>	C7H5IN2O3	292.031	Iniparib (BSI-201)
Selleck					
Chemicals	S1190	<chem>C(Nc1ccc(C#N)c(C(F)(F)F)c1)(=O)C(O)(C)CS(c2ccc(F)cc2)(=O)=O</chem>	C18H14F4N2O4S	430.373	Bicalutamide
Selleck					
Chemicals	S1095	<chem>c1(C=CC(=O)NO)ccc(CN(CCc2c3c(ccc3)[nH]c2)CCO)cc1</chem>	C22H25N3O3	379.452	LAQ824 (Dacinostat)
Selleck					
Chemicals	S1200	<chem>[C@H]1(N2C(=O)N=C(N)N=C2)C[C@H](O)[C@@H](CO)O1</chem>	C8H12N4O4	228.205	Decitabine
Selleck					
Chemicals	S1104	<chem>C(O)Cn1cc(c2cc3c(C(=NO)CC3)cc2)c(c4cncnc4)n1</chem>	C19H18N4O2	334.372	GDC-0879
Selleck					Fluorouracil (5-Fluoracil, 5-
Chemicals	S1209	<chem>C1(=O)NC=C(F)C(=O)N1</chem>	C4H3FN2O2	130.077	FU)
Selleck					Dexrazoxane HCl (ICRF-
Chemicals	S1222	<chem>N1C(=O)CN(C[C@H](C)N2CC(=O)NC(=O)C2)CC1=O.Cl</chem>	C11H17ClN4O4	304.73	187, ADR-529)
Selleck		<chem>c1(N(C)C)c2c(C(=O)C(=C3O)[C@]([H])(C)[C@]4([H])(C@@)3(O)C(=O)C(C(N)=O)=C(O)[C@@H]4N(C)C)C2)c(O)c(NC(=O)CNC(C)(C)C)c1</chem>	C29H39N5O8	585.649	Tigecycline
Chemicals	S1403				
Selleck					
Chemicals	S1234	<chem>C(#N)C(=Cc1cc(C(C)(C)C)c(O)c(Br)c1)C#N</chem>	C14H13BrN2O	305.17	AG-1024
Selleck					
Chemicals	S1425	<chem>c1ccc(C)c(NC(CN2CCN(CC(COc3c(OC)cccc3)O)CC2)=O)c1C.Cl.Cl</chem>	C24H35Cl2N3O4	500.458	Ranolazine 2HCl
Selleck					
Chemicals	S1250	<chem>c1(F)cc(N2C(C)(C)C(=O)N(c3cc(C(F)(F)F)c(C#N)cc3)C2=S)ccc1C(=O)NC</chem>	C21H16F4N4O2S	464.436	Enzalutamide (MDV3100)
		<chem>[O-]C(=O)[C@@H](C)C[C@H](C(=O)C(C)=C[C@H](C)[C@]1([H])[C@@H](C[C@@H](O)C[C@@]2(O)[C@](C)([C@@]3([H])C[C@H](OC4CC[C@H](OC)[C@@H](C)O4)[C@@H](C)[C@@]5(O)[C@]([H])([C@]6([H])[C@H](C)C[C@@H](C)[C@](O)(CO)O6)C[C@H]5C)O3)CC2)O1)C.[Na+]</chem>	C47H77NaO14	889.096	Nanchangmycin
Selleck	S1450				
Chemicals	S1264	<chem>n1cc2c(nc(NC(=O)NC(C)(C)C)c(c3cc(OC)cc(OC)c3)c2)nc1NCCCCN(CC)CC</chem>	C28H41N7O3	523.67	PD173074
Selleck					
Chemicals	S1458	<chem>c1c(F)c(SC2=NN3C(=C(c4c(Cl)cccc4Cl)C(=O)N=C3)C=C2)ccc1F</chem>	C19H9Cl2F2N3OS	436.262	VX-745
Selleck		<chem>c(cccc1)(Oc2c(cc(Cl)cc2)[C@]3([H])[C@]4([H])CN(C)C3)c14.C(O)(=O)C=CC(O)=O</chem>	C21H20ClNO5	401.84	Asenapine
Chemicals	S1283				
Selleck					
Chemicals	S1472	<chem>c1(F)cc(COc2ccc(CN[C@@H](C)C(=O)N)cc2)ccc1.CS(O)(=O)=O</chem>	C18H23FN2O5S	398.449	Safinamide Mesylate
Selleck		<chem>O1[C@H]([C@H]12)C[C@H](C(=Cc3ccc(C)n3)C)O[C@]([H])(O)C(C)(C)C(=O)[C@H](C)[C@@H](O)[C@H](C)CCC2</chem>	C26H39NO6S	493.656	Epothilone A
Chemicals	S1297				
Selleck					
Chemicals	S1484	<chem>c1cc(C(=O)C=Cc2cc(C=CC(=O)NO)n(C)c2)cc(F)c1</chem>	C17H15FN2O3	314.311	MC1568
Selleck					
Chemicals	S1326	<chem>C1(C)=NN(c2ccccc2)C(=O)C1</chem>	C10H10N2O	174.199	Edaravone
Selleck		<chem>n1c(N)c2c(cc(C(C#C)c3ccc(C(=O)N[C@H](C(O)=O)CCC(=O)O)cc3)n2)nc1N</chem>	C23H23N7O5	477.473	Pralatrexate
Chemicals	S1497				
Selleck					
Chemicals	S1358	<chem>C1C(=C2c3c(cc(Cl)cc3)CCc4c2cccc4)CCN(C(OC)=O)C1</chem>	C22H23ClN2O2	382.883	Loratadine
Selleck		<chem>C1(CC(C)C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(C(C)C)C(=O)N(C)C([C@H](O)[C@H](C)CC=CC)C(=O)N(C)C(C)C(=O)N(C)C(C)C(=O)N(C)C(C)C(=O)N1C</chem>	C62H111N11O12	1202.611	Cyclosporine
Chemicals	S1514				
Selleck		<chem>C1C[C@@]2([H])C(C[C@]3([H])[C@@]2([H])CC[C@@]4(CC)[C@@]3([H])C=C[C@@]4(C#C)O)=CC1=O</chem>	C21H26O2	310.43	Gestodene
Chemicals	S1376				
Selleck					
Chemicals	S1528	<chem>c1ncc(c2cc([C@]3(C)CCSC(N)=N3)c(F)cc2F)cn1</chem>	C15H14F2N4S	320.36	LY2811376
Selleck					
Chemicals	S1387	<chem>c1(OCC(O)CN2CCN(c3c(OC)cccc3)CC2)cccc4c1cccc4.Cl.Cl</chem>	C24H30Cl2N2O3	465.413	Naftopidil DiHCl
Selleck		<chem>[C@@]([H])(CCC1)([C@H](C(N[C@H](C(CNC2CC2)=O)=O)CCC)=O)N(C([C@@H](N([C@H](C3CCCCC3)NC(c4cncnc4)=O)=O)C(C)(C)C(=O)C5)[C@@]15[H])</chem>	C36H53N7O6	679.849	Telaprevir (VX-950)
Chemicals	S1538				
Selleck					
Chemicals	S1007	<chem>c(ccc(Oc1ccccc1)c2)(c(O)c(C(=O)NCC(=O)O)nc3C)c23</chem>	C19H16N2O5	352.341	FG-4592
Selleck					
Chemicals	S1114	<chem>n1c2c(cc(C(F)(F)F)c3nnc4n3nc(c5cn(C)nc5)cc4)cc2)ccc1</chem>	C19H13F2N7	377.35	JNJ-38877605
Selleck		<chem>[C@H]1(OC)[C@@H](OP(C)(=O)C)CC[C@@H](C[C@@H](C)[C@H]2OC(=O)[C@@]3([H])N(CCCC3)C(=O)C(=O)[C@](O)(O)[C@@]4([H])C[C@H](OC)C(C)=CC=CC=C[C@H](C)[C@@H](C)C(=O)[C@H](OC)[C@H](O)C(C)=C[C@H](C)C(=O)C2)[C@H](C)CC4)C1</chem>	C53H84NO14P	990.206	Ridafolorimus (Defolorimus, MK-8669)
Chemicals	S1022				

Selleck		<chem>c(ccc1)(c(Nc2n[nH]c(C3CC3)c2)nc(N4[C@](C(Nc5cnc(F)cc5)=O)(C)CCC4)n6)n16</chem>	C23H24FN9O	461.495	BMS-754807
Chemicals	S1124				
Selleck		<chem>c1(C(Nc2cc(n3cnc(C)c3)cc(C(F)(F)F)c2)=O)cc(Nc4nc(c5ccccc5)ccn4)c(C)c c1</chem>	C28H22F3N7O	529.516	Nilotinib (AMN-107)
Chemicals	S1033				
Selleck		<chem>C(Nc1ccc([N+])([O-])=O)c(C(F)(F)F)c1(=O)[C@](O)(C)COc2ccc(NC(C)=O)cc2</chem>	C19H18F3N3O6	441.358	Andarine
Chemicals	S1140				
Selleck		<chem>c1(F)cc2c(NC(=O)C2=Cc3c(C)c(C(=O)NCCN(CC)CC)c(C)[nH]3)cc1.C(=O)(O)C[C@H](O)C(=O)O</chem>	C26H33FN4O7	532.561	Sunitinib Malate
Chemicals	S1042				
Selleck		<chem>c1(Cl)cc2c([nH]cc2C(c3c(F)ccc(NS(CCC)(=O)=O)c3F)=O)nc1</chem>	C17H14ClF2N3O3S	413.826	PLX-4720
Chemicals	S1152				
Selleck		<chem>c1ccc(C(=S)N(C)NC(=O)CC(=O)NN(C(c2ccccc2)=S)C)cc1</chem>	C19H20N4O2S2	400.518	Elesclomol (STA-4783)
Chemicals	S1052				
Selleck		<chem>O1C[C@@H](OCc2ccc(OC(F)(F)F)cc2)Cn3c1nc([N+])([O-])=O)c3</chem>	C14H12F3N3O5	359.257	PA-824
Chemicals	S1162				
Selleck		<chem>c1c(C(F)(F)F)c(C(C#N)=C(N)Sc2ccc(N)cc2)ccc1</chem>	C16H12F3N3S	335.347	SL-327
Chemicals	S1066				
Selleck		<chem>c1(N2CCN(C)CC2)ccc(Nc3nc(OC4cccc(NC(=O)C=C)c4)c(Cl)cn3)cc1</chem>	C24H25ClN6O2	464.947	WZ3146
Chemicals	S1170				
Selleck		<chem>n1ccc(c2[nH]c(c3ccc(S(=O)C)cc3)nc2c4ccc(F)cc4)cc1</chem>	C21H16FN3OS	377.435	SB203580
Chemicals	S1076				
Selleck		<chem>c1(N2CCN(C)CC2)ccc(Nc3nc(Sc4cccc(NC(=O)C=C)c4)c(Cl)cn3)cc1</chem>	C24H25ClN6OS	481.013	WZ8040
Chemicals	S1179				
Selleck		<chem>c(c(c1cccc(OCc2ccccc2)c1)cn3[C@H]4[C@H](CN5CCCC5)C4)(c(N)ncn6)c36</chem>	C28H31N5O	453.579	NVP-ADW742
Chemicals	S1088				
Selleck		<chem>c1(O)cc(c2cc1)C[C@@H](CCCCCCCCC(CCCC(F)(F)F)(F)F)=O)[C@]([H])([C@]23[H])([C@]23[H])([H])([H])([C@]4(C)CC3)CC[C@H]4O</chem>	C32H47F5O3S	606.771	Fulvestrant
Chemicals	S1191				Quisinstat (JNJ-26481585)
Selleck		<chem>c1cc2c(n(C)cc2CNCC3CCN(c4ncc(C(NO)=O)cn4)CC3)cc1</chem>	C21H26N6O2	394.47	
Chemicals	S1096				
Selleck		<chem>S(=O)(=O)([O-])CCSSCCS(=O)(=O)[O-].[Na+].[Na+]</chem>	C4H8Na2O6S4	326.342	Dimesna
Chemicals	S1201				
Selleck		<chem>c1cc2c(OC(N3CCOCC3)=CC2=O)c(c4ccccc4)c1</chem>	C19H17NO3	307.343	LY294002
Chemicals	S1105				
Selleck		<chem>n1c(N)c2c(ncc(CN(C)c3ccc(C(=O)N[C@H](C(O)=O)CCC(O)=O)cc3)n2)nc1N</chem>	C20H22N8O5	454.439	Methotrexate
Chemicals	S1210				
Selleck		<chem>[Pt+2].[O-]C(=O)C(=O)[O-].C1C[C@H](N)[C@H](N)CC1</chem>	C8H14N2O4Pt	397.286	Oxaliplatin
Chemicals	S1224				
Selleck		<chem>C(C#N)(C[C@@]1(C)[C@@]2CC[C@]3([H])([C@@]1([H])CC[C@@]4(C)[C@@]3([H])CC[C@H]4O)[C@]5([H])O2)=C5O</chem>	C20H27NO3	329.433	Trilostane
Chemicals	S1404				
Selleck		<chem>N1(C)C(=O)n2c(c(C(=O)N)nc2)N=N1</chem>	C6H6N6O2	194.151	Temozolomide
Chemicals	S1237				
Selleck		<chem>c1(OC)cc(CC(=O)N[C@H](CC(C)C)c2c(N3CCCC3)cccc2)ccc1C(=O)O</chem>	C27H36N2O4	452.586	Repaglinide
Chemicals	S1426				
Selleck		<chem>C1(=O)C=C(C=C2[C@]3([H])([C@@]([H])([C@@]4(C)CC2)CC[C@]4(CC#N)O)CC1)CC3</chem>	C20H25NO2	311.418	Dienogest
Chemicals	S1251				
Selleck		<chem>n1c(Nc2ccc(CC(=O)N3CCN(CC)CC3)cc2)nc(Nc4ccc(C(=O)Nc5c(Cl)cccc5)c c4)c(F)c1</chem>	C31H31ClFN7O2	588.075	Aurora A Inhibitor I
Chemicals	S1451				
Selleck		<chem>c1cc(c2nc(N3CCOCC3)c4c(n(C5CCN(C(O)C)=O)CC5)nc4)n2)ccc1NC(=O)OC</chem>	C24H29N7O5	495.531	WYE-354
Chemicals	S1266				
Selleck		<chem>c1(Nc2ncnc2)nc(C(=O)NCc3ccccc3)cs1</chem>	C15H13N5OS	311.362	Thiazovivin
Chemicals	S1459				
Selleck		<chem>c1cccc(C(O)(C2C(CC3C2)C=C3)CCN4CCCC4)c1.Cl</chem>	C21H30ClNO	347.922	Biperiden HCl
Chemicals	S1285				
Selleck		<chem>C1(=O)NC(C)=C(C(=O)Nc2cc3c([nH]nc3)cc2F)C(c4ccc(C(F)(F)F)cc4)C1</chem>	C21H16F4N4O2	432.371	GSK429286A
Chemicals	S1474				
Selleck		<chem>O1[C@H](N2C(=O)NC(=O)C(F)=C2)C[C@H](O)[C@H]1CO</chem>	C9H11FN2O5	246.192	Floxuridine
Chemicals	S1299				
Selleck		<chem>c1c(N(C(=O)C)S(=O)(=O)c2ccc(OC)cc2)c(C=Cc3cc[n+](([O-])cc3)ccc1</chem>	C22H20N2O5S	424.47	HMN-214
Chemicals	S1485				
Selleck		<chem>n1(C(c2ccccc2)C)cncc1C(=O)OCC</chem>	C14H16N2O2	244.289	Etomidate
Chemicals	S1329				
Selleck		<chem>C1=C[C@@]2(C)C(CC[C@]3([H])([C@@]2F)[C@H](O)C[C@@]4(C)[C@ @]3([H])C[C@H](C)[C@@]4(O)C(=O)C)=CC1=O</chem>	C22H29FO5	392.461	Betamethasone
Chemicals	S1500				
Selleck		<chem>c1(C=C2SC(=O)NC2=O)cc3c(nc3c4ccncc4)cc1</chem>	C18H11N3O2S	333.364	GSK1059615
Chemicals	S1360				
Selleck		<chem>c1(C=CC(=O)NO)cc2c(n(CCN(CC)CC)c(CCCC)n2)cc1</chem>	C20H30N4O2	358.478	Pracinostat (SB939)
Chemicals	S1515				

Selleck		<chem>C1C[C@@]2(C)C([C@@]3([H])([C@]([H])(C3)[C@]4([H])(C@@]2([H])CC[C@@]5(C)[C@@]4([H])(C@@]6([H])(C@]([H])(C6)[C@]57CCC(=O)O)7)=CC1=O</chem>	C24H30O3	366.493	Drosiprenone
Chemicals	S1377				
Selleck		<chem>c1(NS(=O)(=O)CC)cc2c(NC(=O)C2=Nc3ccc(CN4CCCC4)cc3)c5cccc5</chem>	C29H32N4O3S	516.654	Hesperadin
Chemicals	S1529				
Selleck					
Chemicals	S1390	<chem>c1cc2c(n(C)c3c2C(=O)C(Cn4ccnc4C)CC3)cc1.Cl</chem>	C18H20ClN3O	329.824	Ondansetron HCl
Selleck		<chem>C1C(CC(CC2([C@H](N)C(=O)N3[C@@]4([H])(C@]([H])(C4)C[C@H]3C#N)C5)(O)CC15)C2</chem>	C18H25N3O2	315.41	Saxagliptin
Chemicals	S1540				
Selleck					
Chemicals	S1008	<chem>c1c(C(=O)NOCOC)c(Nc2c(Cl)cc(Br)cc2)c(F)c3c1n(C)cn3</chem>	C17H15BrClFN4O3	457.681	Selumetinib (AZD6244)
Selleck		<chem>c1cc(c2ccc([C@@H](C(F)(F)F)N[C@@H](CC(F)(C)C(CNC3(CC3)C#N)=O)cc2)ccc1S(C)=O</chem>	C25H27F4N3O3S	525.559	Odanacatib (MK-0822)
Chemicals	S1115				
Selleck					
Chemicals	S1023	<chem>c1(NC(c2c(cc(OCOC)c(OCOC)c2)N=C3=N3)cc(C#C)ccc1.Cl</chem>	C23H27ClN3O4	444.931	Erlotinib HCl (OSI-744)
Chemicals	S1129				
Selleck		<chem>n1c(c2ncc1C(Nc3cccc3c4cn(c5n4)c(CN6CCNCC6)cs5)=O)cccc2.Cl</chem>	C25H24ClN7O5	506.022	SRT1720
Chemicals	S1034	<chem>c1cc(Oc2ccccc2)cc(c3c4c(ncn4N)([C@H]5C[C@@H](CN6CCC6)C5)c3)c1</chem>	C27H29N5O	439.552	NVP-AEW541
Selleck		<chem>C(NCC=C)(C1=O)=C(C[C@@H](C)(C)[C@H](O)(C)[C@H](O)[C@@H](C)C=C(C)[C@H](O)(C)N)=O)[C@@H](O)C=C(C)C(=O)N2C(=O)C2=C1</chem>	C31H43N3O8	585.688	17-AAG (Tanespimycin)
Chemicals	S1141				
Selleck		<chem>c1c2c(c(N3CCN(C(=O)Nc4ccc(OC(C)C)cc4)CC3)ncn2)cc(O)c1OCCCN5CCCC5</chem>	C31H42N6O4	562.703	Tandutinib (MLN518)
Chemicals	S1043				
Selleck					
Chemicals	S1153	<chem>n1c(N[C@H](CC)CO)nc(NCc2cccc2)c3c1n(C(C)C)cn3</chem>	C19H26N6O	354.449	Roscovitine (Seliciclib, CYC202)
Selleck					
Chemicals	S1053	<chem>c1cc(C(=O)Nc2c(N)cccc2)ccc1CNC(=O)OCc3ccccc3</chem>	C21H20N4O3	376.409	Entinostat (MS-275)
Selleck					
Chemicals	S1163	<chem>C(c1cc(C(C)C)c(O)cc1O)(N2Cc(c3C2)cc(CN4CCN(C)CC4)cc3)=O</chem>	C24H31N3O3	409.521	AT13387
Selleck					
Chemicals	S1067	<chem>c1nc(c2c(c3ccc4c(OCO4)c3)nc(c5ccc(C(N)=O)cc5)[nH]2)ccc1</chem>	C22H16N4O3	384.387	SB431542
Selleck					
Chemicals	S1171	<chem>c1(Nc2ccc(N3CCOCC3)cc2)nc(c4c(C)nc(N)s4)ccn1</chem>	C18H20N6OS	368.456	CYC116
Selleck					
Chemicals	S1077	<chem>c1cc(c2c(c3ccncc3)[nH]c(c4ccc(O)cc4)n2)ccc1F</chem>	C20H14FN3O	331.343	SB202190 (FHP1)
Selleck					
Chemicals	S1180	<chem>c1c(C(F)(F)F)ccc(c2nc3c(CSCC3)c(O)n2)c1</chem>	C14H11F3N2OS	312.31	XAV-939
Selleck					
Chemicals	S1089	<chem>c1(NS(=O)(=O)C2(CC2)[C@H](O)C)c(Nc3c(F)cc(1)cc3)c(F)c(F)cc1OC</chem>	C19H20F31N2O5S	572.337	Refametinib (RDEA119, Bay 86-9766)
Selleck		<chem>C(O)=O)[C@@H](NC(c1sc(N(C)Cc2ccc(c3c2)N=C(C)Nc3=O)cc1)=O)CC</chem>			
Chemicals	S1192	<chem>C(O)=O</chem>	C21H22N4O6S	458.488	Raltitrexed
Selleck		<chem>c1(C(F)(F)F)cc2c(SC(N3CCC4(OC(C)CO4)CC3)=NC2=O)c([N+])([O-])=O)c1</chem>	C17H16F3N3O5S	431.386	BTZ043 Racemate
Chemicals	S1097				
Selleck		<chem>C1=C[C@@]2(C)[C@@]([H])(CC[C@]3([H])(C@@]2([H])CC[C@@]4(C)[C@@]3([H])CC[C@H]4C(=O)Nc5c(C(F)(F)F)ccc(C(F)(F)F)c5)NC1=O</chem>	C27H30F6N2O2	528.53	Dutasteride
Chemicals	S1202				
Selleck					
Chemicals	S1106	<chem>c(cccc1)(c2c(cc3n(c4ccc(NC(=O)CN)cc4)nc(C(F)(F)F)c3)cc2)cc5)c15</chem>	C26H19F3N4O	460.45	OSU-03012 (AR-12)
Selleck					
Chemicals	S1212	<chem>c1cc2c(nc(CCCC(=O)O)n2C)cc1N(CCCl)CCCl.Cl</chem>	C16H22Cl3N3O2	394.724	Bendamustine HCl
Selleck		<chem>[C@@]([H])([H])(C(=O)OC1)([C@@H](c2cc(OC)c(O)c(OC)c2)c3c(cc4c(OCO4)c3)[C@H]5O[C@@]6([H])(C@@H)(O)[C@@H](O)[C@@]7([H])(C@@]([H])(CO[C@@H](CO7)O6)[C@]15[H]</chem>	C29H32O13	588.557	Etoposide
Chemicals	S1225	<chem>C1CCN([C@H]2C[C@@]3(C)[C@@]([H])(CC[C@]4([H])(C@@]3([H])CC[C@@]5(C)[C@@]4([H])C[C@H]([N+](6C)CCCC6)[C@H]5O(C(=O)C)[C@@H]2O(C(=O)C)C1.[Br-]</chem>	C34H57BrN2O4	637.731	Vecuronium Bromide
Chemicals	S1405				
Selleck		<chem>c1(O)c(c([C@@]2(C(=O)OC)C[C@@]3([H])CN(C[C@@](CC)(O)C3)CCc4c2[nH]c5c4cccc5)cc6c(N(C=O)[C@]7([H])(C@]6(CC8)[C@@]([H])(N89)[C@@](CC)(C=CC9)[C@@H](OC(C)=O)[C@]7(O)C(=O)OC)c1.S(O)(O)(=O)</chem>	C46H58N4O14S	923.036	Vincristine
Chemicals	S1241				
Selleck					
Chemicals	S1430	<chem>c1(OC2CCCC2)cc(C3CC(=O)NC3)ccc1OC</chem>	C16H21NO3	275.343	Rolipram
Selleck					
Chemicals	S1255	<chem>C(N)(=O)Cc1ccc(C(=O)c2cccc2)c1N</chem>	C15H14N2O2	254.284	Nepafenac
Selleck		<chem>c1cccc(CN2C([C@@H](C(C)C)N(C(=O)c3ccc(C)cc3)CCCN)=Nc4c(ccc(Cl)c4)C2=O)c1</chem>	C30H33ClN4O2	517.062	Ispinesib (SB-715992)
Chemicals	S1452				
Selleck					
Chemicals	S1267	<chem>c1(c2ccc(Cl)cc2)cc3c([nH]cc3C(c4c(F)ccc(NS(CCC(=O)=O)=O)c4F)=O)nc1</chem>	C23H18ClF2N3O3S	489.922	Vemurafenib (PLX4032, RG7204)
Selleck					
Chemicals	S1460	<chem>c1cc2c(c3c(c4[nH]n3)c(ccc4)C2=O)cc1</chem>	C14H8N2O	220.226	SP600125

Selleck		<chem>C1=C[C@@]2(C)C(C)[C@]3([H])[C@@]2([H])[C@H](O)[C@@]4(C)[C@@]3([H])[C@@]4(C)[C@@]5(C)[C@@]4(C)(=O)CO)O[C@]([H])(CCCO5)=CC1=O</chem>	C25H34O6	430.534	Budesonide
Chemicals	S1286				
Selleck		<chem>c1c(F)c(Nc2c(C(=O)N)[C@H](O)CO)ccnc2)ccc1</chem>	C15H15FIN3O3	431.201	Pimasertib (AS-703026)
Chemicals	S1475				
Selleck		<chem>N1C(=O)C(F)=CN([C@H]2CCCCO2)C1=O</chem>	C8H9FN2O3	200.167	FT-207 (NSC 148958)
Chemicals	S1300				
Selleck		<chem>c1nc2c(cc3ccc(CN4CCN(CC)CC4)cc3)[nH]2c(N[C@H](C)c5ccccc5)n1</chem>	C27H32N6	440.583	AEE788 (NVP-AEE788)
Chemicals	S1486				
Selleck		<chem>c1(C(O)(Cn2cncn2)Cn3cncn3)ccc(F)cc1F</chem>	C13H12F2N6O	306.271	Fluconazole
Chemicals	S1331				
Selleck		<chem>c(C(=O)OC1)(c(O)c(CC=C(C)CCC(=O)OCCN2CCOCC2)c(O)c3C)c13</chem>	C23H31NO7	433.495	Mycophenolate Mofetil
Chemicals	S1501				
Selleck		<chem>c1(CC(=O)NC(=S)Nc2cc(F)c(Oc3ccnc4c3sc(c5cn(C)cn5)c4)cc2)ccccc1</chem>	C26H20FN5O2S2	517.598	MGCD-265 analog
Chemicals	S1361				
Selleck		<chem>[C@@H]1(N)[C@@H](O)[C@]([H])(O)[C@@H]2[C@]([H])(O)[C@]3(O)[C@@H](O)[C@@]4([H])[C@H](O4)C=CC(=O)O[C@H](C)CC=CC=CC=C</chem>			
Chemicals	S1517				
Selleck		<chem>C=C2[C@H](C(O)=O)[C@@H](O)C3O[C@H](C)[C@H]1O</chem>	C33H47NO13	665.725	Natamycin
Chemicals	S1378				
Selleck		<chem>n1c(c2cnn([C@H](C3CCCC3)CC#N)c2)c4c([nH]cc4)nc1</chem>	C17H18N6	306.365	Ruxolitinib (INCB018424)
Chemicals	S1530				
Selleck		<chem>c1cc2c(NC(=O)C2=C(C3CCCCC3)Nc4cccc(CN(C)C)c4)cc1C(=O)NC</chem>	C26H26N4O2	426.51	BIX 02188
Chemicals	S1392				
Selleck		<chem>c1(OCC)cc2c(c(Nc3ccc(F)c(Cl)c3)c(C#N)cn2)cc1NC(=O)C=CCN(C)C</chem>	C24H23ClFN5O2	467.923	Pelitinib (EKB-569)
Chemicals	S1392				
Selleck		<chem>[nH]1c2c(cc(Cl)cc2)c3c1C(C(N)=O)CCC3</chem>	C13H13ClN2O	248.708	EX 527 (Selisistat)
Chemicals	S1541				
Selleck		<chem>c1c(F)c2c(c(NC(=O)Nc3ccc(N(C)C)cc3)cc(C)n2)cc1F</chem>	C19H18F2N4O	356.369	SB408124
Chemicals	S1545				
Selleck		<chem>c1c(C(=O)O)ccc(n2nc(c3c(O)cccc3)nc2c4c(O)cccc4)c1</chem>	C21H15N3O4	373.362	Deferasirox
Chemicals	S1712				
Selleck		<chem>c1(Cl)ccc(C2(CCNCC2)c3ccc(c4cn[nH]c4)cc3)cc1</chem>	C20H20ClN3	337.846	AT 7867
Chemicals	S1558				
Selleck		<chem>c1cc2c(ccccc2CN(CC=CC#CC(C)(C)C)cc1</chem>	C21H25N	291.43	Terbinafine
Chemicals	S1725				
Selleck		<chem>c1ccc(S(=O)(=O)N2CCCNCC2)c3c1cnc3.Cl</chem>	C14H18ClN3O2S	327.83	Fasudil (HA-1077) HCl
Chemicals	S1573				
Selleck		<chem>C1=C[C@@]2(C)C(C)[C@]3([H])[C@@]2([H])[C@H](O)[C@@]4(C)[C@@]3([H])[C@@]4(C)[C@@]5(C)[C@@]4(C)(=O)CO)=CC1=O</chem>	C21H28O5	360.444	Prednisolone
Chemicals	S1737				
Selleck		<chem>C(C)(C)[C@H](O)C(=O)N[C@@H](C)C(=O)N[C@H]1C(=O)N(C)CCc2c1ccc2</chem>	C19H27N3O4	361.435	Semagacestat (LY450139)
Chemicals	S1594				
Selleck		<chem>c1nc(C(N)=O)cnc1</chem>	C5H5N3O	123.113	Pyrazinamide
Chemicals	S1762				
Selleck		<chem>c1(N)ccc(S(=O)(=O)Nc2ccc(OC)cn2)cc1</chem>	C11H12N4O3S	280.303	Sulfameter
Chemicals	S1618				
Selleck		<chem>c1nc2c(ncn2[C@H]3O[C@H](CO)[C@@H](O)[C@@H]3O)c(N)n1</chem>	C10H13N5O4	267.241	Vidarabine
Chemicals	S1784				
Selleck		<chem>C1(=O)O[C@@H](C[C@@H](OC([C@@H](NC=O)CC(C)C)=O)CCCCC</chem>			
Chemicals	S1629				
Selleck		<chem>CCCCC[C@H]1CCCCC</chem>	C29H53NO5	495.735	Orlistat
Chemicals	S1806				
Selleck		<chem>c1nc(C(O)=O)c[n+](O-)[c]1C</chem>	C6H6N2O3	154.123	Acipimox
Chemicals	S1806				
Selleck		<chem>c1([N+])(=O)[O-])oc(C=NNC(=O)N)cc1</chem>	C6H6N4O4	198.136	Nitrofuril
Chemicals	S1644				
Selleck		<chem>c1c(Cl)c(SC(Cc2ccc(Cl)cc2)Cn3ccnc3)c(Cl)cc1.[N+](O)(=O)[O-]</chem>	C19H18Cl3N3O3S	474.789	Butoconazole nitrate
Chemicals	S1833				
Selleck		<chem>c1cc(CCN(C)CCOc2ccc(NS(=O)(=O)C)cc2)ccc1NS(=O)(=O)C</chem>	C19H27N3O5S2	441.565	Dofetilide
Chemicals	S1658				
Selleck		<chem>c1cc2c(OC=C(C3ccc(O)cc3)C2=O)cc1O</chem>	C15H10O4	254.238	Daidzein
Chemicals	S1849				
Selleck		<chem>NCCN.N1(C)C(=O)c2c(nc[nH]2)N(C)C1=O.N3(C)C(=O)c4c(nc[nH]4)N(C)C3=O</chem>	C16H24N10O4	420.426	Aminophylline
Chemicals	S1673				
Selleck		<chem>C(l)(C(=O)NC(=O)N1[C@H]2C[C@H](O)[C@@H](CO)O2)=C1</chem>	C9H11N2O5	354.099	Idoxuridine
Chemicals	S1883				
Selleck		<chem>CS(=O)(=O)OCCCCOS(=O)(=O)C</chem>	C6H14O6S2	246.302	Busulfan
Chemicals	S1692				
Selleck		<chem>c1ccc(Cl)c(Nc2ccccc2CC(=O)[O-])c1Cl.[Na+]</chem>	C14H10Cl2NNaO2	318.13	Diclofenac Sodium
Chemicals	S1903				
Selleck		<chem>c1cc(S(=O)(=O)Nc2nc(C)c2C)ccc1N</chem>	C11H13N3O3S	267.304	Sulfisoxazole
Chemicals	S1916				

Selleck					
Chemicals	S2134	<chem>c1c(F)c(NC2=C(C(=O)NOC(=O)C=C(C)C(=O)N2C)ccc1I</chem>	C16H17F1N3O4	461.227	AZD8330
Selleck					
Chemicals	S1952	<chem>C1=Cc2c(c(OC)c3c(ccc3)c2)OC1=O</chem>	C12H8O4	216.19	Methoxsalen
Selleck		<chem>c(nc(Nc1ccc(C(F)(F)F)cc1)n2C)(cc(Oc3cc(c4ncc(C(F)(F)F)[nH]4)ncc3)cc5)</chem>			
Chemicals	S2161	<chem>c25</chem>	C24H16F6N6O	518.414	RAF265 (CHIR-265)
Selleck					
Chemicals	S1974	<chem>CNC[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO</chem>	C7H17NO5	195.214	Meglumine
Selleck		<chem>c1cccc(CC2=C([C@@H](C(C)C)N(CCCN)C(c3ccc(C)cc3)=O)Oc4c(ccc(Cl)c4)C2=O)c1.Cl</chem>	C31H34Cl2N2O3	553.519	SB743921
Chemicals	S2182	<chem>N1(C)C(=O)C(O)=C(C(=O)NCC2ccc(F)cc2)N=C1C(C)(C)NC(=O)Cc3oc(C)nn3</chem>	C20H21FN6O5	444.416	Raltegravir (MK-0518)
Selleck					
Chemicals	S2201	<chem>n1ccc(Oc2c(F)cc(NC(=O)C(C(=O)C(c3ccc(F)cc3)=CN4=C4)cc2)c(Cl)c1N</chem>	C23H15ClF2N4O3	468.84	BMS-794833
Selleck		<chem>O=C1O[C@]2([H])[C@@](O)([C@]3(O4)C(C)[C@]([H])(O)C(=O)O5([C@H]45)[C@]([H])(C(C)(C)C)O6)([C@]6([H])O C3=O)C2)[C@]1([H])C</chem>	C20H24O9	408.399	Ginkgolide A
Chemicals	S2026				
Selleck		<chem>n1c(N)c2c(n(C(C)C)nc2c3cc4c(ccc(O)c4)[nH]3)nc1</chem>	C16H16N6O	308.338	PP242
Chemicals	S2218				
Selleck		<chem>c1(cccc(O)c1)N(CC2=NCCN2)c3ccc(C)cc3.CS(=O)(=O)O</chem>	C18H23N3O4S	377.458	Phentolamine Mesylate
Chemicals	S2038				
Selleck		<chem>c1ccc(c2cc(C(=O)O)ccc2)c(O)c1NN=C3C(C)=NN(c4cc(C)c(C)cc4)C3=O</chem>	C25H22N4O4	442.467	Eltrombopag
Chemicals	S2229				
Selleck		<chem>C(Cl)(C(O)=CC(=O)N1)=C1</chem>	C5H4ClNO2	145.544	Gimeracil
Chemicals	S2055				
Selleck		<chem>c1ccc([C@H](C(C)C)C(=O)Nc2ccc(C(=O)NO)cc2)cc1</chem>	C18H20N2O3	312.363	AR-42
Chemicals	S2244				
Selleck		<chem>n1c(Cl)c(NC(NCC2=N2)c(OC)nc1C</chem>	C9H12ClN5O	241.677	Moxonidine
Chemicals	S2066	<chem>[C@@H]1(O)CC[C@]2(C)[C@]([H])(CCC(=C)[C@@H]2CC=C3C(O)CO C3=O)[C@]1(C)CO</chem>	C20H30O5	350.449	Andrographolide
Selleck					
Chemicals	S2097	<chem>[C@H](C(OC)(c1cccc1)c2ccccc2)(C(=O)O)Oc3nc(C)cc(C)n3</chem>	C22H22N2O4	378.421	Ambrisentan
Selleck		<chem>[C@@H]1(O)[C@H](C(O)=O)O[C@H](Oc2cc3c(C(=O)C=C(c4ccccc4)O3)c(O)c2O)[C@H](O)[C@H]1O</chem>	C21H18O11	446.361	Baicalin
Chemicals	S2269				
Selleck		<chem>c1(O)c(CN(C(C)C)c2c(n(C)c(CSc3ccccc3)c2C(=O)OCC)cc1Br.Cl</chem>	C22H26BrClN2O3S	513.875	Arbidol HCl
Chemicals	S2120				
Selleck		<chem>C([C@H](C[C@@H]1C2)CNC1)(=CC=CC3=O)N23</chem>	C11H14N2O	190.242	Cytisine
Chemicals	S2287				
Selleck		<chem>c1(C#N)cc(c2nc(C)c(C(=O)O)s2)ccc1OCC(C)C</chem>	C16H16N2O3S	316.375	Febuxostat
Chemicals	S1547				
Selleck		<chem>c1ccc(NC(=O)C2=C(O)Cc3c(cccc3)S(=O)(=O)N2C)nc1</chem>	C15H13N3O4S	331.346	Piroxicam
Chemicals	S1713	<chem>c1(Cl)c(Oc2c(F)cc(NC(C3=C(OCC)C=CN(c4ccc(F)cc4)C3=O)=O)cc2)ccnc1N</chem>	C25H19ClF2N4O4	512.893	BMS-777607
Selleck					
Chemicals	S1729	<chem>c1c(C)c(OCCCC(C)(C)C(O)=O)cc(C)c1</chem>	C15H22O3	250.333	Gemfibrozil
Selleck		<chem>c1cc(OCCN2CCOCC2)c3c(cccc3)c1NC(=O)Nc4n(c5ccc(C)cc5)nc(C(C)(C)C)c4</chem>	C31H37N5O3	527.657	BIRB 796 (Doramapimod)
Chemicals	S1574				
Selleck		<chem>c1cccc(c2ccc(Cn3c4c(c(C)cc(c5nc6c(cccc6)n5C)p4)nc3CCC)cc2)c1C(=O)O</chem>	C33H30N4O2	514.617	Telmisartan
Chemicals	S1738	<chem>c(c1c(cc(OC)cc1)[nH]2)(CCN3[C@]4([H])C[C@@]5([H])[C@]([H])(C[C@@H](OC)c6cc(OC)c(OC)c(OC)c6)=O)[C@H](OC)[C@H]5C(=O)OC)C3)c24</chem>	C33H40N2O9	608.679	Reserpine
Selleck		<chem>c1(C=NN2CCN(C)CC2)c(O)c(c(C(=O)[C@]3(C)O4)c45)c(c(O)c5C)c(O)c1N</chem>			
Chemicals	S1601	<chem>C(=O)C(C)=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@H](C)[C@H](OC(C)=O)[C@H](C)[C@H](OC)C=CO3</chem>	C43H58N4O12	822.94	Rifampin
Selleck		<chem>[C@]([H])([H])(OCC1)(OC[C@@]2(O C(=O)N[C@@]([C@@]([H])CN(S(=O)(=O)Cc3ccc(N)cc3)CC(C)C([H])Cc4ccccc4)[H])[C@@]12[H].CCO</chem>	C29H43N3O8S	593.732	Darunavir Ethanolate
Chemicals	S1764	<chem>c1c2c(O CO2)cc3c1[C@@H](O)[C@@H]4O[C@H]5[C@@H](O)[C@H](c6sccc6)O C5)[C@H](O)[C@H]4O)[C@@H]7[C@]([H])(C(=O)OC7)[C@H]3c8</chem>	C32H32O13S	656.654	Teniposide
Selleck		<chem>cc(OC)c(O)c(OC)c8</chem>			
Chemicals	S1787				
Selleck		<chem>C(NC(=O)c1c2[nH]nc1)=N2.[Na+]</chem>	C5H4N4NaO	159.101	Allopurinol Sodium
Chemicals	S1631				
Selleck		<chem>OCCOCn1cnc2c1N=C(N)NC2=O</chem>	C8H11N5O3	225.205	Aciclovir
Chemicals	S1807				
Selleck		<chem>c1cc(C(=O)c2cc(C(C)C(=O)O)ccc2)ccc1</chem>	C16H14O3	254.281	Ketoprofen
Chemicals	S1645				

Selleck	Chemicals	S1835	<chem>[C@@H]1(O)[C@@H](C)N(C)C[C@@H](C)C[C@](O)(C)[C@H](O)[C@@H]2C@@H](O)[C@@H](N(C)C)C[C@@H](C)O2)[C@@H](C)[C@H](O)[C@@H]3O[C@@H](C)[C@H](O)[C@@](OC)(C)C3[C@H](C)C(=O)O[C@H](CC)[C@@]1(C)O</chem>	C38H72N2O12	748.984	Azithromycin
Selleck	Chemicals	S1662	<chem>c1cc2c(non2)c(C3C(C(=O)O)C(C)C)=C(C)NC(C)=C3C(OC)=O)c1</chem>	C19H21N3O5	371.387	Isradipine
Selleck	Chemicals	S1855	<chem>c1(F)cc2c(N(CC)C=C(C(=O)=O)C2=O)cc1N3CCN(C)CC3.S(O)(=O)(=O)C</chem>	C18H24FN3O6S	429.463	Pefloxacin Mesylate
Selleck	Chemicals	S1676	<chem>c1cc(CC(C)CN2C[C@@H](C)O[C@@H](C)C2)ccc1C(C)(C)CC.Cl</chem>	C21H36ClNO	353.97	Amorolfine HCl
Selleck	Chemicals	S1884	<chem>[C@@H]1(C)CN(c2c(F)c(N)c3c(N(C4CC4)C=C(C(=O)O)C3=O)c2F)C[C@H](C)N1</chem>	C19H22F2N4O3	392.4	Sparfloxacin
Selleck	Chemicals	S1701	<chem>C1=C[C@@]2(C)C(C[C@]3([H])[C@@]2([H])[C@H](O)C[C@@]4(C)[C@@]3([H])C[C@]5([H])[C@]4(C=O)CO)OC(C)(C)O5)=CC1=O</chem>	C24H32O6	416.507	Desonide
Selleck	Chemicals	S1904	<chem>c1cc(C(=O)CC(=O)c2ccc(C(C)(C)C)cc2)ccc1OC</chem>	C20H22O3	310.387	Avobenzone
Selleck	Chemicals	S1917	<chem>c1c(N(C)C)ccc(C(=C2C=CC(=[N+](C)C)C=C2)c3ccc(N(C)C)cc3)c1.[Cl-]</chem>	C25H30ClN3	407.979	Crystal Violet
Selleck	Chemicals	S2149	<chem>c1(c2ccc(S(C)(=O)=O)cc2)nc(OCC3CCN(c4onc(C(C)C)n4)CC3)cc1</chem>	C23H28N4O4S	456.558	GSK1292263
Selleck	Chemicals	S1956	<chem>c1cc(C(Cn2cnc2)OCc3c(Cl)cc(C)cc3)c(Cl)cc1Cl.O[N+][([O-])=O</chem>	C18H15Cl4N3O4	479.141	Miconazole Nitrate
Selleck	Chemicals	S2162	<chem>c1(Nc2cc(C)[nH]n2)c(Cl)cnc(N[C@@H](C)c3ncc(F)cn3)n1[Br-].[C@@]1([H])(C[C@H](OC(=O)[C@H](CO)c2ccccc2)C3([N+](C)(C)[C@]3([H])[C@@]4([H])[C@]1([H])O4</chem>	C14H14ClFN8	348.766	AZD1480
Selleck	Chemicals	S1978	<chem>C(Nc1ccc(c2c1)ncnc2Nc3ccc(OCc4ccccc(F)c4)c(Cl)c3)(=O)C=C.c5c(S(=O)(=O)O)ccc(C)c5</chem>	C18H24BrNO4	398.291	Methscopolamine
Selleck	Chemicals	S2185		C31H26ClFN4O5S	621.078	AST-1306
Selleck	Chemicals	S2006	<chem>n1c(N)c(c2ccc(Cl)cc2)c(CC)nc1N</chem>	C12H13ClN4	248.711	Pyrimethamine
Selleck	Chemicals	S2202	<chem>c(cnn1C)(c(Nc2c(C)ccc(C(=O)Nc3cc(C(F)(F)F)ccc3)c2)nc(c4cnccc4)n5)c15</chem>	C26H20F3N7O	503.479	NVP-BHG712
Selleck	Chemicals	S2028	<chem>c1cc(C(C#N)c2c(Cl)cc(N3C(=O)NC(=O)C=N3)cc2)ccc1Cl</chem>	C17H9Cl3N4O2	407.638	Diclazuril
Selleck	Chemicals	S2219	<chem>c1cc(Nc2nc(c3ccc(C(=O)NCC#N)cc3)cn2)ccc1N4CCOCC4</chem>	C23H22N6O2	414.46	CYT387
Selleck	Chemicals	S2040	<chem>c1c(NS(C)(=O)=O)c(Oc2ccccc2)cc([N+][([O-])=O])c1</chem>	C13H12N2O5S	308.31	Nimesulide
Selleck	Chemicals	S2230	<chem>c1(C)nc(c2c(c3c4c(ccc(C(N)=O)c4)nc3)c5n(CCC5)n2)ccc1</chem>	C22H19N5O	369.419	LY2157299
Selleck	Chemicals	S2058	<chem>c1(cccc(C)c1)N(C)C(=S)Oc2cc3c(cccc3)cc2</chem>	C19H17NOS	307.409	Tolnaftate
Selleck	Chemicals	S2247	<chem>c1c(C(F)(F)F)c(c2cc(N3CCOCC3)nc(N4CCOCC4)n2)cn1N</chem>	C18H21F3N6O2	410.394	Buparlisib
Selleck	Chemicals	S2067	<chem>c1cc(C=CC(=O)O)ccc1Cn2ccnc2.Cl</chem>	C13H13ClN2O2	264.708	Ozagrel HCl
Selleck	Chemicals	S2262	<chem>c1c(O)cc2c(C(=O)C=C(c3ccc(O)cc3)O2)c1O</chem>	C15H10O5	270.237	Apigenin
Selleck	Chemicals	S2098	<chem>c(C(C)(C)CCC1(C)C)(cc(C)c(C(=C)c2ccc(C(O)=O)cc2)c3)c13</chem>	C24H28O2	348.478	Bexarotene
Selleck	Chemicals	S2270	<chem>[C@H]1(CO)O[C@]2([H])[C@]([H])(O)C(=O)c3c2c(O)c(OC)c(O)c3)[C@@H](O)[C@@H]1O</chem>	C14H16O9	328.271	Bergenin
Selleck	Chemicals	S2121	<chem>c1(c(CC(O)=O)n2c(CC(C)(C)C2)c1c3ccccc3)c4ccc(Cl)cc4</chem>	C23H22ClNO2	379.879	Licofelone
Selleck	Chemicals	S2290	<chem>C1[C@H](C)[C@@]2([H])[C@]([O3]([C@]4([H])O[C@@]3(C)CC2)[C@]([H])([C@@H](C)[C@H](O)O4)C1</chem>	C15H24O5	284.348	Dihydroartemisinin (DHA)
Selleck	Chemicals	S1548	<chem>c1([C@H]2[C@@H](O)[C@H](O)[C@H](O)[C@H](CO)O2)cc(Cc3ccc(OCC)cc3)c(Cl)cc1</chem>	C21H25ClO6	408.873	Dapagliflozin
Selleck	Chemicals	S1714	<chem>N(C(=O)N([C@H]1C(F)(F)[C@H](O)[C@@H](CO)O1)C=C2)=C2N</chem>	C9H11F2N3O4	263.198	Gemcitabine
Selleck	Chemicals	S1565	<chem>c(OC(F)(F)O1)(ccc(C2(CC2)C(=O)Nc3ccc(C)c(c4cc(C(=O)O)ccc4)n3)c5)c15</chem>	C24H18F2N2O5	452.407	VX-809 (Lumacaftor)
Selleck	Chemicals	S1730	<chem>c1cc(Cl)c(S(=O)(=O)N)cc1C(=O)NN2C(C)Cc3c2ccccc3</chem>	C16H16ClN3O3S	365.835	Indapamide
Selleck	Chemicals	S1575	<chem>O=C1[C@H](NC(=O)C(C)C(=O)NCC(F)(F)C(F)(F)F)c2c(cccc2)c3c(ccc(c3)N1</chem>	C22H20F5N3O3	469.405	RO4929097

Selleck					
Chemicals	S1739	<chem>n1c(c2nc3c(cccc3)[nH]2)csc1</chem>	C10H7N3S	201.248	Thiabendazole
Selleck					
Chemicals	S1603	<chem>c1(C(=O)O)c(NCc2cccc2)cc(C)c(S(=O)(=O)N)c1</chem>	C12H11ClN2O5S	330.744	Furosemide
Selleck		<chem>C1(C(C)=C(C=C(C(C)=CC=CC(C)=CC=C(C(C)=CC(C(C)(C)CCC2=C2C)C(C)C)CC1</chem>	C40H56	536.873	Beta Carotene
Chemicals	S1767	<chem>C1=C[C@@]2(C)C(C[C@]3([H])[C@@]2([H])C(=O)C[C@@]4(C)[C@@]3([H])CC[C@]4(O)C(=O)CO)=CC1=O</chem>	C21H26O5	358.428	Prednisone
Chemicals	S1622	<chem>[C@@H]1(O)[C@@H](C)[C@@H](O)[C@H](C)C=CC=C(C)C(=O)Nc2c(O)c(c(c(C(=O)[C@]3(C)OC=C[C@H](O)C[C@@H](C)[C@@H](OC(=O)C)[C@@H]1C)c4O3)c5c2n6c(cc(C)cc6)n5)c(O)c4C</chem>	C43H51N3O11	785.879	Rifaximin
Selleck	S1790	<chem>c(n(C)cc1Cc2c(OC)cc(C(NS(=O)(=O)C3C(C)cccc3)=O)cc2)(ccc(NC(=O)OC4CCCC4)c5)c15</chem>	C31H33N3O6S	575.675	Zafirlukast
Selleck					
Chemicals	S1811	<chem>c1(Cl)nc(C(=O)NC(=N)N)c(N)nc1N.Cl</chem>	C6H9Cl2N7O	266.088	Amiloride HCl
Selleck					
Chemicals	S1646	<chem>c1ccc(C(=O)c2n3c(C(C(=O)=O)CC3)cc2)cc1.OCC(N)(CO)CO</chem>	C19H24N2O6	376.404	Ketorolac
Selleck					
Chemicals	S1836	<chem>c1(S(=O)CCC)cc2c(nc(NC(OC)=O)[nH]2)cc1</chem>	C12H15N3O3S	281.331	Albendazole Oxide
Selleck		<chem>c1cc2c(C[C@]3([H])[C@@]2([H])CC[C@]4(C)[C@@]3([H])CCC4=O)c</chem>	C18H22O2	270.366	Estrone
Chemicals	S1665	<chem>c1O</chem>			
Selleck					
Chemicals	S1859	<chem>c1(O)ccc(C(CC)=C(CC)c2ccc(O)cc2)cc1</chem>	C18H20O2	268.35	Diethylstilbestrol
Selleck					
Chemicals	S1677	<chem>c1cc([C@@H](O)[C@@H](CO)NC(C(Cl)Cl)=O)ccc1[N+](=[O-])=O</chem>	C11H12Cl2N2O5	323.129	Chloramphenicol
Selleck					
Chemicals	S1889	<chem>c1c(O)c2c(C(=O)c3c(c(NCCNCCO)ccc3NCCNCCO)C2=O)c(O)c1</chem>	C22H28N4O6	444.481	Mitoxantrone
Selleck					
Chemicals	S1702	<chem>[C@H]1(CO)O[C@@H](n2cnc3c2N=CNC3=O)CC1</chem>	C10H12N4O3	236.227	Didanosine
Selleck					
Chemicals	S1907	<chem>n1(c(C)nc1[N+](=[O-])=O)CCO</chem>	C6H9N3O3	171.154	Metronidazole
Selleck					
Chemicals	S1928	<chem>c1c(CC=C)cc(C(NCCO)=O)c(O)c1OC</chem>	C13H17NO4	251.278	Alibendol
Selleck		<chem>c1(NC(=O)c2cccc(c3ccc(OC(F)(F)F)cc3)c2C)cnc(N4C[C@@H](C)O[C@@H](C)C4)cc1</chem>	C26H26F3N3O3	485.498	LDE225 (NVP-LDE225, Erismodegib)
Chemicals	S2151				
Selleck					
Chemicals	S1957	<chem>c1cc(S(=O)(=O)Nc2nnc(C)s2)ccc1N</chem>	C9H10N4O2S2	270.331	Sulfamethizole
Selleck					
Chemicals	S2170	<chem>c1c(CN(CC)CC)cc2c(cc(COC(=O)Nc3ccc(C(=O)NO)cc3)cc2)c1.O.Cl</chem>	C24H30ClN3O5	475.965	Givinostat (ITF2357)
Selleck					
Chemicals	S1979	<chem>c1(OCCN(CC)CC)c(l)cc(C(c2c3c(cccc3)oc2CCCC)=O)cc1.Cl</chem>	C25H30Cl2NO3	681.773	Amiodarone HCl
Selleck					
Chemicals	S2186	<chem>c1(C)nc(c2c(c3ccc4c(OCO4)c3)nc(C(C)(C)C)[nH]2)ccc1</chem>	C20H21N3O2	335.4	SB505124
Selleck					
Chemicals	S2007	<chem>c1c(C=C2C(C)=C(CC(O)=O)c3c2ccc(F)c3)ccc(S(=O)C)c1</chem>	C20H17FO3S	356.411	Sulindac
Selleck					
Chemicals	S2205	<chem>c1c(Nc2c3c(cc(OCOC)c(OCOC)c3)ncn2)cccc1C#C.Cl</chem>	C21H22ClN3O4	415.87	OSI-420
Selleck					
Chemicals	S2029	<chem>C1=CC(=O)NC(=O)N1[C@H]2[C@@H](O)[C@H](O)[C@@H](CO)O2</chem>	C9H12N2O6	244.201	Uridine
Selleck					
Chemicals	S2220	<chem>n1c(c2ccc(OCCN(C)C)cc2)[nH]c(c3cc4c(C(=NO)CC4)cc3)c1c5ccncc5</chem>	C27H27N5O2	453.536	SB590885
Selleck		<chem>[C@@H]1(C2)[C@@H]2[C@@]3(C)C(C(C)Cl)=C[C@]4([H])[C@@]3([H])CC[C@@]5(C)[C@@]4([H])CC[C@]5(OC(=O)C(C)=O)=CC1=O</chem>	C24H29ClO4	416.938	Cyproterone Acetate
Chemicals	S2042				
Selleck					
Chemicals	S2231	<chem>n1nc(OCc2ccnc(C(NC)=O)c2)c3c(ccc3)c1Nc4ccc(Cl)cc4</chem>	C20H16ClN5O3	409.826	Telatinib
Selleck					
Chemicals	S2059	<chem>c(cc(OC)c(C)C)c1(nc(N2CCN(C(=O)C3OCCC3)CC2)nc4N)c14.Cl.O.O</chem>	C19H30ClN5O6	459.924	Terazosin HCl
Selleck					
Chemicals	S2248	<chem>c1cc2c(c3c(cc(C(O)=O)cc3)nc2Nc4cccc(Cl)c4)cn1</chem>	C19H12ClN3O2	349.77	CX-4945 (Silmilasertib)
Selleck					
Chemicals	S2074	<chem>c1cc2c(c(C(OC)=O)c(C)n2C)cc1O</chem>	C13H15NO3	233.263	Mecarbinatate
Selleck					
Chemicals	S2263	<chem>[C@H]1(CO)O[C@@H](Oc2ccc(O)cc2)[C@H](O)[C@H](O)[C@@H]1O</chem>	C12H16O7	272.251	Arbutin
Selleck					
Chemicals	S2101	<chem>c1(O(C(CCCCCNC(=N)N)=O)ccc(C(=O)OCC)cc1.O=S(C)(O)=O</chem>	C17H27N3O7S	417.477	Gabexate Mesylate
Selleck					
Chemicals	S2271	<chem>c1cc2c(c[n+]3c(c4c(cc5c(OCO5)c4)CC3)c2)c(O)c1OC.[CH]</chem>	C20H18ClNO4	371.814	Berberine HCl

Selleck		<chem>c1cc2c(Cc1C[C@]3([H])[C@@]2([H])C[C@]4(C)[C@]3([H])C[C@]4(O)C#C)cc1OC</chem>	C21H26O2	310.43	Mestranol
Chemicals	S2125				
Selleck		<chem>[C@]1([O])[C@H](O)[C@H](C)O[C@@H](O)C[C@H]2O[C@]1(O)c3c(O)c4c(OC(c5ccc(OC)c(O)c5)=CC4=O)c3[C@H](O)[C@@H](O)[C@@H]2O</chem>	C28H32O15	608.545	Diosmin
Chemicals	S2292				
Selleck		<chem>c1cc2c(Cc1C[C@]([H])([C@H](O)CN[C@]1C@H(O)[C@@]3([H])Oc4c(cc(F)c4)CC3)O2)cc1F.Cl</chem>	C22H26ClF2NO4	441.896	Nebivolol
Chemicals	S1549				
Selleck					
Chemicals	S1715	<chem>c1(S(=O)(=O)NC(=O)NC2CCCC2)ccc(CCN(C(=O)c3ncc(C)nc3)cc1</chem>	C21H27N5O4S	445.535	Glipizide
Selleck					
Chemicals	S1567	<chem>c1c(N)c2c(C(=O)N(C3CCC(=O)NC3=O)C2=O)cc1</chem>	C13H11N3O4	273.244	Pomalidomide
Selleck					
Chemicals	S1732	<chem>c1cc(C(C(Cl)Cl)c2ccccc2Cl)ccc1Cl</chem>	C14H10Cl4	320.041	Mitotane
Selleck					
Chemicals	S1576	<chem>c1(ncccc1)NS(=O)(=O)c2ccc(N=Nc3ccc(O)c(C(O)=O)c3)cc2</chem>	C18H14N4O5S	398.393	Sulfasalazine
Selleck		<chem>[C@]1(C)[C@@H](O)C(=CO[C@]2(C)C(=O)c(c3c4C(=O)C=C(C)NC5CCN(CC(C)C)CC5)C3=N6)NC(=O)C(C)=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](O)C(C(=O)O)c(O2)c(C)c4O</chem>	C46H62N4O11	847.005	Rifabutin
Chemicals	S1741				
Selleck		<chem>[C@]([H])([C@@](NC(=O)C(=NO)c1csc(N)n1)([H])C2=O)(SCC(C(=C)C3C(=O)O)N23</chem>	C14H13N5O5S2	395.414	Cefdinir
Chemicals	S1605				
Selleck		<chem>N(C(=O)[C@@H]1NC(C(2nc(N)sc2)=NOC)=O)(C(C)OCO(C(=O)C(C)(C)=O)=O)=O)C(C=Cc3c(C)ncs3)CS4][C@@]14[H]</chem>	C25H28N6O7S3	620.721	Cefditoren Pivoxil
Chemicals	S1768				
Selleck					
Chemicals	S1623	<chem>C(=O)N[C@@]([H])(CS)C(=O)O)C</chem>	C5H9NO3S	163.195	Acetylcysteine
Selleck		<chem>C1[C@@H](OC(C(C)C)CC)=O)[C@@]2([H])C(C=C[C@H](C)[C@H]2C[C@]3([H])C[C@@H](O)CC(=O)O3)=C[C@@H]1C</chem>	C25H38O5	418.566	Simvastatin
Chemicals	S1792				
Selleck		<chem>C1[C@@](O)(C)[C@H](O[C@H]2OC(C)C[C@@H](N(C)C)[C@H]2O)[C@@H](C)[C@H](O[C@H]3O[C@H](C)[C@@H](O)[C@](C)(OC)C3)[C@@H](C)C(=O)O[C@H](CC)[C@@](C)(O)[C@H](O)[C@@H](C)C(=O)[C@@H</chem>	C37H67NO13	733.927	Erythromycin
Chemicals	S1635				
Selleck					
Chemicals	S1816	<chem>c1nc(C(c2ccc(Cl)cc2)CCN(C)C)ccc1.C(=O)(O)C=CC(=O)O</chem>	C20H23ClN2O4	390.861	Chlorpheniramine Maleate
Selleck					
Chemicals	S1647	<chem>O1[C@H](n2cnc3c2ncnc3N)[C@H](O)[C@H](O)[C@H]1CO</chem>	C10H13N5O4	267.241	Adenosine
Selleck					
Chemicals	S1839	<chem>c1c(Cl)c(O)c2c(cccn2)c1Cl</chem>	C9H5Cl2NO	214.048	Chloroxine
Selleck					
Chemicals	S1666	<chem>C1(=O)N=C(N)C(F)=CN1</chem>	C4H4FN3O	129.092	Flucytosine
Selleck					
Chemicals	S1866	<chem>c1cccc(C(OCN(C)C)c2ccccc2)c1.Cl</chem>	C17H22ClNO	291.816	Diphenhydramine HCl
Selleck					
Chemicals	S1679	<chem>c1(F)cc([C@H](C)C(=O)O)ccc1c2ccccc2</chem>	C15H13FO2	244.261	Flurbiprofen
Selleck					
Chemicals	S1891	<chem>c1(O)cc(C[C@@](N)(C)C(=O)O)ccc1O</chem>	C10H14N2O4	226.229	Carbidopa
Selleck					
Chemicals	S1704	<chem>N(C(=O)N([C@@H]1CS[C@H](CO)O)C=C2F)=C2N</chem>	C8H10FN3O3S	247.247	Emtricitabine
Selleck					
Chemicals	S1908	<chem>c1([N+]([O-])=O)ccc(NC(=O)C(C)C)cc1C(F)F</chem>	C11H11F3N2O3	276.212	Flutamide
Selleck					
Chemicals	S1929	<chem>c1c(Cl)cc(c2nc(N)nc(N)n2)c(Cl)c1</chem>	C9H7Cl2N5	256.091	Irsogladine
Selleck		<chem>c1(C(N)=NC(=O)OCCCCC)ccc(NCc2nc3c(ccc(C(=O)N(c4ncccc4)CCC(=O)OCC)c3)n2C)cc1</chem>	C34H41N7O5	627.733	Dabigatran Etexilate
Chemicals	S2154				
Selleck					
Chemicals	S1962	<chem>N(S(=O)(=O)c1ccc(N)cc1)c2cc(OC)nc(OC)n2</chem>	C12H14N4O4S	310.329	Sulphadimethoxine
Selleck					
Chemicals	S2177	<chem>c1(Cl)cc(S(=O)(=O)N)cc(S(=O)(=O)N)c1Cl</chem>	C6H6Cl2N2O4S2	305.159	Dichlorophenamide
Selleck		<chem>C1=C[C@@]2(C)C(C[C@]3([H])[C@@]2(Cl)[C@H](O)C[C@@]4(C)[C@@]3([H])C[C@]4H)[C][C@@]4(O)C(c5cccc5)=O)C(=O)CC(=CC1=O</chem>	C27H30Cl2O6	521.429	Mometasone furoate
Chemicals	S1987				
Selleck		<chem>c1c(C(C)C)c(C(C)=O)NS(=O)(=O)Oc2c(C(C)C)cccc2C(C)C(C(C)C)cc1C(C)C</chem>	C29H43NO4S	501.721	Avasimibe
Chemicals	S2187				
Selleck					
Chemicals	S2012	<chem>n1(Cc2ccc(OC)cc2)c(c3cc1)cc(C(NO)=O)cc3</chem>	C17H16N2O3	296.321	PCI-34051
Selleck					
Chemicals	S2207	<chem>C1(Cn2c3c(c(N)ncn3)cn2)=Nc4c(c(C)ccc4)C(=O)N1c5ccccc5C</chem>	C22H19N7O	397.433	PIK-293
Selleck					
Chemicals	S2030	<chem>c1(F)ccc(C(c2ccc(F)cc2)N3CCN(CC=Cc4cccc4)CC3)cc1.Cl.Cl</chem>	C26H28Cl2F2N2	477.417	Flunarizine 2HCl
Selleck		<chem>S(=O)(C)(O)=O.c1cc(C(=O)Nc2ccc(C3(C#N)CCCC3)cc2)c(NCc4cncc4)nc1</chem>	C25H27N5O4S	493.578	Apatinib
Chemicals	S2221				

Selleck					
Chemicals	S2043	Cl.C1(C)(CC(C)(CC2C1)CC3(N)C2)C3	C12H22ClN	215.763	Memantine HCl
Selleck					
Chemicals	S2232	c1cc2c(NC(=O)N(CCN3CCC(C(=O)c4ccc(F)cc4)CC3)C2=O)cc1	C22H22FN3O3	395.427	Ketanserin
Selleck					
Chemicals	S2060	c1(Br)cc(CN(C2CCCCC2)C)c(N)c(Br)c1.Cl	C14H21Br2ClN2	412.591	Bromhexine HCl
Selleck					
Chemicals	S2252	C1(C(C)=O)=C(O)[C@]2(C)C(Oc3c2c(O)c(C)c(O)c3C(=O)C)=CC1=O [Ca+2].n1(c(c2ccc(F)cc2)c(c3ccccc3)c(C(Nc4ccccc4)=O)c1C(C)C)CC[C@ @H](O)C[C@H](O)CC(=O)O-].n5(c(c6ccc(F)cc6)c(c7ccccc7)c(C(Nc8ccccc8)=O)c5C(C)C)CC[C@H](O)C[C@H](O)CC(=O)O[O-]	C18H16O7	344.315	(+)-Usniacin
Selleck					
Chemicals	S2077	C66H68CaF2N4O10	1155.342	Atorvastatin Calcium	
Selleck					
Chemicals	S2264	[C@]([H])(CC1)([C@@]([H])(C)CC2)[C@@]([C@]([H])(O)[C@@]13C)O[C @H](OC)[C@]4(C)[H])(O3)[C@@]24[H] c1(O)cc2c([C@@H](Cc3cc(OC)c(OC)cc3)[N@@+](C)(CCC(=O)O)CCCC CO C(=O)CC[N@@+]4(C)CCc(c5[C@H]4Cc6cc(OC)c(OC)cc6)cc(OC)c(O C)c5)CC2)cc1OC.c7c(S(=O)(=O)[O-])cccc7.c8c(S(=O)(=O)[O-])cccc8 O1[C@]2([H])C3([C@@H](O)C(=O)O2)[C@@]([C@H](O)O4)([C@]4([H])C[C @]3(O)C(C)C)C1=O	C16H26O5	298.375	Artemether
Selleck					
Chemicals	S2113	C65H82N2O18S2	1243.479	Cisatracurium Besylate	
Selleck					
Chemicals	S2276	C15H18O8	326.299	Bilobalide	
Selleck					
Chemicals	S2126	C24H28N2O3	392.491	Naftopidil	
Selleck					
Chemicals	S2295	C15H10O5	270.237	Emodin	
Selleck					
Chemicals	S1550	C19H18N4O2	334.372	Pimobendan	
Selleck					
Chemicals	S1718	C20H32N5O8P	501.471	Adefovir Dipivoxil	
Selleck					
Chemicals	S1568	C16H13BrF3IN2O4	561.089	PD318088	
Selleck					
Chemicals	S1733	C22H30O5	374.471	Methylprednisolone	
Selleck					
Chemicals	S1577	C26H21N3O2S	439.529	Tie2 kinase inhibitor	
Selleck					
Chemicals	S1742	C15H14N4O	266.298	Nevirapine	
Selleck					
Chemicals	S1606	C22H17ClN2	344.837	Clotrimazole	
Selleck					
Chemicals	S1770	C10H10N4O2S	250.277	Sulfadiazine	
Selleck					
Chemicals	S1625	C20H24O2	296.403	Ethinyl Estradiol	
Selleck					
Chemicals	S1793	C23H32N2O5	416.511	Ramipril	
Selleck					
Chemicals	S1636	C47H73NO17	924.079	Amphotericin B	
Selleck					
Chemicals	S1825	C8H11NO4S2	249.307	Erdosteine	
Selleck					
Chemicals	S1651	C10H14N2O5	242.229	Telbivudine	
Selleck					
Chemicals	S1840	C9H16ClN3O2	233.695	Lomustine	
Selleck					
Chemicals	S1667	C8H8Cl3N3O4S2	380.656	Trichlormethiazide	
Selleck					
Chemicals	S1869	C21H24ClNO	341.874	Dapoxetine HCl	
Selleck					
Chemicals	S1680	C10H20N2S4	296.539	Disulfiram	
Selleck					
Chemicals	S1895	C24H40N8O4	504.626	Dipyridamole	
Selleck					
Chemicals	S1705	C21H30O2	314.462	Progesterone	
Selleck					
Chemicals	S1909	C24H25FNNaO4	433.448	Fluvastatin Sodium	

Selleck		<chem>[C@@H]1(C)OC(=O)C[C@H](O)C[C@H](O)C[C@H](O)CC[C@H](O)[C@H](O)C[C@]2(O)O[C@H]([C@H](C(O)=O)[C@@H](O)C2)C[C@H](O)[C@H]3O[C@@H](C)[C@H](O)[C@H](N)[C@H]3O)C=CC=CC=CC=CCC</chem>	C47H75NO17	926.095	Nystatin (Fungicidin)
Chemicals	S1934	<chem>C=CC=C[C@H](C)[C@H](O)[C@H]1C</chem>			
Selleck		<chem>c1cc([C@]2(C(=O)Nc3sc(SCCN4CCCC4)cn3)[C@@H](C5CCCCC5)C2)ccc1S(=O)(=O)C6CC6</chem>	C28H37N3O3S3	559.807	LY2608204
Chemicals	S2155				
Selleck		<chem>C1C(C(C)N)(CC(CC2C3)CC13)C2</chem>	C12H21N	179.302	Rimantadine
Chemicals	S1964				
Selleck		<chem>c(n1c(c2ccc(CN(C)C)cc2)n3)(c3ccc4)c4C(=O)NCC1</chem>	C19H20N4O	320.388	AG-14361
Chemicals	S2178				
Selleck		<chem>C(C(=O)NC(=S)N1)=C1CCC</chem>	C7H10N2OS	170.232	Propylthiouracil
Chemicals	S1988				
Selleck		<chem>c1(OC2CCN(CC(=O)NC)CC2)cc3c(ncnc3Nc4cccc(Cl)c4F)cc1OC</chem>	C23H25ClFN5O3	473.928	AZD8931 (Sapitinib)
Chemicals	S2192				
Selleck		<chem>C(c1cnc2c(c[nH]2)c1OCCCC)(c3c(F)cc(C)cc3F)=O</chem>	C18H17F2N3O2	345.343	BMS-265246
Chemicals	S2014				
Selleck		<chem>C1C[C@@]2(C)C(C[C@]3([H])[C@@]2([H])CC[C@@]4(C)[C@@]3([H])CCC4=O)=C(O)C1=O</chem>	C19H26O3	302.408	Formestane
Chemicals	S2208				
Selleck		<chem>C(Cn1cncc1)(c2c(Cl)cc(Cl)cc2)OCc3ccc(Sc4ccccc4)cc3.[N+](O)(=O)[O-]</chem>	C24H21Cl2N3O4S	518.412	Fenticonazole Nitrate
Chemicals	S2031				
Selleck		<chem>c1(onc(C(=O)N)n1)[C@@H](CC(=O)NO)CCCC2CCCCC2</chem>	C15H24N4O4	324.375	UK 383367
Chemicals	S2224				
Selleck		<chem>C1(c2c(cccc2)C=Cc3c1cccc3)=C4CCN(C)CC4.Cl</chem>	C21H22ClN	323.859	Cyproheptadine HCl
Chemicals	S2044				
Selleck		<chem>[C@H]1(CC)N(C(C)C)c2c(cnc(Nc3c(OC)cc(C(=O)N)[C@H]4CC[C@H](N5C CN(CC6CC6)CC5)CC4)cc3)n2)N(C)C1=O</chem>	C34H50N8O3	618.813	Volasertib (BI 6727)
Chemicals	S2235				
Selleck		<chem>C1[C@@H](O C1[C@@H](C)CC)=O)[C@@]2([H])C(C=C[C@H](C)[C@H]2 CC[C@@H]3C[C@@H](O)CC(=O)O3)=C[C@@H]1C</chem>	C24H36O5	404.54	Lovastatin
Chemicals	S2061				
Selleck		<chem>c1c2c(c(CCCC(=O)O)c[nH]2)ccc1</chem>	C12H13NO2	203.237	3-Indolebutyric acid (IBA)
Chemicals	S2253				
Selleck		<chem>NS(=O)(=O)NC(=N)CCSCc1nc(NC(=N)N)sc1</chem>	C8H15N7O2S3	337.445	Famotidine
Chemicals	S2078				
Selleck		<chem>[C@]([H])(CC1)([C@@]([H])(C)CC2)[C@@]([C@]([H])(O[C@@]13C)O[C@H](OC(CCC(=O)O)=O)[C@]4(C)[H])(OO3)[C@@]24[H]</chem>	C19H28O8	384.421	Artesunate
Chemicals	S2265				
Selleck		<chem>c1(NS(=O)(=O)C(=O)cc2c(cc(CCCC)c2C(c3ccc(OC(CCN(CCCC)CCCC)cc3)=O)cc1.Cl</chem>	C31H45ClN2O5S	593.217	Dronedarone HCl
Chemicals	S2114				
Selleck		<chem>c1cc(C=CC(=O)O)cc(O)c1O</chem>	C9H8O4	180.157	Caffeic Acid
Chemicals	S2277				
Selleck		<chem>c1(OC)ccc([C@@H]2CC(=O)NC2)cc1OC3CCCC3</chem>	C16H21NO3	275.343	S- (+)-Rolipram
Chemicals	S2127				
Selleck		<chem>C1C[C@@]2(C)[C@@]([H])(CC[C@]3(C)[C@]2([H])C(=O)C=C4[C@@]3(C)CC[C@]5(C)[C@@]4([H])C[C@]([C(=O)O)(C)CC5)C(C)[C@@]1([H])</chem>	C30H46O4	470.684	Enoxolone
Chemicals	S2296				
Selleck		<chem>c1(CO)cc(c2ccc3c(nc(N4CCOC[C@@H]4)nc3N5CCOC[C@@H]5C)n2)cc c1OC</chem>	C25H31N5O4	465.545	AZD8055
Chemicals	S1555				
Selleck		<chem>[C@H]1(CO)O[C@@H](N2C=CC(N)=NC2=O)CC1</chem>	C9H13N3O3	211.218	Zalcitabine
Chemicals	S1719				
Selleck		<chem>C1Sc2c(cc(C#Cc3ccc(C(OC)=O)cn3)cc2)C(C)(C)C1</chem>	C21H21NO2S	351.462	Tazarotene
Chemicals	S1569				
Selleck		<chem>C1(C(Nc2sc(C)cn2)=O)=C(O)c3c(cccc3)S(=O)(=O)N1C</chem>	C14H13N3O4S2	351.401	Meloxicam
Chemicals	S1734				
Selleck		<chem>c1c2c(ccnc2)c(S(=O)(=O)NCCNCC=Cc3ccc(Br)cc3)cc1.Cl.Cl</chem>	C20H22BrCl2N3O2S	519.283	H 89 2HCl
Chemicals	S1582				
Selleck		<chem>c1cc(C(O)=O)cn1</chem>	C6H5NO2	123.109	Nicotinic Acid
Chemicals	S1744				
Selleck		<chem>c1c2c(c(CCN(C)C)c[nH]2)cc(Cn3ncnc3)c1.c4cccc(C(=O)O)c4</chem>	C22H25N5O2	391.466	Rizatriptan Benzoate
Chemicals	S1607				
Selleck		<chem>C(C(=O)N)(C(=O)[C@]1(O)[C@@]([H])([C@@H](O)[C@@]2([H])C(=O)c3c(cccc3O)[C@@]2(C)O)C1=O)[C@@H]4N(C)C=C4O</chem>	C22H24N2O9	460.434	Oxytetracycline (Terramycin)
Chemicals	S1773				
Selleck		<chem>c1cc2c(ccc([C@H](C)C(=O)[O-])c2)cc1O.C.[Na+]</chem>	C14H13NaO3	252.241	Naproxen
Chemicals	S1626				
Selleck		<chem>c1cc(C(=O)c2ccc(OC(C)(C)C(=O)OC(C)C)cc2)ccc1Cl</chem>	C20H21ClO4	360.831	Fenofibrate
Chemicals	S1794				
Selleck		<chem>c1cc(S(=O)(=O)N(C(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)O)[C@H]3CCOC3)ccc1N</chem>	C25H35N3O6S	505.627	Amprenavir
Chemicals	S1639				
Selleck		<chem>c1(N)cc(C(=O)OCCN(CC)CC)ccc1OCCC.Cl</chem>	C16H27ClN2O3	330.85	Proparacaine HCl
Chemicals	S1828				
Selleck		<chem>c1cc(O)ccc1OCc2ccccc2</chem>	C13H12O2	200.233	Monobenzene
Chemicals	S1652				

Selleck		C1C[C@@]2(C)[C@]([H])(C[C@H](O)[C@]3([H])[C@@]2([H])CC[C@@			
Chemicals	S1843	J4(C)[C@@]3([H])CC[C@]4([C@H](C)CCC(=O)O)[H])C[C@@H]1O	C24H40O4	392.572	Chenodeoxycholic Acid
Selleck		C1=C[C@@]2(C)C(C[C@]3([H])[C@@]2([H])[C@H](O)C[C@@]4(C)[C			
Chemicals	S1669	@]3([H])CC[C@@]4(OC(=O)OCC(=O)OCC)=CC1=O	C24H31ClO7	466.952	Loteprednol etabonate
Selleck					
Chemicals	S1876	N1C(N)=Nc2c(ncn2COCCOC(=O)[C@@H](N)C(C)C)C1=O.Cl	C13H21ClN6O4	360.797	Valaciclovir HCl
Selleck					
Chemicals	S1685	c1(N)ccc(S(=O)(=O)N)cc1	C6H8N2O2S	172.205	Sulfanilamide
Selleck					
Chemicals	S1896	N(O)C(=O)N	CH4N2O2	76.055	Hydroxyurea
Selleck					
Chemicals	S1706	N(C(=O)N([C@@H]1CS[C@H](CO)O1)C=C2)=C2N	C8H11N3O3S	229.256	Lamivudine
Selleck					
Chemicals	S1910	c1c(Cl)ccc(C(Cn2cncc2)OCc3c(Cl)sc3)c1Cl	C16H13Cl3N2OS	387.711	Tioconazole
Selleck					
Chemicals	S1937	c1c(C(=O)NN)ccnc1	C6H7N3O	137.139	Isoniazid
Selleck					
Chemicals	S2156	c1nc(C(=O)Nc2cc([C@]3(CO)C4[C@@]4([H])CSC(N)=N3)c(F)cc2)ccc1F	C18H16F2N4O2S	390.407	LY2886721
Selleck					
Chemicals	S1965	C1NC(=O)C(c2ccccc2)(CC)C(=O)N1	C12H14N2O2	218.252	Primidone
Selleck					
Chemicals	S2179	c1c(CN2CCOCC2)c3n(c(Cc4c(F)cc(Cl)cc4)c(C)n3)nc1Nc5cc(C)n[nH]5	C23H25ClFN7O	469.942	LY2784544
Selleck		C1=C[C@@]2(C)C([C@@H](F)C[C@]3([H])[C@@]2(F)[C@H](O)C[C@@			
Chemicals	S1992	J4(C)[C@@]3([H])C[C@@H](C)[C@@]4(OC(=O)CC(C=O)SCF)=CC1=O	C25H31F3O5S	500.571	Fluticasone propionate
Selleck		C1CN(Cc2ccc3c(n(c4sc(C(N)=O)c(O[C@@H](c5c(C(F)(F)F)cccc5)C)c4)cn			
Chemicals	S2193	3)c2)CCN1C	C27H28F3N5O2S	543.604	GSK461364
Selleck		c1c(NC(=O)CC[S+])(C(C)ccc(OCC(OCCC)O)c1.c2C(S([O-			
Chemicals	S2015])(=O)=O)ccc(C)c2	C23H33NO7S2	499.641	Suplatast Tosylate
Selleck					
Chemicals	S2214	c1c(F)c(Nc2[nH]c(C)c2)nc(N[C@@H](C)c3ccc(F)cc3)c1C#N	C18H16F2N6	354.357	AZ 960
Selleck					
Chemicals	S2032	c1(ccc(Cl)cc1)C(=O)NC(C(=O)=O)CC(c2c(cccc2)NC3=O)=C3	C19H15ClN2O4	370.786	Rebamipide
Selleck					
Chemicals	S2225	c1cc(S(=O)(=O)N[C@@H](CCCNC(N)=N)C(=O)OC)ccc1C	C14H22N4O4S	342.414	TAME
Selleck					
Chemicals	S2045	N1C(=O)N([C@H]2[C@@H](O)[C@H](O)[C@@H](C)O2)C=C(F)C1=O	C9H11FN2O5	246.192	Doxifluridine
Selleck					
Chemicals	S2238	c1cc(COCc2cc3c(c4c(cc(C(O)C)cc4)C(=O)O3)cc2OC)ccc1OC	C24H22O6	406.428	Palomid 529 (P529)
Selleck					
Chemicals	S2062	C(O)(=O)CNC(=O)C(S)C	C5H9NO3S	163.195	Tiopronin
Selleck					4-Methylumbelliferone (4-
Chemicals	S2256	c1c2c(C(C)=CC(=O)O2)ccc1O	C10H8O3	176.169	MU)
Selleck		c1c(OC)c(OC)cc2c1C[C@H]2CN(C)CCCN3C(=O)Cc4c(cc(OC)c(OC)c4)CC			
Chemicals	S2086	3.Cl	C27H37ClN2O5	505.046	Ivabradine HCl
Selleck		[C@@H]1(O)C[C@@]2(C)[C@@]([H])(CC[C@]3(C)[C@@]2([H])CC=C4[
Chemicals	S2266	C@@]3(C)CC[C@]5(C(=O)O)[C@]4([H])[C@H](C)[C@H](C)CC5)[C@](C)	C30H48O5	488.699	Asiatic Acid
Selleck		(CO)[C@H]1O			
Chemicals	S2116	C(=O)(c1cccc1c2cccc2)Nc3ccc(C(=O)N4CCc5c([nH]c(C)n5)c6c4cccc6)c	C32H27ClN4O2	535.035	Conivaptan HCl
Selleck		c3.Cl			
Chemicals	S2281	c1c(O)cc2c(C(=O)C=C(c3ccccc3)O2)c1O	C15H10O4	254.238	Chrysin
Selleck					
Chemicals	S2128	c1(c2ccc(O)cc2)c(C)c(c3n1Cc4ccc(OCCN5CCCCC5)cc4)cc(O)cc3.Cl	C30H35ClN2O3	507.063	Bazedoxifene HCl
Selleck					
Chemicals	S2298	c(C(=O)C(O)=C(c1ccc(O)c(O)c1)O2)(ccc(O)c3)c23	C15H10O6	286.236	Fisetin
Selleck					
Chemicals	S1556	c1cc(S(=O)(Nc2scnn2)=O)ccc1CCCCCCCCCCCC	C20H31N3O2S2	409.609	PHT-427
Selleck					
Chemicals	S1721	n1c(Sc2n(C)cn2[N+])([O-])=O)c3c(nc[nH]3)nc1	C9H7N7O2S	277.263	Azathioprine
Selleck		c1c2c(Sc3c(cccc3C(OC(N4CCOCC4)=CC5=O)=C5)C2)ccc1NC(=O)CN6C[
Chemicals	S1570	C@@H](C)O[C@@H](C)C6	C30H33N3O5S	547.665	KU-60019
Selleck					
Chemicals	S1735	SCCS(=O)(=O)[O-].[Na+]	C2H5NaO3S2	164.179	Mesna
Selleck					
Chemicals	S1590	c1c(O)cc(OCc2c3c([nH]c(c4cc(N)ccc4)c3)ncn2)cc1	C18H14N4O2	318.329	TWS119
Selleck					
Chemicals	S1756	c1(F)cc2c(N(CC)C=C(C(=O)O)C2=O)nc1N3CCNCC3	C15H17FN4O3	320.319	Enoxacin

Selleck					
Chemicals	S1610	<chem>c1(Cl)cc2c(C(=O)N(c3c(C)cccc3)C(C)N2)cc1S(N)(=O)=O</chem>	C16H16ClN3O3S	365.835	Metolazone
Selleck					
Chemicals	S1777	<chem>c1c(C(N)=S)cc(CC)nc1</chem>	C8H10N2S	166.243	Ethionamide
Selleck					
Chemicals	S1627	<chem>c1c(OC(=O)C)c(C(=O)Nc2sc([N+])([O-])=O)cn2)ccc1</chem>	C12H9N3O5S	307.282	Nitazoxanide
Selleck					
Chemicals	S1799	<chem>c1c(C)c(NC(=O)CN2CCN(CC(O)COc3c(OC)cccc3)CC2)c(C)cc1</chem>	C24H33N3O4	427.537	Ranolazine
Selleck					
Chemicals	S1641	<chem>c1(Cl)cc2c(S(=O)(=O)NC=N2)cc1S(=O)(=O)N</chem>	C7H6ClN3O4S2	295.723	Chlorothiazide
Selleck					
Chemicals	S1830	<chem>S(=O)(c1cccc1)c2ccc3c([nH])c(NC(=O)OC)n3)c2</chem>	C15H13N3O3S	315.347	Oxfendazole
Selleck					
Chemicals	S1653	<chem>C1C(C)(C)C(C=CC(C)=CC=CC(C)=CC(=O)O)=C(C)CC1</chem>	C20H28O2	300.435	Tretinoin
Selleck					
Chemicals	S1847	<chem>c1cc(Cl)ccc1[C@@](C)(c2ccccc2)OCC[C@H]3CCCN3C.O.C(=O)C=CC(=O)O</chem>	C25H30ClNO5	459.962	Clemastine Fumarate
Selleck					
Chemicals	S1671	<chem>NCCCCC(=O)O</chem>	C6H13NO2	131.173	?6-??-?Aminocaproic acid
Selleck					
Chemicals	S1878	<chem>N1C(=O)c2c(n(CO C(CO)CO)cn2)N=C1N</chem>	C9H13N5O4	255.231	Ganciclovir
Selleck					
Chemicals	S1689	<chem>C1=C[C@@]2(C)C(C(C[C@@]3([H])(C@@]2([H])C(=O)C[C@@]4(C)[C@@]3([H])C[C@@H]4C(C)=O)C[C@@H]1O)=CC1=O</chem>	C22H28O5	372.455	Meprednisone
Selleck					
Chemicals	S1899	<chem>c1cc(C(=O)N)cnc1</chem>	C6H6N2O	122.125	Nicotinamide (Vitamin B3)
Selleck					
Chemicals	S1708	<chem>c1(Cl)cc2c(S(=O)(=O)NCN2)cc1S(=O)(=O)N</chem>	C7H8ClN3O4S2	297.739	Hydrochlorothiazide
Selleck					
Chemicals	S1914	<chem>C1C[C@@]2(C)C(=CC[C@@]3([H])(C@@]2([H])CC[C@@]4(C)[C@@]3([H])CC[C@@H]4C(C)=O)C[C@@H]1O</chem>	C21H32O2	316.478	Pregnenolone
Selleck					
Chemicals	S1940	<chem>c(N1[C@@]([H])(C)CO2)(c2c(N3CCN(C)CC3)c(F)c4)c4C(=O)C(C(O)=O)=C1</chem>	C18H20FN3O4	361.368	Levofloxacin
Selleck					
Chemicals	S2158	<chem>c1c2c(c(C=Cc3ccc(C(N4CCNCC4)=O)cc3)n([nH]2)ccc1</chem>	C20H20N4O	332.399	KW-2449
Selleck					
Chemicals	S1969	<chem>C(C(=O)Nc1c(C)cccc1C)N2CCCC2=O</chem>	C14H18N2O2	246.305	Nefiracetam
Selleck					
Chemicals	S2180	<chem>c1c(Cl)c(C(=O)NCC(=O)N[C@@H](CC(C)C)B(O)O)cc(Cl)c1</chem>	C14H19BCl2N2O4	361.029	MLN2238
Selleck					
Chemicals	S2001	<chem>c1cc(Cl)c(F)c(Cc2c(OC)cc3c(C(=O)C(C(=O)O)=CN3[C@@H](CO)C(C)C)c2)c1</chem>	C23H23ClFNO5	447.884	Elvitegravir (GS-9137, JTK-303)
Selleck					
Chemicals	S2195	<chem>n1c(c2ccc(NC(NCC)=O)c(OC)c2)nc(N[C@@H](CCC)c3cnccc3)c(C)c1</chem>	C24H30N6O2	434.534	CYT997 (Lexibulin)
Selleck					
Chemicals	S2021	<chem>c1cc(C2N(C)C(=O)CCS2(=O)=O)ccc1Cl</chem>	C11H12ClNO3S	273.736	Chlormezanone
Selleck					
Chemicals	S2215	<chem>c1(F)cc(CC(C[NiC@H](C(=O)N[C@@H](c2ccccc2)C(OC(C)C)C)=O)C)=O)c c(F)c1</chem>	C23H26F2N2O4	432.46	DAPT (GSI-IX)
Selleck					
Chemicals	S2035	<chem>c1cc(C=C(C)C=C2C(=O)N(CC(=O)O)C(=S)S2)ccc1</chem>	C15H13NO3S2	319.399	Epalrestat
Selleck					
Chemicals	S2226	<chem>c1c(F)c2c(N=C([C@H](CC)Nc3ncnc4c3nc[nH]4)N(c5ccccc5)C2=O)cc1</chem>	C22H18FN7O	415.423	CAL-101 (Idelalisib, GS-1101)
Selleck					
Chemicals	S2047	<chem>N(C(=O)C1=C(C)O)c2c(cc(Cl)s2)S(=O)(=O)N1C)c3cccn3</chem>	C13H10ClN3O4S2	371.819	Lornoxicam
Selleck					
Chemicals	S2239	<chem>[C@@H]1(CSc2nc(c3ccccc3)c(c4ccccc4)o2)O[C@H](c5ccc(NC(CCCCCC(=O)NO)=O)cc5)O[C@H](c6ccc(CO)cc6)C1</chem>	C41H43N3O7S	721.861	Tubacin
Selleck					
Chemicals	S2064	<chem>N1(CCCC(NC)C1)c2c(F)cc3c(N(C4CC4)C=C(C(O)=O)C3=O)c2OC</chem>	C20H24FN3O4	389.421	Balofloxacin
Selleck					
Chemicals	S2259	<chem>c(C(=O)c1c(cccc1O)C2=O)(c(O)cc(CO)c3)c23</chem>	C15H10O5	270.237	Aloe-emodin
Selleck					
Chemicals	S2087	<chem>c1(OC(=O)N(CC)C)cc([C@H](C)N(C)C)ccc1.O.C(=O)[C@H](O)[C@@H](O)C(=O)O</chem>	C18H28N2O8	400.424	Rivastigmine Tartrate
Selleck					
Chemicals	S2267	<chem>O=[N+])([O-])c1[nH]ccn1</chem>	C3H3N3O2	113.075	Azomycin
Selleck					
Chemicals	S2118	<chem>CS(Nc1ccc(C(O)CCCN(CC)CCCCCCC)cc1)(=O)=O.C(O)(=O)C=CC(O)=O</chem>	C44H76N4O10S2	885.225	Ibutilide Fumarate
Selleck					
Chemicals	S2282	<chem>c1cccc2c1c([C@@H](O)[C@]3([H])CC([C@@]([H])(C=C)CN34)CC4)ccn2</chem>	C19H22N2O	294.391	Cinchonidine
Selleck					
Chemicals	S2130	<chem>OS(=O)(=O)O.O.C(=O)O[C@H]1C[C@@]([H])(N(C)[C@@]2([H])C1)CC2)C(CO)c3ccccc3.C(=O)O[C@H]4C[C@@]([H])(N(C)[C@@]5([H])C4)CC5)C(CO)c6ccccc6</chem>	C34H50N2O11S	694.833	Atropine

Selleck	Chemicals	S2299	<chem>c(C(=O)C(c1ccc(OC)cc1)=CO2)(ccc(O)c3)c23</chem>	C16H12O4	268.264	Formononetin
Selleck	Chemicals	S1557	<chem>c1(OC)cc2c(ncnc2Oc3cc(Cl)c(NC(NCCC)=O)cc3)cc1OC</chem>	C20H21ClN4O4	416.858	KRN 633
Selleck	Chemicals	S1723	<chem>c1cc2c(c(CC(=O)O)c(C)n2C(=O)c3ccc(Cl)cc3)cc1OC</chem>	C19H16ClNO4	357.788	Indomethacin
Selleck	Chemicals	S1572	<chem>c1(NCc2ccccc2)n3c(c(C(C)C)n3)nc(NCCCCCN)c1.Cl</chem>	C22H33ClN6	416.991	BS-181 HCl
Selleck	Chemicals	S1736	<chem>c1c(OC)c(OC(CO(C(=O)N)O)ccc1</chem>	C11H15NO5	241.241	Methocarbamol
Selleck	Chemicals	S1593	<chem>n1n(c2ccc(OC)c2)c3c(CCN(c4ccc(N5CCCCC5=O)cc4)C3=O)c1C(=O)N</chem> <chem>c1(C=NN2CCN(C3CCCC3)CC2)c(O)c(c(C(=O)[C@]4(C)O5)c56)c(c(O)c6C)</chem> <chem>c(O)c1NC(=O)C(C)=CC=C[C@H](C)[C@H](O)[C@H](C)[C@H](O)[C</chem> <chem>@H](C)[C@H](O C(C)=O)[C@H](C)[C@H](O)C=CO4</chem>	C25H25N5O4	459.497	Apixaban
Selleck	Chemicals	S1760	<chem>c1cc(OCNC[C@@H](Cc2cc(C(=O)N)c3c(CCN3CCCO)c2)C)c(OC(F)(F)F)</chem> <chem>cc1</chem>	C47H64N4O12	877.031	Rifapentine
Selleck	Chemicals	S1613	<chem>c1cc(OCNC[C@@H](Cc2cc(C(=O)N)c3c(CCN3CCCO)c2)C)c(OC(F)(F)F)</chem> <chem>cc1</chem>	C25H32F3N3O4	495.534	Silodosin
Selleck	Chemicals	S1778	<chem>N1C(=O)C(C(F)(F)F)=CN([C@H]2O[C@H](CO)[C@@H](O)C2)C1=O</chem> <chem>C1=C[C@@@]2(C)C(C)C[C@]3([H])[C@@]2(F)[C@H](O)C[C@@]4(C)[C@</chem> <chem>@]3([H])C[C@@H]5[C@H]4(C(=O)CO)O C(C)(C)O5)=CC1=O</chem>	C10H11F3N2O5	296.2	Trifluridine
Selleck	Chemicals	S1628	<chem>[C@@H]1(O)[C@H](CO)O[C@@H](n2c(N)c(C(N)=O)nc2)[C@@H]1O</chem> <chem>C1C[C@]2(C)[C@]([H])([C]C@H(O)[C@]3([H])[C@@]2([H])CC[C@@]4</chem> <chem>(C)[C@@]3([H])CC[C@@]4([H])[C@@H](CCC(=O)O)C)C[C@H]1O</chem>	C9H14N4O5	258.231	Acadesine
Selleck	Chemicals	S1643	<chem>[C@@H]1(O)[C@H](CO)O[C@@H](n2c(N)c(C(N)=O)nc2)[C@@H]1O</chem> <chem>C1C[C@]2(C)[C@]([H])([C]C@H(O)[C@]3([H])[C@@]2([H])CC[C@@]4</chem> <chem>(C)[C@@]3([H])CC[C@@]4([H])[C@@H](CCC(=O)O)C)C[C@H]1O</chem>	C24H40O4	392.572	Ursodiol
Selleck	Chemicals	S1831	<chem>c1([nH]c2c3ccccc2c3c(OC(C)CNCCOc4c(OC)cccc4)ccc1</chem> <chem>c1cc([C@H](O)CC[C@@H]2[C@H](c3ccc(O)cc3)N(c4ccc(F)cc4)C2=O)</chem> <chem>ccc1F</chem>	C24H26N2O4	406.474	Carvedilol
Selleck	Chemicals	S1655	<chem>c1cc([C@H](O)CC[C@@H]2[C@H](c3ccc(O)cc3)N(c4ccc(F)cc4)C2=O)</chem> <chem>ccc1F</chem>	C24H21F2NO3	409.425	Ezetimibe
Selleck	Chemicals	S1848	<chem>c1(OC)cc(C=CC(=O)C=O)C=Cc2cc(OC)c(O)cc2)ccc1O</chem>	C21H20O6	368.38	Curcumin
Selleck	Chemicals	S1672	<chem>c1(C2(CC)C(=O)NC(=O)CC2)ccc(N)cc1</chem>	C13H16N2O2	232.278	Aminoglutethimide
Selleck	Chemicals	S1881	<chem>c1(CCC)cc(C(=S)N)ccn1</chem>	C9H12N2S	180.27	Protonamide
Selleck	Chemicals	S1691	<chem>c1cc2c(CCN3C2CN(C(=O)C4CCCC4)CC3=O)cc1</chem> <chem>[C@H]1(CC(=O)N)[C@]2([H])N=C(C(C)=C(N=C3C=C(C(N=C4C(C)=C([N-</chem> <chem>]C@@]25C)[C@@H](CCC(=O)N)[C@]5(C)CC(=O)N)[C@@H](CCC(=O)</chem> <chem>N)[C@@]4(CC(=O)N)C)[C@@H](CCC(=O)N)C3(C)C[C@]1(C)CCC(=O)N</chem> <chem>C[C@H](C)OP(=O)([O-</chem> <chem>]O)[C@@H]q[C@H](CO)O[C@H](n7c8c(cc(C)c(C)c8)nc7)[C@@H]6O.[Co</chem> <chem>+2]C#N</chem>	C19H24N2O2	312.406	Praziquantel
Selleck	Chemicals	S1902	<chem>c1cc2c(CC[C@]3([H])[C@@]2([H])CC[C@@]4(C)[C@@]3([H])CC[C@H]4</chem> <chem>O)cc1O</chem>	C63H88CoN14O14P	1355.365	Vitamin B12
Selleck	Chemicals	S1709	<chem>c1cc2c(CC[C@]3([H])[C@@]2([H])CC[C@@]4(C)[C@@]3([H])CC[C@H]4</chem> <chem>O)cc1O</chem>	C18H24O2	272.382	Estradiol
Selleck	Chemicals	S1915	<chem>c1cc(S(=O)(=O)Nc2ncc(C)c2)ccc1N</chem>	C10H11N3O3S	253.278	Sulfamethoxazole
Selleck	Chemicals	S1949	<chem>c1cc2c(C(=O)C=C(C)C2=O)cc1</chem> <chem>[C@]1([H])([C@H](O)C)[C@@]2([H])N(C(C(=O)OCO(C(=O)C(C)(C)C)=C(</chem> <chem>SC3CN(C4=NCCS4)C3)[C@H]2C)C1=O</chem>	C11H8O2	172.18	Menadione
Selleck	Chemicals	S2159	<chem>[C@]1([H])([C@H](O)C)[C@@]2([H])N(C(C(=O)OCO(C(=O)C(C)(C)C)=C(</chem> <chem>SC3CN(C4=NCCS4)C3)[C@H]2C)C1=O</chem>	C22H31N3O6S2	497.628	Tebipenem Pivoxil
Selleck	Chemicals	S1971	<chem>c1cc(C(NCCO[N+])(=O)[O-])=O)cncc1</chem> <chem>c1c(Cl)c(C(=O)NCC(=O)N)[C@@H](CC(C)C)B2O C(=O)CC(C(C)=O)(C(O</chem> <chem>)=O)O2)cc(Cl)c1</chem>	C8H9N3O4	211.175	Nicorandil
Selleck	Chemicals	S2181	<chem>c1cc([C@H](NC(=O)C2CCC(F)(F)CC2)CCN(C3CC4)C4CC(n5c(C(C)C)nn</chem> <chem>c5C)C3)ccc1</chem>	C20H23BCl2N2O9	517.122	MLN9708
Selleck	Chemicals	S2003	<chem>c1cc([C@H](NC(=O)C2CCC(F)(F)CC2)CCN(C3CC4)C4CC(n5c(C(C)C)nn</chem> <chem>c5C)C3)ccc1</chem>	C29H41F2N5O	513.666	Maraviroc
Selleck	Chemicals	S2198	<chem>c1cc2n(c(c3cc(OC(F)(F)F)ccc3)cn2)nc1NCC4CCN(C)CC4</chem>	C20H22F3N5O	405.417	SGI-1776 free base
Selleck	Chemicals	S2024	<chem>c1(scc2)c2C(=C3CCN(C)CC3)c4c(cccc4)CC1=O.C(=O)(O)C=CC(=O)O</chem>	C23H23NO5S	425.497	Ketotifen Fumarate
Selleck	Chemicals	S2216	<chem>c1cc(C=Cc2nc(CO c3ccc(CCCn4ccnn4)cc3)co2)ccc1C(F)(F)F</chem>	C25H23F3N4O2	468.471	Mubritinib (TAK 165)
Selleck	Chemicals	S2036	<chem>C(=O)(O)C[C@H](N)C(=O)N[C@@H](Cc1ccccc1)C(=O)OC</chem>	C14H18N2O5	294.303	Aspartame
Selleck	Chemicals	S2227	<chem>n1c(N)c2c(n(CCC3=Nc4c(c(C)ccc4)C(=O)N3c5ccccc5C)nc2c6cccc(O)c6)nc1</chem>	C28H23N7O2	489.528	PIK-294

Selleck						
Chemicals	S2053	<chem>C1(=O)N=C(N)C=CN1[C@H]2[C@@H](O)[C@H](O)[C@@H](CO)O2</chem>	C9H13N3O5	243.217	Cytidine	
Selleck						
Chemicals	S2243	<chem>c1(Br)nc(C=C(C#N)C=O)N[C@@H](CCC)c2ccccc2ccc1</chem>	C19H18BrN3O	384.27	Degrasyn (WP1130)	
Selleck						
Chemicals	S2065	<chem>c1c(CN2CCCC2)ccnc1OCC=CCNC(=O)CS(Cc3occcc3)=O</chem>	C22H29N3O4S	431.548	Lafutidine	
Selleck						
Chemicals	S2260	<chem>[C@H]1(O)[C@@H](O)[C@@H](CO)O[C@@H](OC[C@H]2O[C@@H](O)[C@@H](C#N)c3ccccc3)[C@H](O)[C@@H](O)[C@@H]2O)[C@@H]1O</chem>	C20H27NO11	457.428	Laetrile	
Selleck						
Chemicals	S2091	<chem>c1c(CCOCC2CC2)ccc(OC(C)CNC(C)C)c1</chem>	C18H29NO3	307.428	Betaxolol	
Selleck						
Chemicals	S2268	<chem>c1(O)cc2c(C(=O)C=C(c3ccccc3)O2)c(O)c1O</chem>	C15H10O5	270.237	Baicalein	
Selleck						
Chemicals	S2119	<chem>c1(C(C)(C)C)cc(SC(C)(C)Sc2cc(C(C)(C)C)c(O)c(C(C)(C)C)c2)cc(C(C)(C)C)c1O</chem>	C31H48O2S2	516.842	Probucol	
Selleck						
Chemicals	S2285	<chem>C1Cc2c(ccc3c2C(=O)C(=O)C4=C3OC[C@H]4C(C)(C)C1</chem>	C19H20O3	296.36	Cryptotanshinone	
Selleck						
Chemicals	S2131	<chem>n1cc(Cl)c(NC(=O)c2cc(OC(C)CC3CC3)c(OC(F)F)cc2)c(Cl)c1</chem>	C17H14Cl2F2N2O3	403.207	Roflumilast	
Selleck						
Chemicals	S2300	<chem>c1cc(C=C(C=O)O)cc(OC)c1O</chem>	C10H10O4	194.184	Ferulic Acid	
Selleck						
Chemicals	S2302	<chem>C1[C@@H]2(C)[C@@H]([H])(CC[C@@H]3(C)[C@@H]2([H])C(=O)C=C4[C@@H]3(C)CC[C@@H]5(C)[C@@H]4([H])C[C@@H](C)(C(=O)O)CC5(C)(C)[C@H]1O[C@@H]6[C@@H](O)[C@H]7[C@@H](O)[C@@H](O)[C@H](O)[C@@H](C(=O)O)O7)[C@@H](O)[C@H](O)[C@@H](C(=O)O)O6</chem>	C42H62O16	822.932	Glycyrrhizic Acid	
Selleck						
Chemicals	S2467	<chem>n1cc2c(n(CCC(COC(=O)C)COC(C)=O)cn2)nc1N</chem>	C14H19N5O4	321.332	Famciclovir	
Selleck						
Chemicals	S2320	<chem>c1(O)cc2c(C(=O)C=C(c3cc(O)c(O)cc3)O2)c(O)c1</chem>	C15H10O6	286.236	Luteolin	
Selleck						
Chemicals	S2480	<chem>c1cc(C2(O)CCN(CCC(c3ccccc3)(c4ccccc4)N(C)C)=O)CC2)ccc1Cl.Cl</chem>	C29H34Cl2N2O2	513.498	Loperamide HCl	
Selleck						
Chemicals	S2337	<chem>c1(OC)c(CC=C(C)C)c2c(C=CC(=O)O2)cc1</chem>	C15H16O3	244.286	Osthole	
Selleck						
Chemicals	S2492	<chem>[C@H]1(O)C(C)(C)O[C@@H](Oc2c(C)c3c(C(O)=C(NC(c4cc(CC=C(C)C)c([O-])cc4)=O)C(=O)O3)cc2)[C@H](O)[C@@H]1OC(=O)N.[Na+]</chem>	C31H35N2NaO11	634.606	Novobiocin Sodium	
Selleck						
Chemicals	S2347	<chem>c1(O)cc2c(C(=O)C(O)=C(c3cc(O)c(O)cc3)O2)c(O)c1.O.O</chem>	C15H14O9	338.266	Quercetin Dihydrate	
Selleck						
Chemicals	S2502	<chem>c1c(OC)cc2c(nc2c2[C@H](O)[C@H]3([H])C[C@@H]([H])([C@H](C=C)CN34)CC4)c1.Cl.O.O</chem>	C20H29ClN2O4	396.908	Quinine HCl Dihydrate	
Selleck						
Chemicals	S2364	<chem>c1(C)c2c(c3c(c4c(c(C)co4)C(=O)C3=O)cc2)cc1</chem>	C18H12O3	276.286	Tanshinone I	
Selleck						
Chemicals	S2515	<chem>C1CN(S(=O)(=O)c2cc(C(NC(=O)c3n4c(CCC)nc3=N4)c(OCC)cc2)CCN1C.C.Cl.O.O.O</chem>	C23H39ClN6O7S	579.11	Vardenafil HCl Trihydrate	
Selleck						
Chemicals	S2377	<chem>c1(O)cc2c(C(=O)C)c3ccc(OC)cc3=CO2)c(O)c1</chem>	C16H12O5	284.263	Biochanin A	
Selleck						
Chemicals	S2534	<chem>c1cc(C(Cn2cnc2)OCc3c(Cl)cccc3Cl)c(Cl)c1Cl.[N+](O)(=O)[O-]</chem>	C18H15Cl4N3O4	479.141	Isoconazole nitrate	
Selleck						
Chemicals	S2390	<chem>[C@@H]1(O)[C@H](O)[C@H](Oc2cc(C=Cc3ccc(O)cc3)cc(O)c2)O[C@H](CO)[C@H]1O</chem>	C20H22O8	390.384	Polydatin	
Selleck						
Chemicals	S2548	<chem>Cl.[C@@H]1([H])(C[C@@H](O)C2N(C)[C@H]2([H])[C@@H]3([H])[C@H]1([H])O3</chem>	C8H14ClNO2	191.655	Scopine HCl	
Selleck						
Chemicals	S2403	<chem>c1c(OC)c(OC)c2c([C@H]3Cc(cc4Oc5ccc(cc5)[C@H]6c(cc7O2)c(CCN6C)cc7OC)ccc4OC)c1CCN3C</chem>	C38H42N2O6	622.75	Tetrandrine	
Selleck						
Chemicals	S2561	<chem>c1cc(C(Cl)=C(c2ccc(OCN(C)CC)cc2)c3ccccc3)ccc1.O.C(=O)CC(O)(C(O)=O)CC(=O)O</chem>	C32H36ClNO8	598.083	Clomifene citrate	
Selleck						
Chemicals	S2412	<chem>O1[C@H](O)[C@@H]2([H])[C@H]([H])(CC=C2CO)C(C(OC)=O)=C1</chem>	C11H14O5	226.226	Genipin	
Selleck						
Chemicals	S2579	<chem>N1C(=O)C(C)=CN([C@H]2[C@H](N=[N+]=[N-])[C@@H](CO)O2)C1=O</chem>	C10H13N5O4	267.241	Zidovudine	
Selleck						
Chemicals	S2446	<chem>C(#N)C=NNc1ccc(C2=NNC(=O)C[C@H]2C)cc1)C#N</chem>	C14H12N6O	280.285	Levosimendan	
Selleck						
Chemicals	S2599	<chem>c1(O)c(l)cc(OCc2c(l)cc(C[C@H](N)C(=O)O)cc2)cc1l</chem>	C15H11I4NO4	776.87	L-Thyroxine	
Selleck						
Chemicals	S2608	<chem>C1=C[C@@H]2(C)C([C@@H](F)C[C@H]3([H])[C@@H]2(F)[C@H](O)C[C@@H]4(C)[C@@H]3([H])C[C@@H]5(C)[C@H]4(C(=O)CO)C(C)O5)=CC1=O</chem>	C26H32F2O7	494.525	Fluocinonide	
Selleck						
Chemicals	S2752	<chem>n1c(c2c(Nc3ccc(OCc4ccn5c(ncn5)c4)c(C)c3)nc1)ccc(c6ccc(CNCCS(C)(=O)=O)o6)c2</chem>	C29H27N7O4S	569.634	HER2-Inhibitor-1	

Selleck							
Chemicals	S2621	<chem>c1cc(Nc2nc(c3n(C(C)C)c(C)nc3)ccn2)ccc1S(=O)(C)=O</chem>	C18H21N5O2S	371.457	AZD5438		
Selleck							
Chemicals	S2768	<chem>C1CCN(c2nc3n(nc3CC)c(NC4c[n+](O-))ccc4c2)[C@H](CCO)C1</chem>	C21H28N6O2	396.486	Dinaciclib (SCH727965)		
Selleck							
Chemicals	S2631	<chem>c1ccc(OC(=O)NC2CCCCC2)cc1c3cc(C(=O)N)ccc3</chem>	C20H22N2O3	338.4	URB597		
Selleck							
Chemicals	S2779	<chem>c1(N(C)C)ccc(C(=O)NCCCCC(C=O)NO)cc1</chem>	C16H25N3O3	307.388	M344		
Selleck							
Chemicals	S2656	<chem>n1(c2cc(N[C@H]3CC[C@H](OC(=O)CN)CC3)c(C(N)=O)cc2)nc(C(F)(F)F)c4c1CC(C)(C)CC4=O</chem>	C25H30F3N5O4	521.532	PF-04929113 (SNX-5422)		
Selleck							
Chemicals	S2790	<chem>n1(C)c(c2nc1C=Cc3ccc(OC)c(OC)c3)C(=O)N(CC)C(=O)N2CC</chem>	C20H24N4O4	384.429	Istradefylline		
Selleck							
Chemicals	S2666	<chem>c1(C(F)(F)F)ccc(OC2cccc(C3CCN(C(=O)Nc4ccnc4)CC3)c2)nc1</chem>	C24H23F3N4O2	456.46	PF-3845		
Selleck							
Chemicals	S2803	<chem>[C@](C)(C(n1nc2c1cccc2)=CC3)(CCC4C5CC=C6[C@]4(C)C[C@H](O)C6)C35</chem>	C26H32N2O	388.545	Galeterone		
Selleck							
Chemicals	S2681	<chem>c(OC(F)(F)O1)(cc(C=C2C(=O)NC(=O)S2)cc3)c13</chem>	C11H5F2NO4S	285.224	AS-604850 CHIR-99021 (CT99021)		
Selleck							
Chemicals	S2924	<chem>c1(NCCNc2ccc(C#N)cn2)nc(c3c(Cl)cc(Cl)cc3)c(c4nc(C)c[nH]4)cn1.Cl</chem>	C22H19Cl3N8	501.799	HCl		
Selleck							
Chemicals	S2692	<chem>c1ccc(Nc2c(C)cn(CNc3ccc(N4CCN(C)CC4)cc3)n2)cc1S(=O)(=O)NC(C)(C)C</chem>	C26H35N7O2S	509.667	TG101209		
Selleck							
Chemicals	S3019	<chem>C(C(=O)N(O)C(C1CCCC1)=C2)=C2C.NCCO</chem>	C14H24N2O3	268.352	Ciclopirox ethanolamine		
Selleck							
Chemicals	S2714	<chem>c1(F)cc([C@H](O)C(=O)N[C@@H](C)C(=O)N[C@@H]2C(=O)N(C)c3c(ccc3)c4c2cccc4)cc(F)c1</chem>	C26H23F2N3O4	479.475	LY411575		
Selleck							
Chemicals	S3061	<chem>c1(O)ccc([C@@H](O)CNC)cc1O.Cl</chem>	C9H14ClNO3	219.665	Epinephrine HCl AG-1478 (Typhostin AG-1478)		
Selleck							
Chemicals	S2728	<chem>c1c(OC)c(OC)cc2c1ncnc2Nc3cccc(Cl)c3</chem>	C16H14ClN3O2	315.754			
Selleck							
Chemicals	S5002	<chem>c1(CCC(CO)(N)CO)ccc(CCCCCC)cc1.Cl</chem>	C19H34ClNO2	343.932	Fingolimod (FTY720) HCl		
Selleck							
Chemicals	S2743	<chem>n1c(C)c2c(N([C@@H]3CC[C@@H](OCCO)CC3)C(=O)C(c4nc(OC)cc4)=C2)nc1N</chem>	C22H27N5O4	425.481	PF-04691502		
Selleck							
Chemicals	S2308	<chem>c1(O)cc2c(C(=O)C[C@@H](c3cc(O)c(OC)cc3)O2)c(O)c1</chem>	C16H14O6	302.279	Hesperetin		
Selleck							
Chemicals	S2468	<chem>c1ccc(Sc2ccc3c([nH]c(NC(=O)OC)n3)c2)cc1</chem>	C15H13N3O2S	299.348	Fenbendazole		
Selleck							
Chemicals	S2322	<chem>C1[C@@]2([H])[C@@]([H])([C@]3([H])[C@]4([H])N(C(=O)CCC4)C2)N(CC3)CC1</chem>	C15H24N2O	248.364	(+)-Matrine		
Selleck							
Chemicals	S2481	<chem>c1([N+])=(O)O-]cccc(C2C(C(=O)OCCN3CCN(C(c4ccccc4)c5ccccc5)CC3)=C(C)NC(C)=C2C(OC)=O)c1</chem>	C35H38N4O6	610.699	Manidipine		
Selleck							
Chemicals	S2338	<chem>C1[C@@]2([H])[C@@]([H])([C@]3([H])[C@]4([H])N(C(=O)CCC4)C2)[N+](O-)](CCC3)CC1</chem>	C15H24N2O2	264.363	Oxymatrine		
Selleck							
Chemicals	S2494	<chem>C1(c2c(cccc2)COc3c1cc(C(C(=O)O)cc3)=CCN(C)C.Cl</chem>	C21H24ClNO3	373.873	Olopatadine HCl		
Selleck							
Chemicals	S2349	<chem>N(CCc1c2[nH]c3c1cccc3)(C(=O)c4c5cccc4)C2=N5</chem>	C18H13N3O	287.315	Rutaecarpine		
Selleck							
Chemicals	S2503	<chem>c1ccc(COC(=O)CNC(=O)C(Cc2ccccc2)CSC(C)=O)cc1</chem>	C21H23NO4S	385.477	Racecadotril		
Selleck							
Chemicals	S2365	<chem>C1Cc2c(ccc3c2C(=O)C(=O)c4c3ccc4C)C(C)(C)C1</chem>	C19H18O3	294.344	Tanshinone IIA		
Selleck							
Chemicals	S2517	<chem>c1cc2c(C3c4c(cccc4)C2(CCCNC)CC3)cc1.Cl</chem>	C20H24ClN	313.864	Maprotiline HCl		
Selleck							
Chemicals	S2378	<chem>[Br-]].c1ccccc1[C@H](CO)C(=O)O[C@@H]2[C@@]([H])([N+](C)(CCCC)[C@@]3([H])C2)[C@]4([H])[C@@]3([H])O4</chem>	C21H30BrNO4	440.371	Butylscopolamine Bromide		
Selleck							
Chemicals	S2535	<chem>c1cc(C(OCc2ccc(Cl)cc2)Cn3cncc3)c(Cl)cc1Cl.[N+](O)(=O)[O-]</chem>	C18H16Cl3N3O4	444.696	Econazole nitrate		
Selleck							
Chemicals	S2391	<chem>c1(O)cc2c(C(=O)C(O)=C(c3cc(O)c(O)cc3)O2)c(O)c1</chem>	C15H10O7	302.236	Quercetin		
Selleck							
Chemicals	S2549	<chem>[Cl-].[C@@]1([H])(Cl)C[C@@H](OC(=O)C(O)(c2ccccc2)c3ccccc3)C4)[N+](CC5)[C@]4([H])CC1</chem>	C25H30ClNO3	427.964	Trospium chloride		
Selleck							
Chemicals	S2404	<chem>c1cc(C=C(C(=O)c2ccc(O)cc2O)ccc1O</chem>	C15H12O4	256.253	Isoliquiritigenin		

Selleck		[C@H]1(NC(c2c(c3c(Cl)cccc3)noc2C)=O)[C@@]4([H])N([C@@H](C([O-])=O)C(C)(C)S4)C1=O.[Na+].O	C19H19ClN3NaO6S	475.878	Cloxacillin Sodium
Chemicals	S2564				
Selleck		C1=C(C(O)=O)[C@]2([H])[C@@]([H])(C(CO)=CC2)[C@H](O)[C@H]3[C@@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O3)O1	C16H22O10	374.34	Geniposidic acid
Chemicals	S2413				
Selleck		c1cc([C@H](O)[C@@H](CO)NC(=O)C(Cl)Cl)ccc1S(=O)(=O)C	C12H15Cl2NO5S	356.222	Thiamphenicol
Chemicals	S2583				
Selleck		C1(CC(N)(CC2C1)CC3C2)C3.Cl	C10H18ClN	187.71	Amantadine HCl
Chemicals	S2451				
Selleck		c1cc(S(=O)(=O)NC(=O)NN2CC3C(CCC3)C2)ccc1C	C15H21N3O3S	323.411	Gliclazide
Chemicals	S2601				
Selleck		OC[C@@H](O)[C@@H](O)[C@@H](O)CO	C5H12O5	152.146	Ribitol
Chemicals	S2612				
Selleck		c(ccc(NC1=N[C@H](C)CO1)c2)(ncnc3Nc4ccc(OCc5nccs5)c(Cl)c4)c23	C22H19ClN6O2S	466.943	Varlitinib
Chemicals	S2755				
Selleck		c1(c2c3c(ncnc3N)n(C4CCCC4)n2)cc5c([nH]cc5)nc1	C17H17N7	319.364	PP121
Chemicals	S2622				
Selleck		n1c(C[C@]2(C(O)=O)CC[C@H](O)c3cccc(Cl)c3F)CC2)cccc1Nc4nccs4	C22H21ClFN3O3S	461.937	MK-5108 (VX-689)
Chemicals	S2770				
Selleck		c1c(OC)c2c(ncc2C(=O)C(=O)N3CCN(C(c4cccc4)=O)C[C@H]3C)[nH]c1	C22H22N4O4	406.434	BMS-378806
Chemicals	S2632				
Selleck		c1(OC)cc2c(ncc3c2N([C@@H](c4ncccc4)C)(=O)N3)cc1c5c(C)noc5C	C23H21N5O3	415.445	I-BET151 (GSK1210151A)
Chemicals	S2780				
Selleck		c1(S(Nc2cc(c3ccc(c4c3)cccc4c5ccnnc5)cn2O2C)(=O)=O)ccc(F)cc1F	C25H17F2N5O3S	505.496	GSK2126458 (GSK458)
Chemicals	S2658				
Selleck		N1C(=O)C(c2c(c3nc(N4CCN(C)CC4)n2)cccc3)=C(c5c(c6[nH]c5)cccc6)C1=O	C25H22N6O2	438.481	Sotrastaurin
Chemicals	S2791				
Selleck		c1(F)ccc(CNC(=O)C(C(=O)C(O)=C2N3C[C@@]4([H])N([C@@H](C)CCO4)C2=O)=C3)c(F)c1	C20H19F2N3O5	419.379	Dolutegravir (GSK1349572)
Chemicals	S2667				
Selleck		c1(S(Nc2cccc(c3c(c4ccnc(N)n4)sc(C(C)(C)C)n3)c2F)(=O)=O)c(F)cccc1F	C23H20F3N5O2S2	519.562	Dabrafenib (GSK2118436)
Chemicals	S2807				
Selleck		c1(F)ccc(c2ccc(C=C3SC(=O)NC3=O)o2)cc1	C14H8FNO3S	289.282	CAY10505
Chemicals	S2682				
Selleck		N1(C)C(C(C=C2)CC1S([O-])(=O)=O)=CC(=O)C2=NNC(N)=O.[Na+]	C10H11N4NaO5S	322.273	Carbazochrome sodium sulfonate (AC-17)
Chemicals	S3000				
Selleck		c1(c2nc3c(sc(CN4CCN(C(=O)[C@H](C)O)CC4)c3C)c(N5CCOCC5)n2)cn(C(N)nc1	C23H30N8O3S	498.601	GDC-0980 (RG7422)
Chemicals	S2696				
Selleck		S1CCC=C[C@@H]2CC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](C(=O)NC(=CC)C(=O)N[C@@H](C(C)C)C(=O)O2)CS1	C24H36N4O6S2	540.696	Romidepsin (FK228, Depsipeptide)
Chemicals	S3020				
Selleck		c1(Cl)cc2c([nH]c(C(=O)N[C@@H](Cc3ccccc3)[C@@H](O)C(N(C)C)=O)c2)cc1	C21H22ClN3O3	399.871	CP-91149
Chemicals	S2717				
Selleck		c1cc(Cc([O-])(=O)c(Nc2c(Cl)cccc2Cl)cc1.[K+]	C14H10Cl2KNO2	334.239	Diclofenac Potassium
Chemicals	S3062				
Selleck		C1(=O)NC(=O)C(Nc2ccc(O)c(Cl)c2)=C1c3ccccc3[N+]([O-])=O	C16H10ClN3O5	359.721	SB415286
Chemicals	S2729				
Selleck		[C@H]1(O)C[C@@H](O)CC[C@@H](C=C(C)[C@H]2OC(=O)[C@@]3([H])N(CCCC3)C(=O)C(=O)[C@](O)(O)[C@H]4[C@@H](OC)C[C@@H](C)CC(C)=C[C@@H](CC=C)C(=O)C[C@H](O)[C@H]2C)[C@H](C)C[C@@H]4O)C1	C44H69NO12	804.018	Tacrolimus (FK506)
Chemicals	S5003				
Selleck		c1(Br)c(N2CCN(Cc3noc(C)c3)CC2)c4c([nH]c(c5ccc(N6CCN(C)CC6)cc5)n4)nc1	C26H31BrN8O	551.481	CCT137690
Chemicals	S2744				
Selleck		[C@H]1(CO[C@@H]2O[C@@H](C)[C@H](O)[C@H](O)[C@H]2O)O[C@@H](Oc3cc4c(C(=O)C[C@@H](c5cc(O)c(OC)cc5)O4)c(O)c3)[C@H](O)[C@@H](O)[C@@H]1O	C28H34O15	610.561	Hesperidin
Chemicals	S2309				
Selleck		C1=C[C@@]2(C)C([C@](F)([H])C[C@]3([H])[C@@]2(F)[C@H](O)C[C@@]4(C)[C@@]3([H])C[C@]5([H])[C@@]4(C(=O)CO)OC(C)(CO)5)=CC1=O	C24H30F2O6	452.488	Fluocinolone Acetonide
Chemicals	S2470				
Selleck		[C@H]1(O)[C@@H](C)O[C@@H](O[C[C@H]2O[C@@H](Oc3cc4c(C(=O)C[C@@H](c5ccc(O)c(OC)cc5)O4)c(O)c3)[C@H](O)[C@H](O)[C@@H]2O)[C@H](O)[C@@H]1O.CO	C29H38O16	642.602	Methyl-Hesperidin
Chemicals	S2323				
Selleck		c1([N+](=O)[O-])ccc(C2C(C(=O)OCCN3CCN(C(c4cccc4)c5ccccc5)CC3)=C(C)NC(C)=C2C(OC)=O)c1.Cl.Cl	C35H40Cl2N4O6	683.621	Manidipine 2HCl
Chemicals	S2482				
Selleck		c1(C(C)=O)ccc(OC)cc1O	C9H10O3	166.174	Paeonol
Chemicals	S2339				
Selleck		c1(C(C)C)C(C)cc(C)c(CC2=NCCN2)c(C)c1O.Cl	C16H25ClN2O	296.835	Oxymetazoline HCl
Chemicals	S2495				
Selleck		[C@H]1(C)O[C@@H](Oc2c(CO)cccc2)[C@H](O)[C@@H](O)[C@@H]1O	C13H18O7	286.278	Salicin
Chemicals	S2351				

Selleck							
Chemicals	S2504	<chem>O1[C@H](n2nc(C(=O)N)nc2)[C@H](O)[C@H](O)[C@H]1CO</chem>	C8H12N4O5	244.205	Ribavirin		
Selleck					Taxifolin		
Chemicals	S2366	<chem>c1(O)cc2c(C(=O)[C@H](O)[C@@H](c3ccc(O)c(O)c3)O2)c(O)c1</chem>	C15H12O7	304.252	(Dihydroquercetin)		
Selleck							
Chemicals	S2522	<chem>c1(O)cc([C@H](CNC)O)ccc1O</chem>	C9H13NO3	183.204	L-Adrenaline		
Selleck							
Chemicals	S2379	<chem>[C@H]1(O)[C@H](O)[C@]([H])(O)[C@@H]2[C@H](CO)O[C@@]([H])(O)[C@@H]3CC[C@@]4(C)C(=CC[C@]5([H])[C@@]4([H])CC[C@@]6(C)[C@@]5([H])C[C@@]7([H])[C@@]6([H])[C@@H](C)[C@@]8CC[C@@H](C)CO8)O7C3)[C@H](O)[C@]9([H])O[C@@H](C)[C@H](O)[C@@H](O)[C@H]9O)[C@H]2O)O[C@@H](C)[C@@H]1O</chem>	C45H72O16	869.044	Dioscin		
Selleck							
Chemicals	S2536	<chem>c1(Cl)cc(Cl)c(COC(Cn2cncc2)c3ccc(Cl)cc3Cl)cc1</chem>	C18H14Cl4N2O	416.129	Miconazole		
Selleck							
Chemicals	S2392	<chem>c(OCCO1)cc([C@@H]2[C@@]3([H])[C@@]([H])([C@@H](c4ccc5c(OCCO5)C4)OC3)CO2)cc6)c16</chem>	C20H18O6	354.353	Sesamin		
Selleck							
Chemicals	S2552	<chem>c1cc2c(C(Cc3ccc(Cl)cc3)=NN(C4CCCN(C)CC4)C2=O)cc1.Cl</chem>	C22H25Cl2N3O	418.359	Azelastine HCl		
Selleck							
Chemicals	S2405	<chem>C(C[C@@]1([H])N(C[C@@]2([H])[C@]([H])(N3CC2)[C@@]1([H])CCC3)C4=O)=C4</chem>	C15H22N2O	246.348	Sophocarpine		
Selleck							
Chemicals	S2565	<chem>c1(O)ccc([C@@H](N)C(=O)N[C@@H]2C(=O)N3[C@]2([H])SC(C)(C)[C@H]3C([O-])=O)cc1.[Na+]</chem>	C16H18N3NaO5S	387.386	Amoxicillin Sodium		
Selleck							
Chemicals	S2415	<chem>[C@@H]1(O)CO[C@@H](O[C@H]2CC[C@]([C3]([C@@]3CC[C@@]4(C)[C@@]5(C)C[C@H](O)[C@@]4([H])[C@@]6(C)O[C@@H](C(O)(C)C)CC6)[C@]57([H])[C@@]([H])([C@@H](O[C@H]8[C@@H](O)[C@@H](O)[C@H]9O)[C@H](CO)O8)C7)C2(C)[C@H](O)[C@H]1O</chem>	C41H68O14	784.97	Astragaloside A		
Selleck							
Chemicals	S2584	<chem>C1=C[C@@]2(C)C(C[C@]3([H])[C@@]2(F)[C@]([H])(O)C[C@@]4(C)[C@@]3([H])C[C@]([H])(C)[C@@]4(O)C(=O)CC)C(=O)CCl)=CC1=O</chem>	C25H32ClFO5	466.97	Clobetasol propionate		
Selleck							
Chemicals	S2453	<chem>c1(O)ccc(CNNC(=O)C(CO)N)c(O)c1O.Cl</chem>	C10H16ClN3O5	293.704	Benserazide HCl		
Selleck							
Chemicals	S2602	<chem>Cc1c(CC(=O)OCC(=O)O)c2c(ccc(OC)c2)n1C(c3ccc(Cl)cc3)=O</chem>	C21H18ClNO6	415.824	Acemetacin		
Selleck							
Chemicals	S2613	<chem>c1(C(=C(Cl)Cl)Cl)cc(N)c(S(=O)(=O)N)cc1S(=O)(=O)N</chem>	C8H8Cl3N3O4S2	380.656	Clorsulon		
Selleck							
Chemicals	S2758	<chem>C1(=O)O[C@H](CO C)[C@@]2(C)c(c3C(=O)C4=C2[C@@H](OC(C)=O)C[C@@]([C]([C@]45[H])C(=O)CC5)c1cc3</chem>	C23H24O8	428.432	Wortmannin		
Selleck					Omecamtiv mecarbil (CK-		
Chemicals	S2623	<chem>c1(C)ccc(NC(=O)Nc2cccc(CN3CCN(C(C)C(=O)CC3)c2F)cn1</chem>	C20H24FN5O3	401.435	1827452)		
Selleck					Dalcetrapib (JTT-705,		
Chemicals	S2772	<chem>c1c(NC(=O)C2(CC(CC)CC)CCCC2)c(SC(=O)C(C)C)ccc1</chem>	C23H35NO2S	389.595	RO4607381)		
Selleck							
Chemicals	S2633	<chem>c1(Cl)c(C#N)c(O[C@H](O)CNC(C)(C)Cc2cc3c(ccc3)cc2)ccc1</chem>	C24H25ClN2O2	408.921	NPS-2143		
Selleck							
Chemicals	S2781	<chem>o1c(c2sc(CO)cc2)ccc1c3sc(CO)cc3</chem>	C14H12O3S2	292.373	RITA (NSC 652287)		
Selleck					5-hydroxymethyl		
Chemicals	S2659	<chem>c1c([C@@H](CCN(C(C)C(C)C)c2cc(CO)ccc2O)cccc1</chem>	C22H31NO2	341.487	Tolterodine (PNU 200577,		
Selleck					5-HMT, 5-HM)		
Chemicals	S2792	<chem>c(cc(C(F)(F)F)cc1)[C@H](N(Cc2cc(C(F)(F)F)cc(C(F)(F)F)c2)C(OC)=O)C[C@@H](CC)N3C(=O)OCC)c13</chem>	C26H25F9N2O4	600.473	Torcetrapib		
Selleck							
Chemicals	S2670	<chem>c1cc(C[C@H](N)COc2ncc(c3ccc4c(c(C)n[nH]4)c3)c2)ccc1</chem>	C22H22N4O	358.436	A-674563		
Selleck							
Chemicals	S2808	<chem>C1N(C(=O)[C@H](CNC(C)C)c2ccc(Cl)cc2)CCN(C3ncnc4c3[C@H](C)C[C@@H]4O)C1</chem>	C24H32ClN5O2	457.996	GDC-0068		
Selleck							
Chemicals	S2683	<chem>C1(=O)Nc2c(cc(Cl)cc2)C(N[C@@H]3CN(CCC34)CC4)=C1c5[nH]c6c(cccc6)n5</chem>	C23H22ClN5O	419.907	CHIR-124		
Selleck							
Chemicals	S3001	<chem>N1C(=O)N([C@@H]2[C@@H](F)[C@@H](O)[C@H](CO)O2)C=C(C)C1=O</chem>	C10H13FN2O5	260.219	Clevudine		
Selleck							
Chemicals	S2697	<chem>c1(c2c(O)cccc2)ccc(c3c4c(NC(=O)C(C#N)=C4O)sc3)cc1</chem>	C20H12N2O3S	360.386	A-769662		
Selleck							
Chemicals	S3022	<chem>[C@@](C)(C(=O)[C@H](OC)C(C)C)[C@@]1(O)[C@@H]2OC(c3cccc3)=O=C(C)[C@@H](OC(=O)[C@H](O)[C@H](c4cccc4)NC(=O)OC(C)(C)C)C1)([C@H](OC)C[C@]5([H])[C@@]6(O)C(=O)CO5)[C@]26[H]</chem>	C45H57NO14	835.932	Cabazitaxel		
Selleck							
Chemicals	S2718	<chem>C1CC(NC(=O)c2cc(c3cccc(S(=O)(=O)CC)c3)c4c([nH]c5c4cc(C)cn5)c2)CCN1C</chem>	C28H32N4O3S	504.644	TAK-901		
Selleck							
Chemicals	S3117	<chem>c1c(C(O)(C(=O)OCC#CCN(CC)CC)C2CCCC2)cccc1.Cl</chem>	C22H32ClNO3	393.947	Oxybutynin chloride		
Selleck							
Chemicals	S2730	<chem>c1cc2c(nc(n3c4c(cc(OCC5(C)CO5)cc4)nc3)cc2)c(N6CCC(N)CC6)c1</chem>	C26H29N5O2	443.541	Crenolanib (CP-868596)		

Selleck		<chem>c1(C=[N+](O-))C(C)(C)C(S([O-])(=O)=O)cc(S(=O)(=O)[O-])cc1.[Na+].[Na+]</chem>	C11H13NNa2O7S2	381.333	NXV-059
Chemicals	S6002				
Selleck		<chem>c1(C(C)(C)C#N)cc(C(=O)Nc2cc(Nc3ccc4c(C(=O)N(C)C=N4)c3(C)cc2)ccc1</chem>	C27H25N5O2	451.52	AZ 628
Chemicals	S2746				
Selleck		<chem>c1(O)ccc(c2c(O)ccc(CC=C)c2)cc1CC=C</chem>	C18H18O2	266.334	Honokiol
Chemicals	S2310				
Selleck		<chem>c1(OC[C@H](C)(CC(C)CC)c(OC[C@H](C)(CC(C)CC)c(OC[C@H](C)(CC(C)CC)ccc1.[I-].[I-].[I-]</chem>	C30H60I3N3O3	891.529	Gallamine Triethiodide
Chemicals	S2471				
Selleck		<chem>c1(O)cc2c(C(=O)C(O)=C(c3c(O)cc(O)cc3)O2)c(O)c1.O</chem>	C15H12O8	320.251	Morin Hydrate
Chemicals	S2325				
Selleck		<chem>n1ccc(C(C=C(C#N)C(=O)N2)=C2C)cc1</chem>	C12H9N3O	211.219	Milrinone
Chemicals	S2484				
Selleck		<chem>C1C=C(C)CC[C@@H]2[C@H](OC(=O)C2=C)[C@H]3[C@](C)(O3)C1</chem>	C15H20O3	248.318	(-)-Parthenolide
Chemicals	S2341				
Selleck		<chem>c1cc(C=CC(=O)O)ccc1Cn2ccnc2</chem>	C13H12N2O2	228.247	Ozagrel
Chemicals	S2496				
Selleck		<chem>[C@@]([H])([H])(CC(=O)O)O1([C@@]2(C)[C@]([H])(C)(C)CCC2)CC3)[C@]13C</chem>	C16H26O2	250.376	Sciareolide
Chemicals	S2355				
Selleck		<chem>[C@@]1(C)(O)[C@H](O)[C@@H](C)C(=NOCOCOC)[C@H](C)C[C@](O)(C)[C@H](O)[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@@H](C)[C@@H](O)[C@H]3C[C@](O)(C)[C@H](O)[C@H](C)O3)[C@@H](C)C(=O)O[C@H]1CC</chem>	C41H76N2O15	837.047	Roxithromycin
Chemicals	S2506				
Selleck		<chem>c1(O)cc2c(C(Cc3cc(OC)c(OC)cc3)NCC2)cc1OC.Cl</chem>	C20H26ClNO4	379.878	Tetrahydropapaverine HCl
Chemicals	S2367				
Selleck		<chem>c1cc2c(C(=O)C(=C3O)[C@]([H])([C@@H](O)[C@]4([H])[C@@]3(O)C(=O)C(C(=O)N)=C(O)[C@@H]4N(C)C)C2=C)c(O)c1.Cl</chem>	C22H23ClN2O8	478.88	Methacycline HCl
Chemicals	S2527				
Selleck		<chem>c1(O)cc2c(C(=O)C=C(c3cc(O)c(OC)cc3)O2)c(O)c1</chem>	C16H12O6	300.263	Diosmetin
Chemicals	S2380				
Selleck		<chem>n1(c(C)nc1[N+])(=O)[O-])CC(O)C</chem>	C7H11N3O3	185.181	Secnidazole
Chemicals	S2537				
Selleck		<chem>c1(O)cc2c(C(=O)C[C@@H](c3ccc(O)cc3)O2)c(O)c1</chem>	C15H12O5	272.253	Naringenin
Chemicals	S2394				
Selleck		<chem>c1(O)c(O)c2c(C=CC(=O)O2)cc1</chem>	C9H6O4	178.142	Daphnetin
Chemicals	S2554				
Selleck		<chem>c1cc2c(C(=O)c3c(cc(C)cc3O)C2=O)c(O)c1</chem>	C15H10O4	254.238	Chrysophanic Acid
Chemicals	S2406				
Selleck		<chem>c1cc(C(CNC(C)C)O)cc(O)c1O.Cl</chem>	C11H18ClNO3	247.719	Isoprenaline HCl
Chemicals	S2566				
Selleck		<chem>[C@H]1(O)C[C@@]2(C)[C@]([H])(C(=O)C=C3[C@@]2([H])CC[C@@]4(C)[C@@]3(O)CC[C@H]4[C@](O)(C)[C@H](O)CCC(C)(O)C)[C@H]1O</chem>	C27H44O7	480.634	20-Hydroxyecdysone
Chemicals	S2417				
Selleck		<chem>C(OC)(=O)C=CC(OC)=O</chem>	C6H8O4	144.125	Dimethyl Fumarate
Chemicals	S2586				
Selleck		<chem>[N+](C)(C)(C)CC(C)OC(=O)N.[Cl-]</chem>	C7H17ClN2O2	196.675	Bethanechol chloride
Chemicals	S2455				
Selleck		<chem>c1(O)cc2c(SC(=O)O2)cc1</chem>	C7H4O3S	168.17	Tioxolone
Chemicals	S2603				
Selleck		<chem>N1(C)CC(C(=O)OC)=CCC1.Br</chem>	C8H14BrNO2	236.106	Arecoline
Chemicals	S2614				
Selleck		<chem>c1c(C(=O)NO)cnc(N(Cc2sc3c(nc4cnc(OC)cc4)nc3N5CCOCC5)c2)C)n1</chem>	C23H24N8O4S	508.553	CUDC-907
Chemicals	S2759				
Selleck		<chem>n1c(N)c2n(c([C@H]3CC[C@H](C(O)=O)CC3)nc2c4cc5c(c(OC)ccc5)[nH]4)n</chem>	C21H22N6O3	406.438	OSI-027
Chemicals	S2624				
Selleck		<chem>N(c1cccc1Br)C(N[C@@H]2CCN(c3ncc(C(F)(F)F)cc3)C2)=O</chem>	C17H16BrF3N4O	429.234	SB705498
Chemicals	S2773				
Selleck		<chem>c1(NC(=O)Nc2cc(C(C)(C)C)nn2c3ccc4c(ccn4)c3)ccc(OC5ccnc(C(=O)NC)c5)cc1F</chem>	C30H28FN7O3	553.587	DCC-2036 (Rebastinib)
Chemicals	S2634				
Selleck		<chem>c1cc2c(nc(N3CCOC[C@@H]3C)nc2N4CCOC[C@@H]4C)nc1c5cccc(C(=O)NC)c5</chem>	C25H30N6O3	462.544	AZD2014
Chemicals	S2783				
Selleck		<chem>c1c(Cl)ccc(S(=O)(=O)[C@]2(c3cc(F)ccc3)CC[C@H](CCC(O)=O)CC2)c1</chem>	C21H21ClF2O4S	442.904	MK-0752
Chemicals	S2660				
Selleck		<chem>[C@H]1(CO[P@](=O)(Oc2ccccc2)N[C@H](C)C(=O)OC(C)O[C@@H](N3C=CC(=O)NC3=O)[C@@](F)(C)[C@@H]1O</chem>	C22H29FN3O9P	529.453	Sofosbuvir (PSI-7977, GS-7977)
Chemicals	S2794				
Selleck		<chem>c1(F)ccc(c2ccc(C=C3C(=O)NC(=O)S3)o2)c(O)c1</chem>	C14H8FNO4S	305.281	AS-252424
Chemicals	S2671				
Selleck		<chem>n1c(N)c2c(n(C(C)C)nc2c3ccc4c(nc(N)j4)c3)nc1</chem>	C15H15N7O	309.326	INK 128 (MLN0128)
Chemicals	S2811				
Selleck		<chem>c1c(O)c(C(=O)c2cc(OC)c(OCN3CCOCC3)cc2)c(CC(=O)N(CCO)CCO)cc(C)cc1O</chem>	C30H42N2O9	574.662	KW-2478
Chemicals	S2685				

Selleck		[C@@H]1(NC(N)=N)[C@H](NC(=O)C)[C@]([H])([C@@H]([C@@H](CO)O)O)OC(C(O)=O)=C1	C12H20N4O7	332.31	Zanamivir
Chemicals	S3007				
Selleck					
Chemicals	S2699	n1cc(c2nc(N3CCOCC3)nc4c2CCN4S(=O)(=O)C)cnc1N	C15H19N7O3S	377.421	CH5132799
Selleck					
Chemicals	S3023	c1(CC(NO)=O)ccc(OCCCC)cc1	C12H17NO3	223.268	Bufexamac
Selleck					
Chemicals	S2719	c1cnc(OC2ccc(Nc3nnc(c4cc(C)cs4)c5c3cccc5)cc2)c(c6ccnc(N)n6)c1	C28H21N7OS	503.578	AMG-900
Selleck					Cabozantinib malate
Chemicals	S4001	c(cc(OC)c(OC)c1)(nccc2Oc3ccc(NC(=O)C4(CC4)C(=O)Nc5ccc(F)cc5)cc3)c12.C(O)(=O)C[C@@H](C(O)=O)O	C32H30FN3O10	635.593	(XL184)
Selleck					
Chemicals	S2731	c1(OC2CCN(C)CC2)ccc(Nc3ncc4c(N(C5CCCC5)C(=O)N4C)n3)c(OC)c1	C24H32N6O3	452.549	AZ 3146
Selleck					
Chemicals	S6003	c1c(C(O)=O)cccc1c2nc(c3c(F)cccc3)on2	C15H9FN2O3	284.242	Ataluren (PTC124)
Selleck					
Chemicals	S2747	N1(CC(O)(C)C)C(C)=C(C(Nc2ncc(OC3c(c4ncc3)ccc(OC)c4)cc2)=O)C(=O)N1c5cccc5	C30H29N5O5	539.582	AMG-458
Selleck					Hydoxychoic acid
Chemicals	S2311	C1C[C@@]2(C)[C@]([H])([C@@H](O)C[C@]3([H])(C@@)2([H])CC[C@@]4(C)[C@@]3([H])CC[C@H]4[C@@H]([C@@H](CCC(=O)O)O)C)[C@@H]1O	C24H40O4	392.572	(HDCA)
Selleck					
Chemicals	S2473	c1c(O)ccc([C@H](CC)[C@@H](c2ccc(OC)c2)CC)c1	C18H22O2	270.366	Hexestrol
Selleck					
Chemicals	S2326	c1(O)cc2c(C(=O)C(O)=C(c3cc(O)c(O)c(O)O2)c(O)c1	C15H10O8	318.235	Myricetin
Selleck					
Chemicals	S2485	c1c(O)c2c(C(=O)c3c(c(NCCNCCO)ccc3NCCNCCO)C2=O)c(O)c1.Cl.Cl	C22H30Cl2N4O6	517.403	Mitoxantrone HCl
Selleck					
Chemicals	S2342	c1(O)cc(O)c(C(=O)CCc2ccc(O)cc2)c(O)c1	C15H14O5	274.269	Phloretin
Selleck					
Chemicals	S2497	[C@H]1([N+](C)CCCC2)C[C@@]3(C)[C@@]([H])(CC[C@]4([H])([C@@]3([H])CC[C@@]5(C)[C@@]4([H])C[C@H]([N+](C)CCCC6)[C@H]5OC(=O)C)C[C@@]4([H])O)C(=O)C.[Br-].[Br-]	C35H60Br2N2O4	732.67	Pancuronium dibromide
Selleck					
Chemicals	S2356	C1=C(C(O)=O)C[C@@H](O)C(O)C1O	C7H10O5	174.151	Shikimic Acid
Selleck					
Chemicals	S2508	O([C@@H]1C[C@@]([H])(N(C)[C@@]2([H])C1)[C@]3([H])(C@@)2([H])O3)C(=O)[C@H](CO)c4cccc4.Br	C17H22BrNO4	384.265	Scopolamine HBr
Selleck					
Chemicals	S2370	C1C[C@@]2(C)[C@@]([H])(CC[C@]3(C)[C@@]2([H])CC=C4[C@@]3(C)CCC5[C@]4([H])([C@H](C)[C@H](C)C[C@H]5C(O)=O)C(C)[C@H]1O	C30H48O3	456.7	Ursolic Acid
Selleck					
Chemicals	S2528	C1CC(C2=CC(C)=CC(=O)N2O)CCC1	C12H17NO2	207.269	Ciclopirox
Selleck					
Chemicals	S2381	OC[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)CO	C6H14O6	182.172	D-Mannitol
Selleck					
Chemicals	S2542	c1ccc(CCNC(=N)NC(N)=N)cc1.Cl	C10H16ClN5	241.721	Phenformin HCl
Selleck					
Chemicals	S2395	c1(C)cc2c(C(=O)c3c(cc(OC)cc3O)C2=O)c(O)c1	C16H12O5	284.263	Rheochrysidin
Selleck					
Chemicals	S2555	[C@@]1(C)(O)[C@H](O)[C@@H](O)C(=O)[C@H](C)C[C@@](C)(OC)[C@H](O)[C@H]2[C@@H](O)[C@@H](N(C)C)C[C@H](CO2)[C@@H](C)[C@@H](O)[C@H]3O[C@@H](C)[C@H](O)[C@@](OC)(C)C3)[C@@H](C)C(=O)O[C@@H]1CC	C38H69NO13	747.953	Clarithromycin
Selleck					
Chemicals	S2407	C1(=C)C[C@](O)[C@]23[C@@]1([H])CC[C@H]2C)(O)[C@H](C(C)C)C3	C15H24O2	236.35	Curcuml
Selleck					Medroxyprogesterone
Chemicals	S2567	C1C[C@@]2(C)C([C@@H](C)C[C@]3([H])(C@@]2([H])CC[C@@]4(C)[C@@]3([H])CC[C@]4(O)C(=O)C(C)=O)=CC1=O	C24H34O4	386.524	acetate
Selleck					
Chemicals	S2420	C1N2[C@@]([H])([C@]3([H])C[C@@]([H])([C@@]4([H])C(CCCN4)=C3)C2)CCC1	C15H24N2	232.364	Aloperine
Selleck					
Chemicals	S2589	[C@@H]1(O)[C@H](O)[C@H](O)[C@@H](CO)N(CCO)C1	C8H17NO5	207.224	Miglitol
Selleck					
Chemicals	S2457	[C@H]1(O)[C@H](SC)O[C@H]([C@@H](NC([C@@H]2C[C@@H](CCC)N2C)=O)C(Cl)C)[C@H](O)[C@@H]1O.Cl	C18H34Cl2N2O5S	461.444	Clindamycin HCl
Selleck					Dehydroepiandrosterone
Chemicals	S2604	C1C[C@@]2(C)C(=CC[C@]3([H])(C@@]2([H])CC[C@@]4(C)[C@@]3([H])CCC4=O)C[C@H]1O	C19H28O2	288.424	(DHEA)
Selleck					Noradrenaline bitartrate
Chemicals	S2615	c1(O)cc([C@@]([H])(O)CN)ccc1O.O.C(=O)[C@]([H])(O)[C@@]([H])(O)C(=O)O.O	C12H19NO10	337.28	monohydrate
Selleck					
Chemicals	S2760	[C@H]1(CO)O[C@H](c2ccc(C)c(Cc3ccc(c4ccc(F)cc4)s3)c2)[C@H](O)[C@@H](O)[C@@H]1O	C24H25FO5S	444.516	Canagliflozin
Selleck					
Chemicals	S2626	c1c(OC[C@H]2OCCNC2)c(NC(=O)Nc3ncc(C)n3)cc(Br)c1C	C18H22BrN5O3	436.303	LY2603618
Selleck					
Chemicals	S2775	C(OC)(=O)Nc1[nH]c2c(ccc(C(c3sccc3)=O)c2)n1	C14H11N3O3S	301.32	Nocodazole

Selleck					
Chemicals	S2635	<chem>n1c(N2CC(Cc3ccc(Cl)cc3)(N)CC2)c4c([nH]cc4)nc1</chem>	C18H20ClN5	341.838	CCT 128930
Selleck		<chem>c(ccn1CCNC(C(C)(C)O)=O)(ncnc2Nc3cc(Cl)c(Oc4cc(C(F)(F)F)ccc4)cc3)c</chem>			
Chemicals	S2784	12	C26H25ClF3N5O3	547.957	TAK-285
Selleck		<chem>c1(N2CC(OC3C2)CC3)c4c(n(C5CCC6(OCCO6)CC5)nc4)nc(c7ccc(NC(NC)=O)cc7)n1</chem>	C27H33N7O4	519.595	WYE-125132 (WYE-132)
Chemicals	S2795	<chem>c1cc(C(=O)Nc2ccc(F)cc2F)ccc1OCCCC</chem>	C17H17F2NO2	305.319	VU 0357121
Selleck		<chem>C1(=O)C(C)=C2C(C(=O)N(C3CC3)C(=O)N2c4cccc(NC(=O)C)c4)=C(Nc5c(F)cc(I)cc5)N1C</chem>	C26H23FIN5O4	615.395	Trametinib (GSK1120212)
Chemicals	S2814	<chem>N1(C(Nc2nc(C)c(c3ccnc(C(C)(C)F)(F)F)c3)s2=O)CCC[C@@H]1C(N)=O</chem>	C19H22F3N5O2S	441.47	BYL719
Selleck		<chem>c1c(c2cc(F)c(CN3CCOCC3)c(F)c2)c4c(ncc(c5cnn(C6CCNCC6)c5)n4)cc1.Cl</chem>	C27H30Cl2F2N6O	563.47	NVP-BSK805 2HCl
Chemicals	S2686				
Selleck					
Chemicals	S3008	<chem>c1cc2c(Sc3c(cc(C(C)O)=O)C)cc3)CC2=O)cc1</chem>	C17H14O3S	298.356	Zaltoprofen
Selleck					
Chemicals	S2700	<chem>c1cc(c2cnc(C(C(=O)N)Cc3ccccc3)cc2)ccc1OCCN4CCOCC4</chem>	C26H29N3O3	431.527	KX2-391
Selleck					
Chemicals	S3025	<chem>c1(CS(F)(=O)=O)cccc1</chem>	C7H7FO2S	174.193	PMSF
Selleck					
Chemicals	S2720	<chem>c1(N(C)C)cc(C(=O)Nc2ccc(C)c(NC(=O)C3ccc(F)cc3)c2)ccc1</chem>	C23H23N3O3	389.447	ZM 336372
Selleck		<chem>c1c(F)c(C[C@@H](N)CC(=O)N2CCn3c(nnc3C(F)(F)F)C2)cc(F)c1F.P(OO)</chem>			Sitagliptin phosphate
Chemicals	S4002	<chem>(=O)=O.[H].O</chem>	C16H20F6N5O6P	523.324	monohydrate
Selleck					
Chemicals	S2735	<chem>c1(c(c2cnn(C)c2)cn3)n3c(N)c(Br)c([C@@H]4CCCCN4)n1</chem>	C15H18BrN7	376.254	MK-8776 (SCH 900776)
Selleck					
Chemicals	S6005	<chem>c1cc(F)c(N(C(N)=O)c2ccc(C(=O)N)c(c3ccc(F)cc3F)n2)c(F)c1</chem>	C19H12F4N4O2	404.318	VX-702
Selleck		<chem>c1cc(c2c(OC)cc(F)c(C(C)C)c2)c(CN3[C@@H](C)[C@@H](c4cc(C(F)(F)F)cc(C(F)(F)F)c4)OC3=O)cc1C(F)(F)F</chem>	C30H25F10NO3	637.508	Anacetrapib (MK-0859)
Chemicals	S2748	<chem>[C@@H]1(CO)OC(Oc2c(CC=C(C)C)c3c(C(=O)C)OC4[C@@H](O)[C@@H](O)[C@@H](O)[C@@H](O)C4)O4=C(c5ccc(OC)cc5)O3)c(O)c2[C@@H](O)[C@@H](O)[C@@H]1O</chem>	C33H40O15	676.662	Icariin
Selleck					
Chemicals	S2475	<chem>n1ccc(c2cnccc2)nc1Nc3c(C)ccc(NC(c4ccc(CN5CCN(C)CC5)cc4)=O)c3</chem>	C29H31N7O	493.603	Imatinib (ST1571)
Selleck					
Chemicals	S2328	<chem>C(N(CC)c1c(ccc(C)n1)C2=O)=C2C(=O)O</chem>	C12H12N2O3	232.235	Nalidixic acid
Selleck					
Chemicals	S2486	<chem>C1CN(C(=N)NC(=N)N)CCO1.Cl</chem>	C6H14ClN5O	207.661	Moroxydine HCl
Selleck		<chem>c1(O)c(C(=O)CCc2ccc(O)cc2)c(O[C@@H]3[C@@H](O)[C@@H](O)[C@@H](O)[C@@H](CO)O3)cc(O)c1</chem>	C21H24O10	436.409	Phlorizin
Chemicals	S2343				
Selleck					
Chemicals	S2498	<chem>OCC(C)(C)[C@@]([H])(O)C(=O)NCCC(=O)O</chem>	C9H17NO5	219.235	D-Pantothenic acid
Selleck		<chem>[C@@H]1(CO)OC2c(cc([C@@H]3Oc4c(c(O)cc(O)c4)C(=O)[C@@H]3O)cc2)O[C@@H]1c5cc(OC)c(O)cc5</chem>	C25H22O10	482.436	Silibinin
Chemicals	S2357				
Selleck					
Chemicals	S2509	<chem>c1(C(O)CNC(C)C)ccc(NS(=O)(=O)C)cc1.Cl</chem>	C12H21ClN2O3S	308.825	Sotalol
Selleck		<chem>[nH]1c2c(cccc2)c3c1[C@@]4([H])N(C[C@@]5([H])[C@@]([H])([C@@H](C(=O)OC)[C@@H](O)CC5)C4)CC3.Cl</chem>	C21H27ClN2O3	390.904	Yohimbine HCl
Chemicals	S2373				
Selleck					
Chemicals	S2529	<chem>c1(O)cc(CCN)ccc1O.Cl</chem>	C8H12ClNO2	189.639	Dopamine HCl
Selleck					
Chemicals	S2384	<chem>[C@](O)(Cc1c2cc(O)c(O)c1)(COc3c4ccc(O)c3O)[C@]24[H]</chem>	C16H14O6	302.279	Hematoxylin
Selleck		<chem>N(C(=O)[C@@]1(NC(=O)C(c2csc(N)n2)=NO)[H])(C(C(=O)O)=C(CSC(=O)c3ccco3)CS4)[C@@]14[H].Cl</chem>	C19H18ClN5O7S3	560.024	Ceftiofur HCl
Chemicals	S2543				
Selleck		<chem>[C@@H]1(CO)O[C@@H](OCCc2ccc(O)cc2)[C@@H](O)[C@@H](O)[C@@H]1O</chem>	C14H20O7	300.304	Salidroside
Chemicals	S2396				
Selleck					
Chemicals	S2556	<chem>c1cc(N(C)CCOC2ccc(CC3C(=O)NC(=O)S3)cc2)nc1</chem>	C18H19N3O3S	357.427	Rosiglitazone
Selleck		<chem>c1cc([C@@H](NC(=O)C)C)=CC([C@@H](O)C(=O)O[C@@H]2C(C)=C3C(C)(C)[C@@](O)([C@@H](OC(=O)c4ccccc4)[C@@]5([H])[C@@](C)([C@@H](O)[C@@H]6[C@@]5(O)C(C)=O)CO6)C(=O)[C@@H]3O)C(C(=O)C2)ccc1</chem>	C45H53NO14	831.901	Cephalomannine
Chemicals	S2408				
Selleck					
Chemicals	S2569	<chem>c1(O)cc([C@@]([H])(O)CNC)ccc1.Cl</chem>	C9H14ClNO2	203.666	Phenylephrine HCl
Selleck					
Chemicals	S2422	<chem>c1cc2c(OC=C(c3ccccc3)C2=O)cc1OC(C)C</chem>	C18H16O3	280.318	Ipriflavone (Osteofix)
Selleck					
Chemicals	S2593	<chem>C(N1c2c(cc(Cl)cc2)C(O)CCC1)(=O)c3ccc(NC(c4c(C)cccc4)=O)cc3C</chem>	C26H25ClN2O3	448.941	Tolvaptan

Selleck					
Chemicals	S2458	<chem>c1c(Cl)c(NC2=NCCN2)c(Cl)cc1.Cl</chem>	C9H10Cl3N3	266.555	Clonidine HCl
Selleck					
Chemicals	S2605	<chem>C1(=O)C(C)=C(CCCCCCCCCO)C(=O)C(O)C=C1OC</chem>	C19H30O5	338.439	Idebenone
Selleck					
Chemicals	S2617	<chem>N1(C[C@H](CO)O)C(=O)C2=C(N(C)C(=O)C(F)=C2Nc3c(F)cc(l)cc3)N=C1</chem>	C17H15F2IN4O4	504.227	TAK-733
Selleck					
Chemicals	S2761	<chem>c1cc2n(c(Cc3cc4c(nc3c4)cc3)cn2)nc1c5cn(C)nc5</chem>	C20H16N6	340.381	NVP-BVU972
Selleck					
Chemicals	S2627	<chem>c1cc(Cn2c3c(ccc3)c4c2CCN(C)C4)ccc1C(=O)NO.Cl</chem>	C20H22ClN3O2	371.861	Tubastatin A HCl
Selleck					
Chemicals	S2776	<chem>S(Cc1cccc1)CC(C)(CCCC(=O)O)SCc2cccc2</chem>	C22H28O2S2	388.587	CPI-613
Selleck					
Chemicals	S2636	<chem>c1c(c2c(C)nc(NC(=O)N3CCC[C@H]3C(N)=O)s2)nc(C(C)(C)C)s1</chem>	C17H23N5O2S2	393.527	A66
Selleck					
Chemicals	S2785	<chem>o1c(c2ccc(Cl)cc2)ccc1C(Nc3cc(OC)cc(OC)c3)=O</chem>	C19H16ClNO4	357.788	A-803467
Selleck					
Chemicals	S2663	<chem>c1(ccccc1O)N2CCN(CCN(C(=O)C3CCCC3)c4ncccc4)CC2.Cl.Cl.Cl</chem>	C25H37Cl3N4O2	531.946	WAY-100635 Maleate
Selleck					
Chemicals	S2796	<chem>C(N[C@H](c1cccc1)C)(=O)C(C#N)=Cc2nc(Br)ccc2</chem>	C17H14BrN3O	356.217	WP1066
Selleck		<chem>c1ccc(NC(=O)Nc2ccc(c3ccc(C([C@H]4[C@@H](C(=O)O)CCC4)=O)cc3)c2)cc1</chem>	C26H24N2O4	428.48	A922500
Chemicals	S2674				
Selleck					
Chemicals	S2820	<chem>c1(N2CCOCC2)ccc(Nc3ncc(Cl)c(Nc4cccc4C(=O)NC)n3)c(OC)c1</chem>	C23H25ClN6O3	468.936	TAE226 (NVP-TAE226)
Selleck					
Chemicals	S2688	<chem>n1c(N)c(C(=O)c2c(OC)ccc(F)c2F)cnc1NC3CCN(S(=O)(C)=O)CC3</chem>	C18H21F2N5O4S	441.452	R547
Selleck					
Chemicals	S3012	<chem>c1(S(N)(=O)=O)cc(Nc2nccc(N(c3cc(c4cc3)nn(C)c4C)C)n2)ccc1C</chem>	C21H23N7O2S	437.518	Pazopanib
Selleck		<chem>n1c(Nc2c(C(NC)=O)c(F)ccc2)c3c([nH]cc3)nc1Nc4cc5c(CCN5C(CN(C)C)=O)cc4OC</chem>	C27H29FN8O3	532.569	GSK1838705A
Chemicals	S2703				
Selleck					
Chemicals	S3026	<chem>c1(O)ccc(C=Cc2cc(O)cc(O)c2)cc1O</chem>	C14H12O4	244.243	Piceatannol
Selleck					
Chemicals	S2722	<chem>c1cc(C(Nc2ccc3c(c(N)cc(C)n3)c2)=O)c(COc4ccc(CC)cc4)cc1.Cl</chem>	C26H26ClN3O2	447.957	JTC-801
Selleck					
Chemicals	S4075	<chem>c1c[n+]2c([S-][Zn+ 2]3([S-]c4[n+](cccc4)[O-]3)[O-]2)cc1</chem>	C10H8N2O2S2Zn	317.722	Zinc Pyrithione
Selleck		<chem>c1(OCCN2CCCC2)ccc(Nc3ncc(C)c(Nc4cc(S(=O)(=O)NC(C)(C)C)ccc4)n3)c1</chem>	C27H36N6O3S	524.678	TG101348 (SAR302503)
Chemicals	S2736				
Selleck		<chem>C1CC=C[C@@]2([H])[C@@]([H])([C]C@H](O)C2)[C@H](O)C=CC(=O)O[C@@H](C)C1</chem>	C16H24O4	280.359	Brefeldin A
Chemicals	S7046				
Selleck		<chem>C(O)(=O)C=CC(O)=O.n1c(c2c3c(N(C)C(=O)N3c4ccc(N5CCNCC5)c(C(F)(F)F)c4)c1ccc(c6ccc(OC)nc6)c2</chem>	C32H29F3N6O6	650.604	BGT226 (NVP-BGT226)
Chemicals	S2749				
Selleck					
Chemicals	S2314	<chem>c1(O)cc2c(C(=O)C(O)=Cc3ccc(O)cc3)O2)c(O)c1</chem>	C15H10O6	286.236	Kaempferol
Selleck		<chem>c1c(N2CCN(c3ccc(N4C=NN(C(C)CC)C4=O)cc3)CC2)ccc(OC[C@H]5CO[C@@]([c6c(Cl)cc(Cl)cc6])(Cn7ncnc7)O5)c1</chem>	C35H38Cl2N8O4	705.633	Itraconazole
Chemicals	S2476				
Selleck		<chem>C1[C@@]2(C)[C@@]([H])(CC[C@@]3(C)[C@@]2([H])CC=C4[C@@]3(C)CCC5[C@@]4([H])CC(C)(C)[C@H]5C(O)=O)C(C)(C)[C@H]1O</chem>	C30H48O3	456.7	Oleanolic Acid
Chemicals	S2334				
Selleck					
Chemicals	S2487	<chem>c(C(=O)OC1)(c(O)c(Cc(CCC(O)=O)C)c(OC)c2C)c12</chem>	C17H20O6	320.337	Mycophenolic acid
Selleck					
Chemicals	S2344	<chem>C1CCCN(C(=O)C=CC=Cc2ccc3c(OCO3)c2)C1</chem>	C17H19NO3	285.338	Piperine
Selleck					
Chemicals	S2499	<chem>c1ccc(OC(C)N(Cc2cccc2)CC)cc1.Cl</chem>	C18H23Cl2NO	340.287	Phenoxybenzamine HCl
Selleck		<chem>c1(OC)ccc2c([C@@]34[C@@]([H])(C(=O)C)C(=O)C3)[C@@H](N(C)CC4)C2)c1O</chem>	C19H23NO4	329.39	Sinomenine
Chemicals	S2359				
Selleck		<chem>[C@H]1(NC)[C@@H](O)[C@]2([H])[C@]([H])(O[C@]3(O)[C@@]([H])(O[C@H](C)CC3=O)O2)[C@@H](NC)[C@H]1O.Cl.Cl</chem>	C14H26Cl2N2O7	405.271	Spectinomycin HCl
Chemicals	S2510				
Selleck					
Chemicals	S2374	<chem>c1(O)cc2c([nH]cc2CC(N)C(=O)O)cc1</chem>	C11H12N2O3	220.225	5-hydroxytryptophan (5-HTP)
Selleck					
Chemicals	S2531	<chem>c1(OC)cc(C=O)c(OC)cc1OC</chem>	C10H12O4	196.2	Asaraldehyde
Selleck					
Chemicals	S2385	<chem>c1cc(CCN(C)C)ccc1O</chem>	C10H15NO	165.232	Hordenine
Selleck					
Chemicals	S2545	<chem>[C@@]1([H])[C]C@H](O)C2N(C)[C@]2([H])[C@@]3([H])[C@]1([H])O3</chem>	C8H13NO2	155.194	Scopine
Selleck					
Chemicals	S2399	<chem>c1(O)cc2c(C(=O)[C@H](O)[C@@H](c3cc(O)c(O)c(O)c3)O2)c(O)c1</chem>	C15H12O8	320.251	Dihydromyricetin

Selleck					
Chemicals	S2557	<chem>c1ccc2c(cccc2CN(C)CC=CC#CC(C)(C)C)c1.Cl</chem>	C21H26ClN	327.891	Terbinafine HCl
Selleck					
Chemicals	S2409	<chem>[C@@](C)(C(=O)[C@H](O)C(=C1C)C(C)[C@H](O)(C[C@@H]1O)[C@H]2OC(c3ccccc3)=O)([C@H](O)C[C@H]4([H])[C@@]5(O(C=O)C)CO4[C@@]25[H])</chem>	C29H36O10	544.59	10-Deacetylbaicatin-III
Selleck					
Chemicals	S2574	<chem>c1c(O)c2c([C@](O)(C)[C@@](C(=C3O)C2=O)([H])C[C@]4([H])[C@@]3(O)C(=O)C(C(=O)N)=C(O)[C@@]4([H])N(C)C)cc1.Cl</chem>	C22H25ClN2O8	480.895	Tetracycline HCl
Selleck					
Chemicals	S2437	<chem>c1cc2c(CN3[C@]([H])(c4c(cc(OC)c(OC)c4)CC3)C2)c(OC)c1OC</chem>	C21H25NO4	355.427	Rotundine
Selleck					
Chemicals	S2594	<chem>C(N1CCCC1=O)C(NCCN(C(C)C)C(C)C)=O</chem>	C14H27N3O2	269.383	Pramiracetam
Selleck					
Chemicals	S2461	<chem>C(N1c2c(cccc2)NC1=O)CCN3CCC(N4C(=O)Nc5c4ccc(Cl)c5)CC3</chem>	C22H24ClN5O2	425.911	Domperidone
Selleck					
Chemicals	S2606	<chem>C1CC(=C([C@H](c2ccc(N(C)C)cc2)C[C@]3(C)[C@@]4([H])CC[C@@]3(C#CC)O)[C@]45[H])C(C5)=CC1=O</chem>	C29H35NO2	429.594	Mifepristone
Selleck					
Chemicals	S2619	<chem>c1ccc(COC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C=O)CC(C)C)cc1</chem>	C26H41N3O5	475.621	MG-132
Selleck					
Chemicals	S2765	<chem>N1=C(C(NC)=O)c2c(c(O)c3n2[C@H](C)CN(CC)C3=O)C(=O)N1Cc4cc(Cl)c(F)cc4</chem>	C21H21ClFN5O4	461.874	MK-2048
Selleck					
Chemicals	S2629	<chem>c1(OC)cc(OC)c(Cl)cc1NC(=O)Nc2cc(C)on2</chem>	C13H14ClN3O4	311.721	PNU-120596
Selleck					
Chemicals	S2777	<chem>c1(C)cnc(c2c(Cl)cnc(N3CCN(C(CCS(=O)(=O)C)=O)CC3)c2)c(C)c1</chem>	C20H25ClN4O3S	436.955	PF-5274857
Selleck					
Chemicals	S2638	<chem>C(C(=O)c1c(c(c2c3c(c4c(cccc4)s3)ccc2)ccc1)O5)=C5N6CCOCC6</chem>	C25H19NO3S	413.488	NU7441 (KU-57788)
Selleck					
Chemicals	S2787	<chem>N1(C)c(c2C(O)=C(C(N(CC)c3ccccc3)=O)C1=O)cccc2Cl</chem>	C19H17ClN2O3	356.803	Laquinimod
Selleck					
Chemicals	S2664	<chem>C1CCCC(c2ccc(OC(C(O)=O)(C)CC)cc2)(c3ccc(OC(C(=O)O)(C)CC)cc3)C1</chem>	C28H36O6	468.582	Clinofibrate
Selleck					
Chemicals	S2797	<chem>C1c2c(ncc(Br)c2)[C@H](C3CCN(C(=O)CC4CCN(C(=O)N)CC4)CC3)c5c(cc(Cl)cc5Br)C1</chem>	C27H31Br2ClN4O2	638.822	Lonafarnib
Selleck					
Chemicals	S2677	<chem>c1ccc(C(c2ccccc2)C(O)CN3CCN(c4cccc(Cl)c4)CC3)cc1.Cl.Cl</chem>	C25H29Cl3N2O	479.87	BRL-15572
Selleck					
Chemicals	S2840	<chem>S=C1N(c2cc(F)c(C(=O)NC)cc2)C3(CCC3)C(=O)N1c4cc(C(F)(F)F)c(C#N)n</chem>	C21H15F4N5O2S	477.435	ARN-509
Selleck					
Chemicals	S2689	<chem>c(cc[nH]1)(cc(c2nc(N3CCOCC3)c4c(n(C5CCN(Cc6cnccc6)CC5)nc4)n2)cc7)c</chem>	C28H30N8O	494.591	WAY-600
Selleck					
Chemicals	S3017	<chem>c1c(C(O)=O)c(OC(=O)C)ccc1</chem>	C9H8O4	180.157	Aspirin
Selleck					
Chemicals	S2711	<chem>c1(F)cc(CC(=O)N[C@@H](C)C(=O)N[C@@H]2C(=O)N(C)c3c(cccc3)c4c2</chem>	C26H23F2N3O3	463.476	YO-01027
Selleck					
Chemicals	S3031	<chem>c1cc2c(c(C)nc(CN3C(=O)c4c(nc(N5CCC[C@@H](N)C5)n4CC#CC)N(C)C3=O)n2)cc1</chem>	C25H28N8O2	472.542	Linagliptin
Selleck					
Chemicals	S2726	<chem>c1(N2C(=O)C(Br)=C(Oc3c(F)cc(F)cc3)C=C2C)cc(C(NC)=O)ccc1C</chem>	C22H19BrF2N2O3	477.299	PH-797804
Selleck					
Chemicals	S4119	<chem>c(cc(N1CCN(C)CC1)c(F)c2)(N(CC)C=C(C(=O)O)C3=O)c23.S(=O)(=O)(O)C.O.O</chem>	C18H28FN3O8S	465.494	Pefloxacin Mesylate Dihydrate
Selleck					
Chemicals	S2738	<chem>c1(ccccc1)CN2CCN(CC(=O)NN=Cc3c(O)c(CC=C)ccc3)CC2</chem>	C23H28N4O2	392.494	PAC-1
Selleck					
Chemicals	S7397	<chem>c1(cc(NC(=O)Nc2ccc(OC3ccnc(C(NC)=O)c3)cc2)ccc1Cl)C(F)(F)F</chem>	C21H16ClF3N4O3	464.825	Sorafenib
Selleck					
Chemicals	S2750	<chem>C(NC1CCOCC1)(=O)c2ccc(c3nccc(c4c[nH]nc4c5ncccc5)c3)cc2</chem>	C25H23N5O2	425.482	GW788388
Selleck					
Chemicals	S2319	<chem>C1(=O)[C@H]2[C@@]3(O2)[C@@](C)(CC[C@@]4([H])[C@]3(C)C(=O)C[C@@]5([H])[C@@]4(COC(=O)C6)[C@@]6([H])OC5(C)C)[C@H](c7ccoc7)O1</chem>	C26H30O8	470.512	Limonin
Selleck					
Chemicals	S2479	<chem>[C@H]1(O)[C@]([H])([C@H](NC([C@H]2N(C)C[C@H](CCC)C2)=O)[C@H](O)C)O[C@H](SC)[C@H](O)[C@H]1O.Cl</chem>	C18H35ClN2O6S	442.998	Lincomycin HCl
Selleck					
Chemicals	S2335	<chem>[C@@]1([H])([C@H]2O)[C@@](CO3)(CC4)[C@]5([C@@]23O)[C@H](O)[C@]4([H])C(=C)C5=O)[C@@H](O)CCC1(C)C</chem>	C20H28O6	364.433	Oridonin
Selleck					
Chemicals	S2489	<chem>C1C[C@@H](C(=O)N[C@@H](C(O)=O)Cc2ccccc2)CC[C@@H]1C(C)c(C(=O)C(c1ccc(O)cc1)=CO2)(ccc(O)c3O[C@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)c23</chem>	C19H27NO3	317.423	Nateglinide
Selleck					
Chemicals	S2346		C21H20O10	432.377	Puerarin
Selleck					
Chemicals	S2500	<chem>c1cc(CCC(=O)c2c(OC(CNCCC)O)cccc2)ccc1</chem>	C21H27NO3	341.444	Propafenone HCl
Selleck					
Chemicals	S2362	<chem>c1cc(C(CNC)O)ccc1O</chem>	C9H13NO2	167.205	Synephrine

Selleck					
Chemicals	S2512	c1nc(NC(C2=C(O)c3c(ccs3)S(=O)(=O)N2C)=O)cc1	C13H11N3O4S2	337.374	Tenoxicam
Selleck		[C@@H]1(CO)[C@H](O)[C@H](O)[C@@H](O)[C@]([H])([C@]2([H])c3c(c			
Chemicals	S2375	c(O)cc(CO)c3C(=O)c4c2ccc4O)O1	C21H22O9	418.394	Aloin
Selleck					
Chemicals	S2533	c1cc([C@@](O)([H])[C@](C)([H])NCCc2ccc(O)cc2)ccc1O.Cl	C17H22ClNO3	323.814	Ritodrine HCl
Selleck					
Chemicals	S2386	c1cc2c(C(=C3C(=O)c4c(cccc4)N3)C(=O)N2)cc1	C16H10N2O2	262.263	Indirubin
Selleck		[Br-			
]O.[C@@]1([H])[C]C@H](OC(=O)C(O)(c2sccc2)c3sccc3)C4)[N+](C)(C			Tiotropium Bromide
Chemicals	S2547	[C@]4([H])[C@H]5[C@@H]1O5	C19H24BrNO5S2	490.432	hydrate
Selleck					
Chemicals	S2401	c1(O)cc(CC(O)C([O-])=O)ccc1O.[Na+]	C9H9NaO5	220.155	Sodium Danshensu
Selleck		C1C[C@@]2(C)C(CCC[C@]3([H])[C@@]2([H])C(=O)C[C@@]4(C)[C@@]3([
Chemicals	S2559	[H])CC[C@@]4(O)C(=O)COC(=O)C=CC1=O	C23H30O6	402.481	Cortisone acetate
Selleck		[C@H]1(CO)O[C@@H](O[C@]23C[C@]([H])([C@]24COC(=O)c5ccccc5)[
Chemicals	S2410	C@](O)(O[C@H]46[H])C[C@]3(C)O6)[C@H](O)[C@@H](O)[C@@H]1O	C23H28O11	480.462	Paeoniflorin
Selleck					
Chemicals	S2576	c1c(C)c(CC2=NCCN2)c(C)cc1C(C)(C)C.Cl	C16H25ClN2	280.836	Xylometazoline HCl
Selleck					
Chemicals	S2438	c1cc(C(O)CNC)ccc1O.Cl	C9H14ClNO2	203.666	Synephrine HCl
Selleck		C1(O)C(O)C(O)C(=O)CCCCCCCCCCCCC)C(SC)OC1C(NC(C2CC(CCC)			
Chemicals	S2596	CN2C)=O)C(C)C.Cl	C34H64Cl2N2O6S	699.853	Clindamycin palmitate HCl
Selleck		c1cc2c(CC[C@]3([H])[C@@]2([H])CC[C@@]4(C)[C@@]3([H])C[C@@H](
Chemicals	S2466	O)[C@H]4O)cc1O	C18H24O3	288.381	Estriol
Selleck					
Chemicals	S2607	c1(OC)cc(OC)c(C(CCCN2CCCC2)=O)c(OC)c1.Cl	C17H26ClNO4	343.846	Buflomedil HCl
Selleck		c1cc(S(=O)(=O)c2cc3c(ccc(C(N)=O)c3Nc4cccc(OC)c4)c(C)c2)cc(C(=O)N(
Chemicals	S2620	C)C)c1	C27H26N4O5S	518.584	GSK256066
Selleck					
Chemicals	S2767	n1c(c2nc1)c(N)ncn2C	C6H7N5	149.153	3-Methyladenine
Selleck		c1ccc(OCCCN(CC(c2ccccc2)c3ccccc3)Cc4c(Cl)c(C)(F)F)ccc4)cc1CC(O)			
Chemicals	S2630	=O.Cl	C33H32Cl2F3NO3	618.513	GW3965 HCl
Selleck					
Chemicals	S2778	c1(Nc2ccc(Cl)cc2Cl)nc(C(NCC3CCOCC3)=O)c(C(F)(F)F)n1	C18H17Cl2F3N4O2	449.254	GW842166X
Selleck		c1c(C(=O)N)c(N[C@H]2CC[C@H](O)CC2)cc(n3c4c(C(=O)CC(C)(C)C4)c(C			
Chemicals	S2639	(F)(F)F)n3)c1	C23H27F3N4O3	464.481	SNX-2112 (PF-04928473)
Selleck					Tofacitinib (CP-
Chemicals	S2789	n1c(N([C@@H]2[C@@H](C)CCN(C(Cc#N)=O)C2)C)c3c([nH]cc3)nc1	C16H20N6O	312.37	690550,Tasocitinib)
Selleck					
Chemicals	S2665	c1cc(OC(C)(C)C(=O)O)ccc1C2CC2(Cl)Cl	C13H14Cl2O3	289.154	Ciprofibrate
Selleck		c1(O)cc(CCc2[nH]nc(NC(c3ccc(N4C[C@@H](C)N[C@@H](C)C4)cc3)=O)			
Chemicals	S2801	c2)cc(OC)c1	C26H33N5O3	463.572	AZD4547
Selleck					
Chemicals	S2680	c1nc2c(c3ccc(Oc4ccccc4)cc3)nn2[C@@H]5CCCN(C(=O)C=C)C5)c(N)n1	C25H24N6O2	440.497	Ibrutinib (PCI-32765)
Selleck		C1OCCN(CC(=O)N[C@@H](CCc2ccccc2)C(=O)N[C@@H](CC(C)C)C(=O)			
Chemicals	S2853	N[C@@H](Cc3ccccc3)C(=O)N[C@@H](CC(C)C)C(=O)[C@@]4(C)CO4)C	C40H57N5O7	719.91	Carfilzomib (PR-171)
Selleck					
Chemicals	S2690	c1(F)ccc(C(=O)N2C[C@@H](c3onc(c4ccc(F)cc4)n3)CCC2)cc1	C20H17F2N3O2	369.365	ADX-47273
Selleck					
Chemicals	S3018	c1(Nc2ccccc(F)(F)F)c2)ncccc1C(O)=O	C13H9F3N2O2	282.218	Niflumic acid
Selleck		C1(OC)=C(C(=O)C2=CC1=O)C[C@H](C)C[C@@H](OC)[C@H](O)[C@H]			
Chemicals	S2713	(C)C=C(C)[C@H](OC(N)=O)[C@@H](OC)C=CC=C(C)C(=O)N2	C29H40N2O9	560.636	Geldanamycin
Selleck					
Chemicals	S3032	C(O)(=O)C(C)(OCc1c(c2h(Cc3ccccc3)n1)cccc2)C	C19H20N2O3	324.374	Bindarit
Selleck					Dacomitinib (PF299804,
Chemicals	S2727	C(N1CCCC1)C=CC(=O)Nc2cc3c(ncnc3Nc4ccc(F)c(Cl)c4)cc2OC	C24H25ClFN5O2	469.939	PF299)
Selleck					
Chemicals	S4273	C(N)(=O)c1cccc(N)c1	C7H8N2O	136.151	3-Aminobenzamide
Selleck					
Chemicals	S2742	c1cc(c2cc3c(CCNc3=O)[nH]2)ccn1	C12H11N3O	213.235	PHA-767491
Selleck					
Chemicals	S8049	c1cc(Cn2c3c(cccc3)c4c2CCN(C)C4)ccc1C(=O)NO	C20H21N3O2	335.4	Tubastatin A
Selleck					
Chemicals	S2751	c1(c2c3c(c(C(=O)N)C)nn3C)C(C)C1)cnc(Nc4ccc(N5CCN(C)CC5)cc4)n2	C25H32N8O	460.575	Milciclib (PHA-848125)
Selleck					
Chemicals	S1333	c1(C(F)(F)F)ccc(OC(c2ccccc2)CCNC)cc1.Cl	C17H19ClF3NO	345.787	Fluoxetine HCl

Selleck					
Chemicals	S3070	<chem>N1(CC(N)=O)CCCC1=O</chem>	<chem>C6H10N2O2</chem>	142.156	Piracetam
Selleck					
Chemicals	S4256	<chem>c1nc(N2CCN(CCCC3C(=O)CC4(CCCC4)CC3=O)CC2)ncc1.Cl</chem>	<chem>C21H32ClN5O2</chem>	421.964	Buspirone HCl
Selleck					
Chemicals	S1189	<chem>N1=C(CN2CCO[C@H](O[C@H](c3cc(C(F)(F)F)cc(C(F)(F)F)c3)C)[C@@H]2c4ccc(F)cc4)NC(=O)N1</chem>	<chem>C23H21F7N4O3</chem>	534.427	Aprepitant
Selleck					
Chemicals	S1441	<chem>C1C(O)(C(c2ccc(O)cc2)CN(C)C)CCCC1.Cl</chem>	<chem>C17H28ClNO2</chem>	313.863	Venlafaxine
Selleck					
Chemicals	S2103	<chem>c1cc2c([C@@]3[C@H]45)[C@@](O)(CCC4=O)[C@H](N(CC6CC6)CC3)C2)c(O5)c1O.Cl</chem>	<chem>C20H24ClNO4</chem>	377.862	Naltrexone HCl
Selleck					
Chemicals	S3024	<chem>n1c(c2ccc(Cl)c2Cl)c(N)nc(N)n1</chem>	<chem>C9H7Cl2N5</chem>	256.091	Lamotrigine
Selleck					
Chemicals	S1438	<chem>[C@H](O(C(C)C)O1)(CO[C@]2(COS(=O)=O)N)[C@H]3OC(C)(C)O2][C@@H]13</chem>	<chem>C12H21NO8S</chem>	339.362	Topiramate
Selleck					
Chemicals	S3175	<chem>C(NC)C[C@H](Oc1cccc1C)c2ccccc2.Cl</chem>	<chem>C17H22ClNO</chem>	291.816	Atomoxetine HCl
Selleck					
Chemicals	S4283	<chem>c(cccc1)(C=Cc2c(cccc2)C3=CCCN(C)C)c13.Cl</chem>	<chem>C20H22ClN</chem>	311.848	Cyclobenzaprine HCl
Selleck					
Chemicals	S1259	<chem>c1cc2c([C@H](CCNC(=O)CC)CC2)c3c1OCC3</chem>	<chem>C16H21NO2</chem>	259.343	Ramelteon
Selleck					
Chemicals	S1444	<chem>c1c2c(snc2N3CCN(CCc4cc5c(NC(=O)C5)cc4Cl)CC3)ccc1.Cl</chem>	<chem>C21H22Cl2N4OS</chem>	449.397	Ziprasidone HCl
Selleck					
Chemicals	S2452	<chem>c1(C(C(NC(C)(C)C)C)=O)cc(Cl)ccc1.Cl</chem>	<chem>C13H19Cl2NO</chem>	276.202	Amfebutamone HCl
Selleck					
Chemicals	S1445	<chem>c1(c(CS(=O)=O)N)no2)c2cccc1</chem>	<chem>C8H8N2O3S</chem>	212.226	Zonisamide
Selleck					
Chemicals	S3180	<chem>[nH]1c(c2c(C[C@H]3CCCN3C)c1)ccc(CCS(c4ccccc4)(=O)=O)c2.Br</chem>	<chem>C22H27BrN2O2S</chem>	463.431	Eletriptan HBr
Selleck					
Chemicals	S4289	<chem>c1(Cl)cc(C(=O)NCCN(CC)CC)c(OC)cc1N.Cl</chem>	<chem>C14H23Cl2N3O2</chem>	336.257	Metoclopramide HCl
Selleck					
Chemicals	S1280	<chem>C1CCN(CC)C1CNC(=O)c2c(OC)cc(N)c(S(=O)=O)CC)c2</chem>	<chem>C17H27N3O4S</chem>	369.479	Amisulpride
Selleck					
Chemicals	S1614	<chem>c(sc(N)n1)(cc(OC(F)(F)F)cc2)c12</chem>	<chem>C8H5F3N2OS</chem>	234.198	Riluzole
Selleck					
Chemicals	S2459	<chem>N1c2c(cc(Cl)cc2)N=C(N3CCN(C)CC3)c4c1cccc4</chem>	<chem>C18H19ClN4</chem>	326.823	Clozapine
Selleck					
Chemicals	S1693	<chem>N1(c2c(cccc2)C=Cc3c1cccc3)C(N)=O</chem>	<chem>C15H12N2O</chem>	236.269	Carbamazepine
Selleck					
Chemicals	S3189	<chem>N1c(c2CC1=O)cccc2CCN(CCC)CCC.Cl</chem>	<chem>C16H25ClN2O</chem>	296.836	Ropinirole HCl
Selleck					
Chemicals	S1281	<chem>c1(OC)ccc(C(=O)N2CCCC2=O)cc1</chem>	<chem>C12H13NO3</chem>	219.237	Aniracetam
Selleck					
Chemicals	S1615	<chem>C(C)(N=C1N(CCCC1)C2=O)=C2CCN3CCC(c4noc5c4ccc(F)c5)CC3</chem>	<chem>C23H27FN4O2</chem>	410.484	Risperidone
Selleck					
Chemicals	S2460	<chem>[C@H]1(NCCC)Cc2c(nc(N)s2)CC1</chem>	<chem>C10H17N3S</chem>	211.327	Pramipexole
Selleck					
Chemicals	S1747	<chem>C(C)(NC(C)=C(C(=O)OCCOC)C1c2cc([N+](O-))=O)ccc2)=C1C(=O)OC(C)C</chem>	<chem>C21H26N2O7</chem>	418.44	Nimodipine
Selleck					
Chemicals	S3199	<chem>c1ccc(O[C@@H]([C@@]2([H])CNCCO2)c3ccccc3)c(OC)c1.CS(=O)(O)=O</chem>	<chem>C20H27NO6S</chem>	409.496	Reboxetine mesylate
Selleck					
Chemicals	S1330	<chem>c1c(C(COC(=O)N)COC(=O)N)cccc1</chem>	<chem>C11H14N2O4</chem>	238.24	Felbamate
Selleck					
Chemicals	S1920	<chem>c1(F)ccc(C(CCCN2CCC(O)(c3ccc(Cl)cc3)CC2)=O)cc1</chem>	<chem>C21H23ClFNO2</chem>	375.864	Haloperidol
Selleck					
Chemicals	S2493	<chem>N1c2c(cccc2)N=C(N3CCN(C)CC3)c4c1sc(C)c4</chem>	<chem>C17H20N4S</chem>	312.433	Olanzapine
Selleck					
Chemicals	S1898	<chem>c1cc2c(N=CC2C(=O)OC3C[C@]([H])(N(C)[C@]4([H])C3)CC4)cc1.Cl</chem>	<chem>C17H21ClN2O2</chem>	320.814	Tropisetron
Selleck					
Chemicals	S3212	<chem>C(NCCN1CCOCC1)(=O)c2ccc(Cl)cc2</chem>	<chem>C13H17ClN2O2</chem>	268.739	Moclobemide (Ro 111163)
Selleck					
Chemicals	S1332	<chem>c1cc2c(C(=O)N(C)Cc3n2cnc3C(OC)=O)cc1F</chem>	<chem>C15H14FN3O3</chem>	303.288	Flumazenil
Selleck					
Chemicals	S1975	<chem>c1cc2c(NC(=O)CC2)cc1OCCCCN3CCN(c4cccc(Cl)c4)CC3</chem>	<chem>C23H27Cl2N3O2</chem>	448.385	Aripiprazole
Selleck					
Chemicals	S2541	<chem>C(CCN(C)C)N1c2c(cccc2)CCc3c1cc(Cl)cc3.Cl</chem>	<chem>C19H24Cl2N2</chem>	351.313	Clomipramine HCl
Selleck					
Chemicals	S2456	<chem>c1ccc2c(Sc3c(cc(Cl)cc3)N2CCCN(C)C)c1.Cl</chem>	<chem>C17H20Cl2N2S</chem>	355.325	Chlorpromazine HCl

Selleck									
Chemicals	S4058	C1CN(CCC)[C@H](C(Nc2c(C)cccc2C)=O)CC1.Cl	C17H27ClN2O	310.862	Ropivacaine HCl				
Selleck									
Chemicals	S1356	C1(=O)OCCCN1[C@@H](CC)C(=O)N	C8H14N2O2	170.209	Levetiracetam				
Selleck									
Chemicals	S2016	C1c2c(cccc2)C3N(CCN(C)C3)c4c1cccn4	C17H19N3	265.353	Mirtazapine				
Selleck									
Chemicals	S3005	[C@@H]1(c2ccc(F)cc2)CCNC[C@H]1COc3ccc4c(OCO4)c3.Cl	C19H21ClFNO3	365.826	Paroxetine HCl				
Selleck									
Chemicals	S2525	C1(c2cccc2)(c3ccccc3)C(=O)NC(=O)N1	C15H12N2O2	252.268	Phenytoin				
Selleck									
Chemicals	S4202	Cl.c1cc(OC)c(OC)cc1C(C(C)C)(C#N)CCCN(CCc2cc(OC)c(OC)cc2)C	C27H39ClN2O4	491.063	Verapamil HCl				
Selleck									
Chemicals	S1391	N1(C(=O)N)c2c(cccc2)CC(=O)c3c1cccc3	C15H12N2O2	252.268	Oxcarbazepine				
Selleck									
Chemicals	S2084	c1cc2c(cccc2)c(O)[C@H](c3cccs3)CCNC)c1.Cl	C18H20ClNOS	333.876	Duloxetine HCl				
Selleck									
Chemicals	S3021	n1(c2ccc(Cl)cc2Cl)c(c3ccc(Cl)cc3)c(C)c(C)(NN4CCCC4)=O)n1	C22H21Cl3N4O	463.787	Rimonabant				
Axon		COc1cccc(c1c1cc(nn1c1ccc(cc1C(C)C)C(=O)N(CCCN(C)C)C)C(=O)NC1(C(=O)O)C2CC3CC1CC(C2)C3)OC	C39H51N5O6	685.85	SR 142948				
Medchem	1255	ONC(=O)C[C@H](C(=O)N)[C@@H](C(C)(C)C)C(=O)N[C@@H](c1ccccc1)C)CCCc1ccc(c(c1)C)c1cccc1	C34H43N3O4	557.72	UK 356618				
Axon	2111								
Medchem									
Cayman									
Chemical	10879	O=C(Oc1ccccc1C(C)C)NCCc1ccc2c(c1)cccc2	C22H23NO2	333.42	JW 480				
Cayman									
Chemical	13942	Nc1cccc(c1)Cn1ncc2c(c1=O)n(C)c1c2sc(c1)S(=O)C	C17H16N4O2S2	372.46	ML-265				
Cayman									
Chemical	15016	COc1ccc2c(c1)ccc(c2)OCC1(CN(C1)C(=O)c1ccc(cc1)F)C(=O)O	C23H20FNO5	409.41	PF-04418948				
Cayman		CCOC(=O)[C@H](CC(=O)N)[C@H](C(=O)N)[C@H](c1ccccc1)C(=O)OCC	C27H35N3O6S	529.65	Ezatiostat				
Chemical	16248)CSCc1ccccc1)N							
Cayman									
Chemical	17924	O=C1CCC(=O)C1C(=O)c1ccc(cc1[N+](=O)[O-])C(F)(F)F	C14H10F3NO5	329.23	Nitisinone				
Chem-									
Impex	22427	O=C(C(=O)c1ccc(cc1)Cl)c1ccc(cc1)Cl	C14H8Cl2O2	279.12	4,4'-Dichlorobenzil				
Cayman									
Chemical	9001740	CCCCCCCCCCCCC(=O)NCCO	C17H35NO2	285.47	Ethanolamide				
Cayman		CC[C@@H]1/C=C/C(=O)/C[C@H](C)C[C@H](OC)[C@H]2O[C@](O)([C@@H](C[C@@H]2O)C)C(=O)C(=O)N2[C@H](C(=O)O)[C@@H](C[C@@H](C[C@@H](C(=O)O)C)/C=C/[C@@H]1CC[C@H](C[C@@H](C1)OC)O)/C)CCC	C43H69NO12	792	Ascomycin				
Axon	11309	COc1cc(C(C)C)c2c(c1)S(=O)(=O)N(C2=O)COc1cc(=O)n2c(n1)c(OCCN1CCCC1)ccc2	C27H32N4O7S	556.63	SSR 69071				
Medchem	1269								
Axon									
Medchem	2118	OC(=O)[C@H]1C[C@@H]1C(=O)c1ccc(c(c1)Cl)Cl	C11H8Cl2O3	259.09	UPF 648				
Cayman		CO[C@@H]1[C@@H](CC[C@@H]2([C@H]1[C@@H]1(C)O[C@@H]1CC=C(C)C)CO2)OC(=O)/C=C/C=C/C=C/C(=O)O	C26H34O7	458.54	Fumagillin				
Chemical	11332	CCc1cc(C)[nH]c(=O)c1CNC(=O)c1cc(cc2c1cnn2C(C)C)c1ccnc(c1)N1CCN	C31H39N7O2	541.69	GSK343				
Cayman	14094	(CC1)C							
Cayman		CCOC(=O)N1[C@H](CC)C[C@@H](c2c1ccc(c2)C(F)(F)F)N(C(=O)OC)Cc1cc(cc(c1)C(F)(F)F)C(F)(F)F	C26H25F9N2O4	600.47	Torcetrapib				
Chemical	15028	COc1ccc(cc1)C[C@@H](C(=O)N)[C@H](C(=O)[C@@H]1(C)CO1)Cc1ccccc1)NC(=O)[C@@H](NC(=O)CN1CCOCC1)C	C31H40N4O7	580.67	ONX 0914				
Cayman									
Chemical	17995	CCCN1CCN(CC1)c1ccc(cc1)C(=O)NC1(CCCCC1)C(=O)NCC#N	C23H33N5O2	411.54	Balicatib				
AstaTech	41123	OC(=O)CNC(=O)[C@@H](Cc1ccccc1)CN1CC[C@@H]([C@H](C1)C)(C)c1ccc(c1)O	C25H32N2O4	424.53	alvimopan				
Cayman									
Chemical	9002002	Clc1ccc2c(c1)cc(a2)C(=O)NNS(=O)(=O)c1ccccc1C(F)(F)F	C16H10ClF3N2O4S	418.77	BCATc Inhibitor 2				
Axon		O[C@@H]([C@@H]([C@@H](NC(=O)c1cc(cc(c1)N(S(=O)(=O)C)C)C(=O)N)[C@@H](c1ccccc1)C)Cc1ccccc1)CNC1CC1	C31H38N4O5S	578.72	BACE-1inhibitor				
Medchem	1125								
Axon									
Medchem	1383	OC(=O)C(=O)c1cn(c2c1cc(cc2)c1ccc(cc1)OC(F)(F)F)Cc1ccccc1	C24H16F3NO4	439.38	Tiplaxtinin				
CHES									
Fine									
Organic	2132	Oc1ccc(cc1)c1ccc2c(c1=O)ccc(c2O)O	C15H10O5	270.24	7,8-Dihydroxy-3-(4-hydroxy-phenyl)-chromen-4-one				
Cayman									
Chemical	11931	O=C(OC(C)(C)C)CN(Cc1ccc(s1)[N+](=O)[O-])Cc1ccc(cc1)Cl	C18H21ClN2O4S	396.89	GSK4112?				
Cayman									
Chemical	14406	CCN(c1nc(N)c(nc1Cl)C(=O)NC(=N)N)C(C)C	C11H18ClN7O	299.76	Amiloride				

Cayman		O[C@H]1C[C@@H](C[C@H]1COS(=O)(=O)N)n1ccc2c1nnc2N[C@H]1C				
Chemical	15217	Cc2c1cccc2	C21H25N5O4S	443.52	MLN4924	
Cayman						
Chemical	16480	CCN1CCN(CC1)c1nc2CCCCCc2c(c1)c1ccc(cc1)F	C23H30FN3	367.5	Blonanserin	
Cayman						
Chemical	17999	CCN(c1ccc(cc1)/C=N/NC(=O)c1ccc(cc1)O)CC	C18H21N3O2	311.38	DY 131	
AstaTech	41281	BrC1csc(c1)COc1nc(N)nc2c1nc[nH]2	C10H8BrN5OS	326.17	LOMEGUATRIB	
Cayman		CCOC(=O)/C=C/[C@@H](NC(=O)[C@@H](NC(=O)[C@H](C(C)C)NC(=O)				
Chemical	10007713)c1cccc(c1C)O)CO)CC(C)C	C26H39N3O7	505.6	HMB-Val-Ser-Leu-VE	
Key		O[C@@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@@H](C(=O)N)C)CCCNC(=N)N)CC(C)				
Organics	HS-2008	C)CCCNC(=O)N)Cc1ccc(cc1)O)NC(=O)[C@@H](Cc1ccnc1)NC(=O)[C@@H](Cc1ccc(cc1)C)NC(=O)[C@@H](Cc1ccc2c(c1)cccc2)NC(=O)C	C70H92ClN17O14	1431.04	Cetrotrelax	
Axon		CCOC(=O)N[C@@H]1CC[C@@H]2[C@@H](C1)C[C@@H]1[C@H]([C@H]2/C=C/C/c2ccc(cn2)c2ccc(c2)F)[C@H](OC1=O)C				
Medchem	1755		C29H33FN2O4	492.58	SCH 530348	
Axon						
Medchem	2148	C[C@@H]1CN(C[C@H]1c1[nH]c(=O)c2c(n1)n(nc2)C1CCOCC1)Cc1ncccn1	C20H25N7O2	395.46	PF 04447943	
Cayman						
Chemical	12018	Clc1cc(COC(=O)N2CCN(CC2)CCC(=O)c2ccc3c(c2)oc(=O)[nH]3)cc(c1)Cl	C22H21Cl2N3O5	478.33	PF-8380	
Cayman					N-(p-amylicinnamoyl)	
Chemical	14531	CCCCCc1ccc(cc1)/C=C/C(=O)Nc1ccccc1C(=O)O	C21H23NO3	337.41	Anthranilic Acid	
Cayman						
Chemical	15362	OC(=O)/C(=N/Nc1sc(c(n1)c1ccc(c(c1)Cl)Cl)/Cc1ccccc1[N+])(=O)[O-]	C18H12Cl2N4O4S	451.28	4EGI-1	
Acros						
Organics						
(US)	17397	CCCCCCCCCCC(=O)O	C11H22O2	186.29	Undecanoic acid, 99%	
Cayman						
Chemical	18002	Oc1cc2c3SCCNC(=O)c3sc2cc1	C11H9NO2S2	251.32	kb NB 142-70	
AstaTech	42077	C[C@H](Nc1ncnc2c1sc2C)CN1CCN(CC1)S(=O)(=O)c1ccc(c(c1)Cl)Cl	C20H23Cl2N5O2S2	500.46	LPA2 ANTAGONIST 1	
Cayman						
Chemical	10008671	CCCc1nn(c2c1[nH]c(nc2=O)c1cc(ccc1OCC)S(=O)(=O)N1CCN(CC1)C)C	C22H30N6O4S	474.58	Sildenafil	
Axon						
Medchem	2097	COc1cccc(c1)c1cn(c2c1c(N)ncn2)c1ccc(cc1)CCN1CCC(CC1)O	C26H29N5O2	443.54	CGP77675	
Axon						
Medchem	1792	Clc1cccc(c1)OCc1nn(c2c1c(N)ncn2)C1CCOCC1	C17H18ClN5O2	359.81	PF 4800567	
Axon						
Medchem	2270	BrC1cccc(c1)NC(=O)c1cccc(c1)S(=O)(=O)N1CCCCC1	C19H21BrN2O3S	437.35	AK 7	
Cayman						
Chemical	12046	COC(=O)c1cnn(c1/C=N/NC(=S)NC(C)(C)C)c1ccc(cc1F)F	C17H19F2N5O2S	395.43	CID-2745687	
Cayman						
Chemical	14603	Fc1nccc(c1)c1ccc(c(c1)C(=O)Nc1ccnc1)OCc1ccccc1	C24H18FN3O2	399.42	GSK2578215	
Cayman		CCCS1c1n([C@@H]2[C@H]2c2ccc(c(c2)F)F)c2c(n1)n(n2)[C@@H]1C[C@@H]([C@H]([C@H]1O)O)OCCO				
Chemical	15425		C23H28F2N6O4S	522.57	Ticagrelor	
Cayman						
Chemical	17501	CCCCCCC(=O)c1c(O)cc(cc1CC(=O)OCC)O	C18H26O5	322.4	Cytosporone B	
Cayman						
Chemical	18377	COc1cccc(c1)c1ccc(c(c1)F)NC(=O)C1=C(CCC1)C(=O)O	C20H18FNO4	355.36	Vidofludimus	
AstaTech	55318	OCCN(CCCOc1ccc2c(c1)ncnc2Nc1n[nH]c(c1)CC(=O)Nc1cccc(c1)F)CC	C26H30FN7O3	507.56	AZD1152-HQPA	
Cayman						
Chemical	10010206	CCc1c(c2ccccc2)c(nn1c1cccc1c1cccc(c1)OCC(=O)O)c1ccccc1	C31H26N2O3	474.55	BMS309403	
Axon						
Medchem	1279	O=C/C=C/C/c1ccnc1)NCCCC1CCN(CC1)C(=O)c1ccccc1	C24H29N3O2	391.5	FK866	
Axon						
Medchem	1907	Clc1cc2nc(c(nc2cc1Cl)NC(C)(C)C)S(=O)(=O)C	C13H15Cl2N3O2S	348.25	GLP-1R agonist DMB	
Axon		N#C/C(=Clc1ccc(c(c1)OC)OCc1ccc(cc1C(F)(F)F)C(F)(F)F)/C(=O)Nc1nnc(s1)C(F)(F)F				
Medchem	2337		C23H13F9N4O3S	596.42	XCT 790	
Cayman						
Chemical	12072	FC(C(C(F)(F)F)c1ccc(cc1)NS(=O)(=O)c1cccs1)O)(F)F	C13H9F6NO3S2	405.34	SR 3335	
Cayman						
Chemical	14745	CCCCCCCn1cc(c2c1ccc(c2)c1cccc(c1)C)CC(=O)N	C25H32N2O	376.53	Cysmethynil	
Cayman						
Chemical	15487	Clc1ccc(c(c1)/C(=N/NC(=O)c1cccc(c1)S(=O)(=O)N1CCOCC1)/C)O	C19H20ClN3O5S	437.9	SP2509	
Cayman		Fc1ccc(cn1)NC(=O)[C@@]1(C)CCCN1c1nc(Nc2n[nH]c(c2)C2CC2)c2n(n1)ccc2				
Chemical	17505		C23H24FN9O	461.49	BMS 754807	
Cayman						
Chemical	18503	NC(=O)Nc1cc(Cl)ccc1OCC(=O)N1CCN(C[C@H]1C)Cc1ccc(cc1)F	C21H24ClFN4O3	434.89	BX 471	

AstaTech Cayman Chemical	70704	CCCC[C@@]1(O)CC[C@H]2[C@H](O1)CC(=O)[C@@H]2CCCCCCC(=O)O)(F)F	C20H32F2O5	390.46	LUBIPROSTONE
AstaTech Cayman Chemical	10010740	O=C1CC(=NN1c1cccc1)c1ccc(cc1)[N+](=O)[O-]	C15H11N3O3	281.27	CAY10550
Axon	16257	Oc1ccc(cc1)C[C@H]1C(=O)N(C[C@H]2N1C(=O)CCN2C(=O)NCc1cccc1)Cc1cccc2c1cccc2	C33H32N4O4	548.6	ICG-001
Medchem Advanced ChemBlocks	1985	CN[C@H](C(=O)N[C@H]1CN(CC[C@@H]2N(C1=O)[C@@H](CC2)C(=O)NC(c1cccc1)c1cccc1)C(=O)CC(C)C	C32H43N5O4	561.71	AT 406
Cayman	10259	OC(=O)c1ccc(nc1)C#Cc1ccc2c(c1)C(C)(C)CCS2	C19H17NO2S	323.41	AGN 190299
Acros Organics (US)	13217	N#Cc1cccc(c1c1[nH]c2c(n1)c1ccc(cc1c1c2cccc1)Cl)C#N	C23H11ClN4	378.81	MF63
Cayman Chemical	14772	Clc1ccc(c(c1)Cl)O	C6H4Cl2O	163	2,4-Dichlorophenol, 99%
Cayman Chemical	16207	C/C=C(\C(=O)O[C@H]1C(=C[C@]23[C@]1(O)[C@H](O)C(=C[C@H](C3=O)[C@H]1[C@@H](C[C@H]2C)C1(C)CO)C)/C	C25H34O6	430.53	Ingenol-3-angelate
Cayman Chemical	17703	CCCCNc1ncc(c(n1)N[C@@H]1CC[C@H](CC1)O)c1ccc(cn1)CN1CCOCC1	C24H36N6O2	440.58	UNC2250
Chem-Impex	21985	O=c1c(O)c(oc2c1cccc2)c1cccc1	C15H10O3	238.24	3-Hydroxyflavone
AstaTech Cayman Chemical	78259	Fc1cccc(c1)c1ccc(cn1)C(=O)NC1CCN(CC1)CC(F)(F)F	C19H19F4N3O	381.37	HPGDS-INHIBITOR-1
Cayman Chemical	10016	O=C[C@@H](NC(=O)[C@@H](NC(=O)[C@H](C)C)NC(=O)[C@H](Cc1ccc(cc1)O)NC(=O)C)CC(=O)O	C23H32N4O8	492.5	Ac-YVAD-CHO
Cayman Chemical	15215	COc1ccc2c(c1)[nH]c1c2C[C@@H]2N([C@H]1CC(C)C)C(=O)[C@@H](NC2=O)CCC(=O)OC(C)(C)C	C26H35N3O5	469.6	ko143
Axon Medchem	1992	NC(=O)c1cnc(nc1NCc1cccc1)NCCc1ccc(c(c1)Cl)O	C20H20ClN5O2	397.86	AS 1517499
Advanced ChemBlocks	10265	O=C(N1CCC[C@@](C1)(Cc1cccc1)C(=O)N(N(C)C)[C@H](NC(=O)C(N)(C)C)Cc1c[nH]c2c1cccc2	C31H42N6O3	546.7	Anamorelin
Cayman Chemical	13243	BrC1ccc(c(c1)/C=N/NC(=O)C)Sc1nc2c([nH]1)cccc2)C)O	C17H15BrN4O2S	419.3	KH7
Cayman Chemical	14806	CCOCc1nc2c(n1CC(O)(C)C)c1cccc1nc2N	C17H22N4O2	314.38	R-848
Cayman Chemical	16239	COc1ccc(cc1NS(=O)(=O)c1cc(C)cc(c1O)Cl)c1cccc1	C19H15Cl2NO4S	424.3	BMS 303141
Cayman Chemical	17737	CNC(=O)c1ccc(cc1)Nc1ncc(c(n1)NCc1nccnc1N(S(=O)(=O)C)C(F)F)	C20H21F3N8O3S	510.49	Defactinib
Chem-Impex	22028	O=c1cc(oc2c1ccc1c2cccc1)c1cccc1	C19H12O2	272.3	a-Naphthoflavone
ChemBridge	4403033	OC(=O)CCn1nnc2c1cccc2	C9H9N3O2	191.19	3-(1H-1,2,3-benzotriazol-1-yl)propanoic acid
Cayman Chemical	17642	CC(OC(=O)N1CCC(CC1)Oc1nccnc1c1cnn2c1ccc(cc1F)S(=O)(=O)C)C	C21H24FN5O5S	477.5	APD668
Selleck Chemicals	S7488	Cc1cc(ccc1Nc1nc(NC2CCCC2)c2c(n1)[nH]cn2)N1CCOCC1	C22H29N7O	407.91	MPI-0479605-HCL
Tocris	3411	CC1(C)CCC(C)(C)C2=CC(=CC=C12)C3(OCCO3)C4=CC(=C(C=C4)C(O)=O	C24H28O4	380.477	SR 11237; SR-11237 FR 180204; 5-(2-PHENYLPYRAZOLO[1,5-A]PYRIDIN-3-YL)-1H-PYRAZOLO[3,4-C]PYRIDAZIN-3-AMINE;
Tocris	3706	NC1=N[NH]C2=C1C=C(N=N2)C3=C4C=CC=C[N]4N=C3C5=CC=CC=C5	C18H13N7	327.343	FR-180204
Tocris	4088	CC1=CC(=C(C)[N]1C2=CC=C(F)C=C2)C(=O)CN3CCCC3	C18H21FN2O	300.371	IU1; IU-1

						olanzapine ODT; Zyprexa 15mg; Lanzapin; Zyprexa; LY-170053; Ran- olanzapine Ir; Zyprexa - 7.5mg; Deprex; Lapozan; Olanzapine-odt; Zyprexa Velotab; Zyprexa - 10mg; Ipg-olanzapine ODT; Olanzapine and Fluoxetine; Act Olanzapine ODT; Apisco; Sandoz Olanzapine ODT; Act Olanzapine; Egolanza; Mar-olanzapine ODT; Teva-olanzapine; Van-olanzapine; CO Olanzapine; Jolyon-MD; Zyprexa Zydys; Ran- olanzapine ODT; Apo- olanzapine ODT; Nu- olanzapine; Caprilon; Olanzapine; Ipg- olanzapine; Olansek; 2- methyl-4-(4-methyl-1- piperaziny)-10H- thieno[2,3- b][1,5]benzodiazepine; Jamp Olanzapine Fc; C07322; Olanzapinum; Accel-olanzapine; Ran- olanzapine; Abbott- olanzapine ODT; Elynza; PMS-olanzapine; Mar- olanzapine; OLANZAPINE; Zyprexa Intramuscular; Sandoz Olanzapine; PMS- olanzapine ODT; Mylan-
Tocris	4349	CN1CCN(CC1)C2=NC3=CC=CC=C3NC4=C2C=C(C)S4	C17H20N4S	312.432		
Tocris	3676	CC(F)(F)CN1CCOC2=C([N](N=C2C1=O)C3=CC=CC=C3Cl)C4=CC=C(C)C =C4	C21H17Cl2F2N3O2	452.281	PF-514273	
J & W PharmLab					(S)-2-(2-Methylpyrrolidin-2- yl)-1H-benzimidazole-4- carboxamide	
LLC	75R0522S	NC(=O)c1cccc2c1nc([nH]2)[C@]1(C)CCCN1	C13H16N4O	317.21		
Cayman						
Chemical	18010	Cc1cnc(nc1NCc1ccc(cc1)n1ncc1)c1cccc1C(C)C	C23H24N6	384.48	ML-323	
Cayman						
Chemical	17034	OC[C@H]1CCCN1Cc1ccc(cc1)COc1cc(C)cc(c1)CS(=O)(=O)c1cccc1	C27H31NO4S	465.6	PF-543	
Medchem						
Express	HY-15846	NC(=O)C[C@]1([H])N=C(c2ccc(cc2)Cl)c2c(n3c1nnc3C)sc(c2C)C	C19H18ClN5OS	399.9	CPI-203	
Medchem		CN(CC(=O)N)[C@]1([H])(NC(=O)c1ccc(c(c1)Cl)OC(C)C)Cc1ccc(cc1)c1nc2n				
Express	HY-10299	(c1)cccc2[C@]1([H])(O)C)C	C32H38ClN5O4	592.13	GSK-923295	
					AM 80; Tamibaro; Tamibarotene; OMS- 0728; tamibarotene; TM- 411; TOS-80; TOS-80T; TAMIBAROTENE; retinobenzoic acid; Amnoid; Amnoleuk; INNO-507; NSC-608000; D01418; Amnolake; Am 80; AM-80; Z-208; C12864	
Tocris	3507	CC1(C)CCC(C)(C)C2=C1C=CC(=C2)NC(=O)C3=CC=C(C=C3)C(O)=O	C22H25NO3	351.439		

						BF 2649 hydrochloride; pitolisant; TIPROLISANT; Pitolisant hydrochloride; Tiprolisant; Pitolisant; pitolisantum; BF-2649; Tiprolisant hydrochloride; FUB-649; Wakix;
Tocris	3743	<chem>ClC1=CC=C(C(CCCOCCCN2CCCCC2)C=C1</chem>	C17H26ClNO	295.847	BF 2.649	
Tocris	4100	<chem>CC1=C(C=C(C([N]1CCCN2CCOCC2)C3=CC=CC=C3)C(=O)NC4=CC=CC(=C4)C(F)(F)F</chem>	C26H28F3N3O2	471.515	HC 067047; HC-067047 Bicifadine hydrochloride; Bicifadine; CL-220075; BICIFADINE HYDROCHLORIDE; BICIFADINE; DOV- 220075; NIH-9542; D03110; Bicifadine HCl;	
Tocris	4357	<chem>CC1=CC=C(C=C1)C23CNCC2C3</chem>	C12H15N	173.254	MCV-4147 Tacrine; Cognex; C01453; 1,2,3,4- tetrahydroacridin-9-amine; TACRINE HYDROCHLORIDE; Tetrahydroaminoacridine; Tacrine hydrochloride; Tacrine HCl; Cl-970; THA; tacrina; THA.HCl; Tacrin hydrochloride; Tacrinum; Talem; TACRINE; Tetrahydroaminacrine; OROS-tacrine; tacrine;	
Tocris	965	<chem>NC1=C2CCCCC2=NC3=CC=CC=C13</chem>	C13H14N2	198.264	Tacrin 4-(5-(3- Hydroxyphenyl)thiophen-2- yl)-2-methylphenol	
Bide Pharmatec h	BD289516	<chem>Oc1cccc(c1)c1ccc(s1)c1ccc(c(c1)C)O</chem>	C17H14O2S	282.36		
Cayman Chemical	19186	<chem>CN(C[C@H](c1cccc1)NC(=O)N1Cc2c(C1(C)C)[nH]nc2Nc1nc(C)nc2c1scc2)</chem>	C25H30N8OS	490.62	PF-3758309	
Cayman Chemical Medchem	19932	<chem>OC[C@H](c1cccc(c1)Cl)NC(=O)c1[nH]cc(c1)c1nc(ncc1C)Nc1ccc(cc1Cl)F</chem>	C24H20Cl2FN5O2	500.35	TCS ERK 11e	
Express	HY-18072	<chem>O=C(N1CCc2c1ccc(c2)c1cn(c2c1c(N)ncn2)C)Cc1cccc(c1)C(F)(F)F</chem>	C24H20F3N5O	451.44	GSK2606414	
AbovChem	HY-18630	<chem>C=CCN(CCCCCCOc1ccc(c(c1)F)C(=O)c1ccc(cc1)Br)C</chem>	C23H27BrFNO2	448.37	Ro 48-8071 KU 55933; KU-55933; KU- 0064 XAV 939; XAV939; NVP- XAV-939; XAV-939	
Tocris	3544	<chem>O=C1C=C(C(O(C=C1)C3=C2SC4=C(SC2=CC=C3)C=CC=C4)N5CCOCC5</chem>	C21H17NO3S2	395.495		
Tocris	3748	<chem>OC1=C2CSCCC2=NC(=N1)C3=CC=C(C(C=C3)C(F)(F)F</chem>	C14H11F3N2OS	312.31		

					Probenecid; Probenecide; Probalan; Probampicin; Benemid Tab 500mg; Probenecida; Probenecid; 4-(N,N-Dipropylsulfamoyl)benzoic acid; Benemid; Probenecid acid; Benuryl; Proben; Probenecidum; probenecid; Probecid; 4-((Dipropylamino)sulfonyl)benzoic acid; C07372; Benecid; D00475; Probenecid and Colchicine; P-(Dipropylsulfamoyl)benzoic acid; 4-(Di-N-propylsulfamoyl)benzoic acid; probenecidum; PROBENECID
Tocris	4107	<chem>CCCN(CCC)[S](=O)(=O)C1=CC=C(C(=C1)C(=O)O)</chem>	C13H19NO4S	285.359	Bosutinib; SKI-606; Bosulif; Bosulif; Bosutinib; D03252; BOSUTINIB; bosutinib.H2O; bosutinib hydrate; bosutinibum; SKI 606; bosutinib; 4-((2,4-Dichloro-5-methoxyphenyl)amino)-6-methoxy-7-(3-(4-methyl-1-piperazinyl)propoxy)-3-quinolinecarbonitrile; Bosutinib Monohydrate; PF-5208763; Bosutinib monohydrate
Tocris	4361	<chem>OCC1=C(Cl)C=C(Cl)C(=C1)NC2=C3C=C(OC)C(=CC3=NC=C2C#N)OCCC</chem>	C26H29Cl2N5O3	530.446	
Apollo Scientific	BI TP1545	<chem>N4CCN(C)CC4OC(=O)C[C@@H]1NC(=O)CNC(=O)[C@H](CCCCNC(=N)N)NC(=O)CCSC[C@H](NC(=O)[C@H]2N(C(=O)[C@@H](NC1=O)Cc1c[nH]c3c1cccc3)CCC2)C(=O)N</chem>	C35H49N11O9S2	831.96	Human Eptifibatide
AstaTech Cayman Chemical	F 16272 10170	<chem>O[C@H]1CCC2(C(=CC[C@H]3[C@@H]2CC2=C(C)[C@]4(CC[C@@H]32)O[C@@H]2[C@H]([C@H]4C)NC[C@H](C2)C)C1)C</chem>	C27H41NO2	411.62	CYCLOPAMINE
Axon		<chem>OB(CCSC[C@@H](C(=O)O)N)O</chem>	C5H12BNO4S	193.03	BEC
Medchem	2003	<chem>COc1cccc(c1C1=NCc2c(c3c1cc(Cl)cc3)nc(nc2)Nc1ccc(c(c1)OC)C(=O)O)F</chem>	C27H20ClFN4O4	518.92	MLN 8237
Medchem Express	HY-16768	<chem>OC(=O)Cc1c(C)n(c2c1ccc2)Cc1ccc(cc1C(F)(F)F)S(=O)(=O)C</chem>	C19H17F3N2O4S	426.41	Fevipirant 4-(6-(4-(piperazin-1-yl)phenyl)pyrazolo[1,5-a]pyrimidin-3-yl)quinoline
ChemShuttle	109785	<chem>N1CCN(CC1)c1ccc(cc1)c1cnc2n(c1)ncc2c1ccnc2c1cccc2</chem>	C25H22N6	406.48	

					zirconium imido; Histamine; Histamine Dihydrochloride; Histamine diphosphate monohydrate; imido vanadium; Alo Therapeutic Massage Pain Relieving; Histamine dihydrochloride; titanium imido dichloride; histamine; histaminium; HISTAMINE HYDROCHLORIDE; HD- O; Arthritis Relief; niobium imido; rhodium imido; Imido; Histamine Phosphate; Histamine Phosphate Injection USP, 1mg/ml; Histamine phosphate; Histamine biphosphate; MX-8899; Histamine diphosphate; Bichlorhydrate d'histamine; Histamine Positive skin test control; HISTAMINE DIHYDROGEN PHOSPHATE; Imido titanium; HISTAMINE; b- Aminoethylglyoxaline; titanium imido; histamine amine; Dr. Freds Miracle Rub; IMIDO DIPHOSPHATE; Histatrol; Histamine Phosphate Injection USP Liq Sc; Histaminium; HISTAMINE
Tocris	3545	NCCC1=C[NH]C=N1	C5H9N3	111.145	
Tocris	3793	OC(=O)C1=C(NC(=O)N2CCC(CC2)C3=C(C=CC=C3)C(F)(F)F)C=CC=C1	C20H19F3N2O3	392.372	A 1120; A-1120; 2-[(4-{2-(trifluoromethyl)phenyl}piperidin-1-yl)carbonyl]amino]benzoic acid
Tocris	4152	4	C21H14ClFN2O2	380.799	TMN 355
Tocris	4370	C1=CN=C(C=C1)NC4=NC2=C(C(CCC3=N[NH]C=C23)S4	C14H13N5S	283.352	TC-N 22A 3-((4-(trifluoromethyl)phenyl)amino)benzoic acid
Oxchem Axon	AX8288312	OC(=O)c1cccc(c1)Nc1ccc(cc1)C(F)(F)F	C14H10F3NO2	281.23	
Medchem Cayman	1130	O=C(N1CCCC1)Nc1cccc(c1)Nc1ccc(c(n1)NCCC1c[nH]cn1)Br	C20H23BrN8O	471.35	BX 912
Chemical Bide Pharmatec	18095	CNc1nc(cc(n1)c1ccc2c(c1)[nH]nc2N)N1C[C@H](CC[C@H]1C)C(=O)NC1CC	C25H34N8O	462.59	GSK2334470
h Medchem	BD237663	COc1cccc(c1c1ccc(cc1)C[C@@H](C(=O)O)NC(=O)c1c(Cl)cccc1Cl)OC	C24H21Cl2NO5	474.33	TR-14035
Express	HY-11004	N#CC(c1cccc(c1)C(=O)Nc1ccc(c(c1)Nc1ccc2c(c1)c(=O)n(cn2)C)C)(C)C	C27H25N5O2	451.52	AZ 628 1-(5-(tert-butyl)isoxazol-3-yl)-3-(4-(7-(2-morpholinoethoxy)benzo[d]imidazo[2,1-b]thiazol-2-yl)phenyl)urea
ChemShutt le	105147	O=C(Nc1noc(c1)C(C)(C)C)Nc1ccc(cc1)c1cn2c(n1)sc1c2ccc(c1)OCCN1CCO	C29H32N6O4S	560.67	

						Dopamine Hydrochloride; dopaminium cation; Hydroxytyramine; Dopamine hydrochloride; Intropin; DA; Dopamina; C03758; Dopamine HCl; 4- (2-Aminoethyl)pyrocatechol; Dynatra; dopamine; Revimine; Dopamine Hcl Inj 4%; DOPAMINE HYDROCHLORIDE; 2- (3,4-Dihydroxyphenyl)ethylami ne; 4-(2-Aminoethyl)catechol; Tensamin; Dopaminum; Dopamine; Hydroxytyramin; Intropin Injection 40mg/ml; Dopamine Hydrochloride and Dextrose; DOPAMINE; dopaminium(1+); dopaminum; Rascordin; Sabax Dopamin; Dopamin- Natterman; Deoxyepinephrine; Dopamine methiodide; Oxytyramine; 3- Hydroxytyramine; Dophamine; Dopamine Hcl; 3,4-Dihydroxyphenethylamine; 4-(2-Aminoethyl)-1,2- benzenediol; 4-(2-Aminoethyl)benzene-1,2- diol; dopamina; Dopamin
Tocris	3548	NCCC1=CC(=C(O)C=C1)O	C8H11NO2	153.178		
Tocris	3826	OC1=C(C2=C(C=C1)C(=O)C=C(O2)C3=CC=CC=C3)O	C15H10O4	254.238	7,8-Dihydroxyflavone; 7,8-DIHYDROXYFLAVONE;	
Tocris	4171	FC1=CC(=CC=C1)N2CNC(=O)C23CCN(CCNC(=O)C4=CC5=CC=CC=C5C=C4)CC3	C26H27FN4O2	446.517	7,8-Dihydroxyflavone VU 0364739 hydrochloride; VU-0364739	
Tocris	4427	CC(C)COC1=CC=C(C=C1C#N)C2=NC(=C(S2)C(O)=O)C	C16H16N2O3S	316.375	Febuxostat; febuxostat; Febuxostat potassium; Adenuric; Febric; Febuxostat; Feburic; Uloric; TEI-6720; Febuxostat lysine salt; Febuxostat triethanolamine salt; Febuxostat sodium; FEBUXOSTAT; TMX-67; Febuxostat choline salt; Febuxostat tromethamine; febuxostatium; Febuxostat triethylamine salt	
Key Organics/B IONET - BioChem als Stock	SS-4313	CCCCCCCCCCCCCOc1ccc(o1)C(=O)O	C19H32O4	324.45	TOFA, RMI 14514	

Cayman Chemical	15403	<chem>CCOC(=O)NCCCC(=O)NCCc1cccc1</chem>	C15H22N2O3	278.35	CAY10683
Cayman Chemical	10008933	<chem>CC(=O)c1ccc2c(c1)[C@@H]1C=CC[C@@H]1[C@@H](N2)c1cc2OCOc2c1Br</chem>	C21H18BrNO3	412.28	G-1 Selisistat S-enantiomer(EX-527 S-enantiomer)
AbovChem Medchem Express	HY-15452A HY-18305	<chem>NC(=O)[C@H]1CCCC2c1[nH]c1c2cc(cc1)Cl</chem> <chem>O=C(C(C)C)Nc1ncc(s1)c1cc(nn1c1c(Cl)cccc1Cl)C(F)F</chem>	C13H13ClN2O C17H14Cl2F2N4OS	248.71 431.29	BMS-5 4-[4-[4-[4-fluoro-3-(trifluoromethyl)phenyl]-1-methylimidazol-2-yl]piperidin-1-yl]-1H-pyrazolo[3,4-d]pyrimidine GSK 650394; GSK-650394 Rotigotine hydrochloride; Rotigotine; Neupro; N-0437; D05768 RWJ 50271; RWJ-50271 4μ 8C N-(2,2,2-trifluoroethyl)-9-(4-(4-(4-(trifluoromethyl)biphenyl-2-ylcarboxamido)piperidin-1-yl)butyl)-9H-fluorene-9-carboxamide
ChemShuttle	134398	<chem>Cn1cc(nc1C1CCN(CC1)c1ncc2c1cn[nH]2)c1ccc(c(c1)C(F)F)F</chem>	C21H19F4N7	445.42	pyrazolo[3,4-d]pyrimidine GSK 650394; GSK-650394
Tocris	3572	<chem>OC(=O)C1=C(C=C(C=C1)C2=C[NH]C3=NC=C(C=C23)C4=CC=CC=C4)C5CCCC5</chem>	C25H22N2O2	382.454	650394 Rotigotine hydrochloride; Rotigotine; Neupro; N-0437; D05768 RWJ 50271; RWJ-50271 4μ 8C N-(2,2,2-trifluoroethyl)-9-(4-(4-(4-(trifluoromethyl)biphenyl-2-ylcarboxamido)piperidin-1-yl)butyl)-9H-fluorene-9-carboxamide
Tocris	3896	<chem>CCCN(CCC1=CC=CS1)C2CCC3=C(C2)C=CC=C3O</chem>	C19H25NOS	315.473	0437; D05768
Tocris	4227	<chem>CC1=C(C=C[N]1)C2=NC(=CS2)C3=CC=CC(=C3)C(F)F)C(=O)NCCCCO</chem>	C18H17F3N4O2S	410.413	RWJ 50271; RWJ-50271
Tocris	4479	<chem>CC1=CC(=O)OC2=C1C=CC(=C2C=O)O</chem>	C11H8O4	204.179	4μ 8C N-(2,2,2-trifluoroethyl)-9-(4-(4-(4-(trifluoromethyl)biphenyl-2-ylcarboxamido)piperidin-1-yl)butyl)-9H-fluorene-9-carboxamide
Shanghai AQBioPharma Co. Ltd.	ABF 12752	<chem>O=C(c1cccc1c1ccc(cc1)C(F)F)NC1CCN(CC1)CCCCC1(C(=O)NCC(F)F)F)c2cccc2c2c1cccc2</chem>	C39H37F6N3O2	693.72	650394 Rotigotine hydrochloride; Rotigotine; Neupro; N-0437; D05768 RWJ 50271; RWJ-50271 4μ 8C N-(2,2,2-trifluoroethyl)-9-(4-(4-(4-(trifluoromethyl)biphenyl-2-ylcarboxamido)piperidin-1-yl)butyl)-9H-fluorene-9-carboxamide
Cayman Chemical	10007927	<chem>OC(=O)CCCCCCCCCN(C(=O)NC12CC3CC(C2)CC(C1)C3</chem>	C23H40N2O3	392.58	AUDA
Cayman Chemical	17408	<chem>[O-][N+](=O)c1ccc(cc2c1non2)Nc1cccc1c1cccc1</chem>	C18H12N4O3	332.31	10074-G5
AbovChem Medchem Express	HY-10442 HY-13259	<chem>Nc1nccc2c1ncc2[C@@H]1C=C([C@H]1([C@H]1O)O)CO</chem> <chem>O=C[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)OCc1cccc1)CC(C)C)CC(C)C)CC(C)C</chem>	C12H14N4O3 C26H41N3O5	262.26 475.62	3-Deazaneplanocin A MG-132
Selleck Chemicals	S7252	<chem>O=C(/C=C\c1n1cnc(n1)c1cc(cc(c1)C(F)F)C(F)F)Nn1cncn1</chem>	C17H11F6N7O	443.31	KPT-330

						Tizanidine hydrochloride; Cimbrar; Sizolan; Sirdalid; Tizanidine; Ternelin; Telzanine; Tizan; DS-103282; Sirdalud; Tizanidine hydrochloride; TIZANIDINE; Tizanidine succinate; Tizalud; Musant; Tizanidina; Tizaflex; DS-103282 ch; Zanaflex; ZANAFLEX; 5-Chloro-4-(2-imidazolin-4-on-2-ylamino)-2, 1, 3-benzothiazdiazole; 5-Chloro-4-(2-imidazolin-2-ylamino)-2, 1, 3-benzothiadiazole; Zanpeak; Tizadin; Pal-tizanidine; Tizanidin; tizanidine; Sirdalud MR; Tizanidinum; Navizan; Mylan-tizanidine; Tizanidine HCl; TIZANIDINE HYDROCHLORIDE; Tizanidine Hydrochloride; Spaslax; Relaxkov; NVD-422; Myores; AN-021A; Tizanidine sulfate;
Tocris	3609	<chem>C1C1=C(NC2=NCCN2)C3=NSN=C3C=C1</chem>	C9H8ClN5S	253.711	Zitanid; C07452	
Tocris	3912	<chem>CN1C2=CC=C(C(C=C2N=C(C3=CC=C(C(C=C3)C(O)=O)C4=CC5=C(C(C=C14)C(C)(C)CCC5(C)C)[N+](O-)=O</chem>	C29H29N3O4	483.558	HX 531; HX-531	
Tocris	4255	<chem>COC1=CC(=CC(=C1)OC)C(=O)NNC(=O)NC2=CC=CC3=C2C=CC=C3</chem>	C20H19N3O4	365.383	TC-O 9311	
					Paliperidone; PALIPERIDONE PALMITATE; R-76477; Ro-76477; PALIPERIDONE; 9-Hydroxyrisperidone; Paliperidone; Invega; D05339; SID90341688; 3-{2-[4-(6-fluoro-1,2-benzoxazol-3-yl)piperidin-1-yl]ethyl}-9-hydroxy-2-methyl-6, 7, 8, 9-tetrahydropyrido[1,2-a]pyrimidin-4-one; paliperidona; Invega Sustenna; paliperidonum; Paliperidone Palmitate; JNS-007ER; RO-76477	
Tocris	4493	<chem>CC5=C(CCN1CCC(CC1)C2=NO C3=CC(=CC=C23)F)C(=O)N4CCCC(O)C4=N5</chem>	C23H27FN4O3	426.484	JNS-007ER; RO-76477	
Pharmablo						
ck - US						
Stock	PBLJ6619	<chem>OC[C@H]1N[C@H]([C@@H]([C@@H]1O)O)c1c[nH]c2c1nc[nH]c2=O</chem>	C11H14N4O4	266.25	Forodesine	
Cayman		<chem>Fc1cc(F)cc(c1)[C@@H](C(=O)N)[C@H](C(=O)N)[C@H]1c2cccc2c2c(N(C1=O)C)cccc2)C)O</chem>	C26H23F2N3O4	479.48	LY411575	
Chemical	16162					
ChemPacifi						
c	33433	<chem>COC(=O)CCc1ccc(cc1)OCC(CNC(C)C)O</chem>	C16H25NO4	295.37	Esmolol	
Medchem		<chem>C#CCC(c1ccc(cc1)C(=O)N)[C@H](C(=O)O)CCC(=O)O)Cc1cnc2c(n1)c(N)n</chem>				
Express	HY-10446	<chem>c(n2)N</chem>	C23H23N7O5	477.47	Pralatrexate	
Medchem						
Express	HY-15667	<chem>[O-][N+](=O)c1cc(sc1Sc1cccc(c1Cl)Cl)C(=O)C</chem>	C12H7Cl2NO3S2	348.22	P005091	
Selleck		<chem>O=C1C=C2C(=CC=C3[C@@H]2(C)CC[C@@H]3(C)CC[C@@H]3(C)[C@@H]2C[C@@H](C)(CC3)C(=O)O)C)C)C(=C1O)C</chem>	C29H38O4	450.61	Celastrol	
Chemicals	S1290					

					Acamprosate calcium; ACAMPROSATE; Campral; Acamprosate calcium; Regtect; Acamprosate Calcium; Zulex; N- Acetylhomotaurine; Sobriol; Acamprosate; CaAOTA; Acamprosato; acamprosate calcium; ACAMPROSATE CALCIUM; N-acetyl homotaurine; calcium acetylhomotaurinate; Acamprosat; Calcium Bisacetyl Homotaurine; Aotal; Acamprosatum; Alcomed; D02780; CA- Aota; 3-Acetamido-1- propanesulfonic acid; calcium acetyl homotaurinate; NS-11; SNC-102; acamprosate(1-); acamprosate; acamprosatum
Tocris	3618	<chem>CC(=O)NCCC[S](=O)(=O)O</chem>	C5H11NO4S	181.21	Pyrimethamine; Chloridine; PYRIMETHAMINE; Primethamine; Pyrimethaminum; pirimecidan; pyrimethamine; EXR-101; Pyrimethamine; Daraprim; Diaminopyritamin; Pirimetamina; 2,4- Diamino-5-chlorophenyl-6- ethylpyrimidine; 2,4- Diamino-5-(4- chlorophenyl)-6- ethylpyrimidine; CD; chloridine; Malacide; Pyrimethamin; Fansidar Tablets; 5-(4- Chlorophenyl)-6-ethyl-2,4- pyrimidinediamine; Chloridyn; Ethylpyrimidine; 5-(4- Chlorophenyl)-6-ethyl-2,4- diaminopyrimidine; 5-(4'- Chlorophenyl)-2,4-diamino- 6-ethylpyrimidine; pirimetamin; Chloridin; 2,4- Diamino-5-(P- chlorophenyl)-6- ethylpyrimidine; D00488; darachlor; Malocide; TRP- 004; C07391; Pyremethamine; Pyrimethamine Hcl
Tocris	3918	<chem>CCC1=C(C(=NC(=N1)N)N)C2=CC=C(C1)C=C2</chem>	C12H13ClN4	248.711	
Tocris	4343	<chem>COC1=CC2=C(NC3CCN(CC3)C(C)C)N=C(N=C2C=C1OCCCN4CCCC4)C5C</chem> <chem>CCCC5</chem>	C30H47N5O2	509.726	UNC 0638; UNC-0638

[illegible]

AbovChem	HY-N0127	<chem>COC(=O)[C@H]1[C@@H](O)CC[C@@H]2[C@@H]1C[C@@H]1N(C2)CCc2c1[nH]c1c2cccc1</chem>	C21H26N2O3	354.44	Yohimbine
Pharmablo					benzamide, n-
ck - US					(cyanomethyl)-4-[2-[[4-(4-
Stock	PBLJ6152	<chem>N#CCNC(=O)c1ccc(cc1)c1ccnc(n1)Nc1ccc(cc1)N1CCOCC1</chem>	C23H22N6O2	414.46	morpholinyl)phenyl]amino]-
Combi-					4-pyrimidinyl]-
Blocks	QE-9393	<chem>Oc1ccc2c(c1)Oc1c(C32OC(=O)c2c3cccc2)ccc(c1)O</chem>	C20H12O5	332.31	Fluorescein
Advanced					
ChemBlock					
s - In					
Stock	G-7963	<chem>CNC(=O)c1ccc(cc1F)N1C(=S)N(C(=O)C1(C)C)c1ccc(c(c1)C(F)(F)F)C#N</chem>	C21H16F4N4O2S	464.44	
Target					
Molecule	T 1803	<chem>OCCNC(=O)c1cccc(c1)c1ncnc(c1)Nc1ccc(cc1)OC(F)(F)F</chem>	C20H17F3N4O3	418.37	GNF-5
Target					
Molecule	T 2504	<chem>O=C(N(c1nc(c(s1)S(=O)(=O)N)C)C)Cc1ccc(c1)c1ccccc1</chem>	C18H18N4O3S2	402.49	BAY 57-1293
Target					
Molecule	T 3067	<chem>O=c1sn(c(=O)n1Cc1ccccc1)c1cccc2c1cccc2</chem>	C19H14N2O2S	334.39	Tideglusib
Target					
Molecule	T 1947	<chem>NCCCCCNc1cc(NCc2ccccc2)n2c(n1)c(cn2)C(C)C</chem>	C22H32N6	380.53	BS-181
AstaTech	41167	<chem>CN(Cc1cccc2c1cccc2)C/C=C/C#CC(C)(C)C</chem>	C21H25N	291.43	TERBINAFINE HCL
Bide					
Pharmatec					
h	BD145505	<chem>CCOc1cc(ccc1C(=O)O)CC(=O)N[C@H](c1ccccc1N1CCCCC1)CC(C)C</chem>	C27H36N2O4	452.59	Repaglinide
Pharmablo					
ck - US					
Stock	PBN2011567	<chem>CCN(CCN(C(=O)Cn1c(SCc2ccc(cc2)F)nc(=O)c2c1CCC2)Cc1ccc(cc1)c1ccc(cc1)C(F)(F)F)CC</chem>	C36H38F4N4O2S	666.77	Darapladib
Cayman					
Chemical	15785	<chem>ONC(=O)c1ccc(cc1)Cn1c2ccccc2c2c1CCN(C2)C</chem>	C20H21N3O2	335.4	Tubastatin A
Vitas M					
Labs - BB	BBL023172	<chem>COc1ccc(cc1)C(=O)C(=O)c1ccccc1</chem>	C15H12O3	240.25	BBL023172
Selleck					
Chemicals	S7500	<chem>Cc1cc(C)c(c(c1)C)S(=O)(=O)n1cc(cc1C)C</chem>	C15H19NO2S	277.38	HJC0350
Target					
Molecule	T0162	<chem>OCCOCCN1CCN(CC1)C1=Nc2ccccc2Sc2c1ccccc2</chem>	C21H25N3O2S	383.51	Quetiapine
Target					
Molecule	T 6278	<chem>CN1CCN(CC1)c1nc2ccccc2c(n1)C1=C(C(=O)NC1=O)c1c[nH]c2c1cccc2</chem>	C25H22N6O2	438.48	Sotrastaurin
Target					
Molecule	T 3032	<chem>O=C(c1nc(cnc1N)c1ccc(cc1)S(=O)(=O)C)Nc1ccccc1</chem>	C18H16N4O3S	368.41	VE-821
Bepharm	B17734	<chem>NC[C@@H]1CC[C@H](CC1)C(=O)O</chem>	C8H15NO2	157.21	Tranexamic acid
Advanced					
ChemBlock					
s - In					
Stock	M15325	<chem>Cc1cc(C(Nc2ccccc2)C)c2h(c1)c(=O)cc(n2)N1CCOCC1</chem>	C21H24N4O2	364.44	663619-89-4
Bide					
Pharmatec					
h	BD113240	<chem>N#Cc1ccccc1Cn1c(cc(=O)n(c1=O)C)N1CCC[C@H](C1)N</chem>	C18H21N5O2	339.39	Alogliptin
Pharmablo					
ck - US					
Stock	THR0011	<chem>CC(=O)c1c(C)c2cnc(nc2n(c1=O)C1CCCC1)Nc1ccc(cn1)N1CCNCC1</chem>	C24H29N7O2	447.53	palbociclib
Cayman					
Chemical	19768	<chem>CCc1oc2c(c1C(=O)c1cc(Br)c(c1)Br)O)cccc2</chem>	C17H12Br2O3	424.08	Benzbromarone
Advanced					
ChemBlock					
s - In					
Stock	M15125	<chem>Cc1cnc(nc1Nc1cccc(c1)S(=O)(=O)NC(C)C)Nc1ccc(cc1)OCCN1CCCC1</chem>	C27H36N6O3S	524.68	
Combi-					
Blocks	QA-4191	<chem>CC(NC(=O)NS(=O)(=O)c1cncccc1Nc1cccc(c1)C)C</chem>	C16H20N4O3S	348.42	Torasemide
Target					
Molecule	T 1611	<chem>CC(=CC=CC(=CC(=O)O)C)C=CC1=C(C)CCCC1(C)C</chem>	C20H28O2	300.44	Isotretinoin
Target					AG-337; Nolatrexed
Molecule	T 2627	<chem>Cc1ccc2c(c1Sc1ccncc1)c(=O)nc([nH]2)N</chem>	C14H12N4OS	357.26	2hydrochloride
Target					
Molecule	T 1943	<chem>COc1ccc(cc1)c1cnc2n(c1)ncc2c1ccccc2c1cccn2</chem>	C22H16N4O	352.39	mL347
Bide					
Pharmatec					
h	BD3002	<chem>N=C(N[N+](=O)[O-])NCCCC[C@H](C(=O)O)N</chem>	C6H13N5O4	219.2	H-Arg(NO2)-OH

Combi-Blocks	QA-9111	CS _c 1nc2c([nH]1)cc(c(c2)Cl)O _c 1cccc(c1Cl)Cl	C14H9Cl3N2O ₅	359.66	Triclabendazole
Medchem Express	HY-13501	FC(c1ccc(cc1)/C=C/c1ccc(n1)CO _c 1ccc(cc1)CCCCn1ncc1)(F)F	C25H23F3N4O ₂	468.47	Mubritinib
Pharmablo ck - US		C=CCn1c(=O)c2c(n1c1cccc(n1)C(O)(C)C)nc(nc2)Nc1ccc(cc1)N1CCN(CC1)C	C27H32N8O ₂	500.6	MK-1775
Stock Cayman Chemical	PBLJ6189 20390	O=C(CNC(=O)C)(Cc1cccc1)CSC(=O)C)OCc1cccc1	C21H23NO ₄ S	385.48	Racecadotril
Advanced ChemBlock s - In		CCc1cc2C(=O)c3c4ccc(cc4[nH]c3C(c2cc1N1CCC(CC1)N1CCOCC1)(C)C)C#N	C30H34N4O ₂	482.62	
Stock Cayman Chemical	I-9209 15987	CC1Nc2cc(Cl)c(cc2C(=O)N1c1cccc1C)S(=O)(=O)N	C16H16ClN3O ₃ S	365.83	Metolazone
Target Molecule	T 1330	CO _c 1cc(C)c(c(c1C)C)C=CC(=CC=CC(=O)O)C)C	C21H26O ₃	326.43	Acitretin
Target Molecule	T 2670	OCc1ccc(o1)c1ccc2c(c1)c(ncn2)NCCc1ccc(o1)C	C19H17N3O ₃	335.36	mL167
Target Molecule	T 2588	O=C(c1c[nH]c2c(c1=O)cccc2)Nc1cc(O)c(cc1C(C)(C)C)C(C)(C)C	C24H28N2O ₃	392.49	Ivacaftor
Bide Pharmatec h	BD235626	O=C1CCC(C(=O)N1)N1C(=O)c2c(C1=O)c(N)ccc2	C13H11N3O ₄	273.24	Pomalidomide
Combi-Blocks	QA-6056	Cc1cnc(s1)NC(=O)C1=C(O)c2cccc2S(=O)(=O)N1C	C14H13N3O ₄ S ₂	351.4	Meloxicam
Medchem Express	HY-50898	Fc1cccc(c1)CO _c 1ccc(cc1Cl)Nc1nnc2c1cc(cc2)c1ccc(o1)CNCCS(=O)(=O)C	C29H26ClFN4O ₄ S	581.06	Lapatinib
J&K Scientific	985371	OC[C@H]1O[C@H](O)[C@@H]([C@H]([C@H]1O)O)O	C6H12O ₆	180.16	D-(+)-Glucose, ACS reagent
Cayman Chemical	14337	OC(=O)[C@H](Cn1ccc(=O)c(c1)O)N	C8H10N2O ₄	198.18	L-Mimosine
Advanced ChemBlock s - In		O=C(Nc1cc(ccc1c1ccsc1)S(=O)(=O)NC1CC1)Nc1cccc(c1)C(F)(F)F	C21H18F3N3O ₃ S ₂	481.51	
Combi-Blocks	QE-1174	C[C@@H]1CC[C@H]([C@@H]([C@H]1O)C)C	C10H20O	156.27	L-Menthol
Enzo Life Sciences	ALX-430-146	C=CCc1cccc(c1O)/C=N/NC(=O)CN1CCN(CC1)Cc1cccc1	C23H28N4O ₂	392.49	PAC-1
Target Molecule	T 6053	CC(O(C=O)C1=CN(CC(c2c1[nH]c1c2cccc1)(C)C)C(=O)c1ccc(c(c1)F)F)C	C25H24F2N2O ₃	438.47	Turofexorate Isopropyl (XL335)
Target Molecule	T 1857	O=C(c1cccc(c1)c1ncc(n1)C(F)(F)F)NCC1(CCOCC1)c1ccc(n1)c1cccc1CC[C@H]1OC(=O)[C@H](C)[C@@H]([C@H]1O)[C@@H]([C@H]([C2](C)OC)O)[C@H](C)[C@@H]([C@H]1O)[C@@H]([C@H]([C@H]2O)N(C)C)[C@H]([C@H]1C(=O)[C@@H]([C@H]([C@H]1(C)O)O)C)C)CO	C25H21F3N4O ₃ S	514.52	N-((4-(4-phenylthiazol-2-yl)tetrahydro-2H-pyran-4-yl)methyl)-3-(5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl)benzamide
Chem-Impex Bide Pharmatec h	126 BD229143	OCCOc1c(C)cc(cc1C)c1nc2cc(OC)cc(c2c(=O)[nH]1)OC	C20H22N2O ₅	370.4	RVX-208
Medchem Express	HY-17386	O=C1NC(=O)C(S1)Cc1ccc(cc1)OCCN(c1ccccn1)C	C18H19N3O ₃ S	357.43	Rosiglitazone
Combi-Blocks	AN-2948	Nc1ccc(cc1)S(=O)(=O)N	C6H8N2O ₂ S	172.2	Sulfanilamide
Cayman Chemical	16128	N#CC(=NNc1ccc(cc1)C1=NNC(=O)C[C@H]1C)C#N	C14H12N6O	280.28	Levosimendan
Advanced ChemBlock s - In		O=C(Nc1ccc(cc1N)F)/C=C/c1cnn(c1)C/C=C/c1cccc1	C21H19FN4O	362.4	
Enamine BB - US					
Stock	EN300-123537	O=c1oc2cccc2c(c1Cc1c(=O)oc2c(c1O)cccc2)O	C19H12O ₆	336.29	107753-78-6

Key Organics/B IONET - BioChemicals Stock	SS-4787	OCc1cc(ccc1OC)c1ccc2c(n1)nc(nc2N1CCOC[C@@H]1C)N1CCOC[C@@H]1C	C25H31N5O4	465.54	AZD8055
Target Molecule	T2044	CCc1c(C(=O)C(=O)N)c2c(n1Cc1cccc1)cccc2OCC(=O)O	C21H20N2O5	380.39	Varespladib
Target Molecule	T0389	CCCCCOC(=O)N=C(c1ccc(cc1)NCc1nc2c(n1C)ccc(c2)C(=O)N(c1ccccn1)CCC(=O)OCC)N	C34H41N7O5	627.73	Dabigatran etexilate
Combi- Blocks Bide	QA-4624	COc1c(C/C=C/C/C(=O)O)\C)c(C)O)c2c(c1C)COC2=O	C17H20O6	320.34	Mycophenolic acid
Pharmatec h Bide	BD218703	OC(=O)COc1ccc(cc1C)SCc1sc(nc1C)c1ccc(cc1)C(F)(F)F	C21H18F3NO3S2	453.5	GW 501516
Pharmatec h	BD55672	OC(=O)C(c1ccc2c(c1)CC(=O)c1c(S2)cccc1)C	C17H14O3S	298.36	Zaltoprofen
Combi- Blocks	OR-1175	O=C(NS(=O)(=O)c1ccc(cc1)C)NN1CC2C(C1)CCC2	C15H21N3O3S	323.41	Gliclazide
Combi- Blocks	QA-2612	Clc1ccc(cc1)OC(C(=O)C(C)(C)C)n1cccc1	C15H17ClN2O2	292.76	Climbazole
Pharmablo ck - US Stock	PBLJ6191	O=C(OCc1cccnc1)NCc1ccc(cc1)C(=O)Nc1ccccc1N	C21H20N4O3	376.41	Entinostat 3-methyl 5-(2-methylpropyl) 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate
Enamine BB - US Stock	EN300-119517	COC(=O)C1=C(C)NC(=C(C1c1cccc1[N+])(=O)[O-])C(=O)OCC(C)C	C20H24N2O6	388.41	
Key Organics/B IONET - BioChemicals Stock	ES-0052	COc1cc2c(ncnc2cc1OCCCN1CCCC1)Oc1ccc2c(c1F)cc([nH]2)C(Cl.Cl.C(CNC(C1=CC=CC=C1)C1=CC=CC=C1)NC(C1=CC=CC=C1)C1=CC=CC=C1	C25H27FN4O3	450.51	AZD2171, Cediranib
Tocris Medchem	2385		C28H30Cl2N2	465.45	AMN 082 dihydrochloride
Express Medchem	HY-A0063A	O=c1[nH]c(CN2CCCC2=N)c(c(=O)[nH]1)Cl	C9H11ClN4O2	242.66	Tipiracil
Express Selleck Chemicals	HY-13946 S1043	Clc1ccc(cc1)Oc1ccc(cc1)c1nc2c([nH]1)ccc(c2)C(=O)N COc1cc2c(cc1OCCCN1CCCC1)ncnc2N1CCN(CC1)C(=O)Nc1ccc(cc1)OC(C)C	C20H14ClN3O2	363.8	BML-277
Maybridge Vitas M Labs	GK01981 STK832240	COC(=O)c1scccc1NC(=O)Cc1cccs1 Oc1ccc(cc1)/C=N/N(Cc1ccccc1)Cc1ccccc1	C31H42N6O4	562.7	Tandutinib (MLN518)
Vitas M Labs	STL321288	C(NC(c1ccccc1)c1ccccc1)CNC(c1ccccc1)c1ccccc1	C12H11NO3S2	281.35	GK01981
Vitas M Labs	STK772817	CCCCn1c(cnc2c1nc1c2c(=O)[nH]c(=O)n1C)c1ccccc1	C21H20N2O	316.4	STK832240
Maybridge	KM03430	CSc1sc(c2c1C(=O)CC(C2)(C)C)c1cn(n1)C(=O)C	C28H28N2	392.54	STL321288
Enamine BB - UA Backorder	EN300-122638	O=C1CN(C(=O)N1)/N=C/c1ccc(o1)c1ccc(cc1)[N+](=O)[O-]	C18H19N5O3	353.38	STK772817
Key Organics/B IONET - Screening and Fragments - Stock	MS-0333	CCCCOc1ccc(cc1)/C=C/1\SC(=O)NC1=O	C16H18N2O2S2	334.46	KM03430 1-({[5-(4-nitrophenyl)furan-2-yl]methylidene)amino}imidazolidine-2,4-dione
Target Molecule	T2456	COc1cc2c(ccnc2cc1OC)Oc1ccc(c(c1)Cl)NC(=O)Nc1noc(c1)C	C13H13NO3S	263.31	5-((Z)-(4-propoxyphenyl)methylidene)-1,3-thiazolane-2,4-dione
AbovChem	HY-15370A	CC1CCN(CC1)CC[C@H]1CCCN1S(=O)(=O)c1ccccc1O	C22H19ClN4O5	454.86	Tivozanib
			C18H28N2O3S	352.49	SB-269970

Enamine Screening Compound						
s	Z274554748	O=C(N1CCOCC1)Oc1nsnc1N1CCCCC1	C12H18N4O3S	298.36	Z274554748	
Maybridge	SPB06189	NC(=N)N/N=C/C/c1ccc(c(c1)Cl)Cl	C8H8Cl2N4	231.08	SPB06189	
Vitas M Labs	STK869906	Fc1ccccc1c1cc(=O)c2c(n1)sc1c2CCCC1	C16H12FNO2S	301.34	STK869906	
Vitas M Labs	STK235555	O=C(N1CCCc2c1cccc2)CSc1nc2c(s1)cccc2	C18H16N2OS2	340.46	STK235555	
Vitas M Labs	STK746869	N#Cc1c(SCC(=O)Nc2nnc(s2)CC)nc(nc1SC)N	C12H13N7OS3	367.47	STK746869	
ChemDiv	D399-0002	Clc1ccc(cc1)S(=O)(=O)N1CCCC1c1cccs1	C14H14ClNO2S2	327.85	D399-0002	
Advanced ChemBlock						
s - In Stock	R16001	Cc1[nH]c2c(n1)CCN(c1c2cccc1)C(=O)c1ccc(cc1)NC(=O)c1ccccc1c1ccccc1	C32H26N4O2	498.57	conivaptan	
Key Organics/B IONET - Screening and Fragments						4-[4-(4-chlorophenyl)phenyl]-4-oxo-2-[(phenylsulfanyl)methyl]butanoic acid
- Stock	12P-030	OC(=O)C(CC(=O)c1ccc(cc1)c1ccc(cc1)Cl)CSc1ccccc1	C23H19ClO3S	410.91		
AbovChem Bide	HY-15979A	Brcc1ccc(cc1)/C=C/CNCCNS(=O)(=O)c1cccc2c1ccnc2	C20H20BrN3O2S	446.36	H 89	
Pharmatec h	BD262844	Clc1ccc(cc1)C1=C(CCC(C1)(C)C)CN1CCN(CC1)c1ccc(c(c1)Oc1nc2c(c1)cc[nH]2)C(=O)NS(=O)(=O)c1ccc(c(c1)[N+](=O)[O-])NCC1CCOCC1	C45H50ClN7O7S	868.44	ABT-199	
ChemDiv	6603-0104	CC(OC(=O)CN1C(=O)C(=O)c2c1c(C)ccc2)C	C14H15NO4	261.27	6603-0104	
Vitas M Labs	STK155799	CCCCC(=O)Nc1c(C)cc(cc1C)Br	C14H20BrNO	298.22	STK155799	
Specs	AG-690/40699390]	C24H23N3O4	417.46	AG-690/40699390	
ChemDiv	0075-0068	CN1CCN(CC1)c1ccc(cc1)Nc1c2ccccc2nc2c1cccc2	C24H24N4	368.47	0075-0068	
Vitas M Labs	STL336112	COc1ccccc1N1CCN(CC1)c1ncnc2c1cnn2c1ccccc1	C22H22N6O	386.45	STL336112	
MolMall Sarl	18650	CN1CCN(CC1)C(=S)SSC(=S)N1CCN(CC1)C	C12H22N4S4	350.59	18650	
Bide Pharmatec h	BD21816	Fc1ccc(cc1)[C@@H]1CCNC[C@H]1COc1ccc2c(c1)OCO2	C19H20FNO3	329.37	(3S,4R)-3-((Benzo[d][1,3]dioxol-5-ylloxy)methyl)-4-(4-fluorophenyl)piperidine	
Key Organics/B IONET - Screening and Fragments						
- Stock	AS-2259	OB(c1ccccc1)O	C6H7BO2	121.93	Phenylboronic acid	
Cayman Chemical	12097	CN(c1ccc2c(c1)nn(c2C)C)c1ccnc(n1)Nc1ccc(c(c1)S(=O)(=O)N)C	C21H23N7O2S	437.52	Pazopanib	
AbovChem Vitas M Labs	HY-10203	Clc1ccc(cc1)Nc1nnc(c2c1cccc2)Cc1ccncc1	C20H15ClN4	346.81	Vatalanib base	
STK416816		Fc1ccc(cc1)S(=O)(=O)n1c(C)nc2c1cccc2	C14H11FN2O2S	290.31	STK416816	
ChemDiv	6030-2123	COc1ccc(cc1OC)CCNC(=O)CC(c1ccccc1O)C)c1ccccc1	C26H29NO4	419.51	6030-2123	
Vitas M Labs	STL019982	COC(=O)c1c(NC(=O)CC2SC(=N)NC2=O)sc(c1C)C	C13H15N3O4S2	341.41	STL019982	
Vitas M Labs	STK066844	Clc1ccc(c(c1)C(=O)Nc1ccc(cc1)Cl)NS(=O)(=O)c1ccc(c(c1)[N+](=O)[O-])Cl	C19H12Cl3N3O5S	500.74	STK066844	
Vitas M Labs	STL304557	CC1(C)OCc2c(C1)c1c(nc2N2CCOCC2)sc2c1ncnc2Nc1cccn1	C24H26N6O2S	462.57	STL304557	
ChemDiv	0988-0215	OC(CN1CCOCC1)COc1c(Br)cc(cc1Br)C(c1cc(Br)c(c1)Br)OCC(CN1CCOCC1)O)C)C	C29H38Br4N2O6	830.24	0988-0215	
Medchem Express	HY-10052	O=C1NC(CN2[C@H]([C@@H]([C@@H](O[C@@H](C3=CC(C(F)(F)F)=CC(C(F)(F)F)=C3)C)OCC2)C4=CC=C(F)C=C4)=NN1	C23H21F7N4O3	534.427	Aprepitant	

TCI						
America	E1096	<chem>C#Cc1c[nH]c(=O)[nH]c1=O</chem>	<chem>C6H4N2O2</chem>	136.11	5-Ethynyluracil	
Medchem						
Express	HY-A0033	<chem>NC(=O)C(c1ccccc1)(c1ccccc1)[C@@H]1CCN(C1)CCc1ccc2c(c1)CCO2</chem>	<chem>C28H30N2O2</chem>	426.55	Darifenacin	
AbovChem	HY-B0109A	<chem>CCN[C@H]1C[C@H](C)S(=O)(=O)c2c1cc(s2)S(=O)(=O)N</chem>	<chem>C10H16N2O4S3</chem>	324.44	Dorzolamide	
Enamine						
Screening						
Compound						
s	Z26397758	<chem>O=C(c1ccc2c(c1)OCO2)NC1CCCc2c1cccc2</chem>	<chem>C18H17NO3</chem>	295.33	Z26397758	
Enamine						
Screening						
Compound						
s	Z32036776	<chem>O=C(c1n[nH]c2c1cccc2)Nc1ccc(cc1)N1CCOCC1</chem>	<chem>C18H18N4O2</chem>	322.36	Z32036776	
Vitas M						
Labs	STK410281	<chem>COc1ccc(cc1)C(=O)Nc1sc(nc1C(=O)N)Nc1ccccc1</chem>	<chem>C18H16N4O3S</chem>	368.41	STK410281	
ChemDiv	4577-1576	<chem>CCOc1ccc(cc1)S(=O)(=O)N(c1ccccc1)CC(=O)N/N=C/C1C(=O)Nc2c1cccc2</chem>	<chem>C24H22N4O5S</chem>	478.52	4577-1576	
InterBioScr						
een	STOCK1N-65052	<chem>O=C(Nc1cccc(c1)C(=O)C)CN1CCc2c(C1)cc1c(c2)OCCCO1</chem>	<chem>C22H24N2O4</chem>	380.44	STOCK1N-65052	
Vitas M		<chem>Clc1ccc(cc1)COc1ccc(cc1)c1nn(cc1/C=C/1\SC(=S)N(C1=O)CCS(=O)(=O)O)c1ccccc1</chem>	<chem>C28H22ClN3O5S3</chem>	612.14	STK810090	
Labs	STK810090	<chem>O=C(N([C@@H](C1=NC2=NC=CC=C2C1N3C=CC=C(OCC)C=C3)=O)C)CC4=CC=CN=C4)CC5=CC=C(O(C(F)(F)F)C=C5</chem>	<chem>C32H28F3N5O4</chem>	603.591	AMG 487	
Medchem		<chem>COc1cc(ccc1Cc1cn(c2c1cc(cc2)NC(=O)OC1CCCC1)C(=O)NS(=O)(=O)c1ccccc1C</chem>	<chem>C31H33N3O6S</chem>	575.68	Zafirlukast	
Express	HY-15319					
Cayman						
Chemical	10008282					
AbovChem	HY-13009	<chem>OC(=O)C[C@@H]1CC[C@H](CC1)c1ccc(cc1)N1CCOc2c(C1=O)c(N)ncn2</chem>	<chem>C21H24N4O4</chem>	396.44	PF-04620110	
AbovChem	HY-70050C	<chem>O=C1N(CCc2c1c1ccccc1n2C)Cc1nc[nH]c1C</chem>	<chem>C17H18N4O</chem>	294.35	Alosetron	
Enamine						
Screening						
Compound						
s	Z55729757	<chem>C1CCn2c(CC1)nnc2C1CC3CC(C2)CC(C1)C3</chem>	<chem>C17H25N3</chem>	271.4	Z55729757	
Vitas M						
Labs	STK841699	<chem>Oc1ccccc1)NC(=O)c1cc2n(n1)c(C)cc(n2)c1ccccc1</chem>	<chem>C20H16N4O2</chem>	344.37	STK841699	
ChemDiv	G748-0054	<chem>CC(=O)Nc1ccc(cc1)C(=O)Nc1sc(nc1C(=O)N)Nc1ccccc1</chem>	<chem>C19H17N5O3S</chem>	395.43	G748-0054	
ChemDiv	D419-2236	<chem>CCCC(=O)Nc1nc(cc(n1)c1ccccc1)c1ccccc1</chem>	<chem>C20H19N3O</chem>	317.38	D419-2236	
Life						
Chemicals	F0748-0306	<chem>COc1ccccc1c1nncc(s1)NC(=O)C(SC1=NCCS1)C</chem>	<chem>C15H16N4O2S3</chem>	380.51	F0748-0306	
Medchem						
Express	HY-B0397	<chem>Clc1cc(cc(c1Cl)S(=O)(=O)N)S(=O)(=O)N</chem>	<chem>C6H6Cl2N2O4S2</chem>	305.16	Dichlorphenamide	
Medchem		<chem>O=C(C1=CC=C(C(C(OC)=C1)NC2=NC=C(N(C3=O)C)C(N([C@@H]3CC)C(C)C)=N2)N[C@H]4C[C@@H](C4)N5CCN(CC5)CC6CC6</chem>	<chem>C34H50N8O3</chem>	618.813	Volasertib	
Express	HY-12137					
Target						
Molecule	T1583	<chem>ONC(=O)CCCCCCC(=O)Nc1ccccc1</chem>	<chem>C14H20N2O3</chem>	264.32	Vorinostat	
Target						
Molecule	T0373	<chem>COCCOc1cc2c(ncnc2cc1OCCOC)Nc1cccc(c1)C#C</chem>	<chem>C22H23N3O4</chem>	393.44	Erlotinib	
Apollo						
Scientific -		<chem>CC(C[C@@H]([C@H](CC(=O)N)[C@H](C(=O)N)[C@H]([C@H](CC(=O)O)O)CC(C)C)C)O)NC(=O)[C@H](C(C)C)NC(=O)[C@H](C(C)C)NC(=O)CC(C)C)C</chem>	<chem>C34H63N5O9</chem>	685.89	Pepstatin A	
Biochemica						
ls - Stock	BIMI2205					
Maybridge	RDR01836	<chem>Cc1csc(n1)Nc1cccc2c1cccc2</chem>	<chem>C14H12N2S</chem>	240.32	RDR01836	
Vitas M						
Labs	STK368746	<chem>CC(COC(=O)N)(c1ccc(cc1)C(C(F)(F)F)(C(F)(F)F)O)C)C</chem>	<chem>C15H17F6NO3</chem>	373.29	STK368746	
ChemDiv	K407-0490	<chem>COc1cc2c(cc1OC)CCN(C2COc1ccc(cc1)O)C(=O)c1ccc(cc1)Cl</chem>	<chem>C26H26ClNO5</chem>	467.94	K407-0490	
Enamine						
Screening						
Compound						
s	Z166688522	<chem>O=C(Nc1cc(C)cc(c1)C)Nc1ccc(cc1)S(=O)(=O)N</chem>	<chem>C15H17N3O3S</chem>	319.38	Z166688522	
Maybridge	S06924	<chem>COc1ccc(c(c1)c1nc2ccccc2c(=O)o1)Br</chem>	<chem>C15H10BrNO3</chem>	332.15	S06924	
AbovChem	HY-15599	<chem>COc1c2ccccc2c(c1C)C(=O)c1ccc(c(c1)C(=O)O)N</chem>	<chem>C18H16N2O4</chem>	324.33	SSR128129E (free acid)	
Medchem		<chem>O=C(N(C1CCCC1)CCNCCC2=C(OCC(N3)=O)C3=C(O)C=C2)CCNCCC4=CC=C(Cl)C(Cl)=C4.O=C(O)C(F)(F)F.O=C(O)C(F)(F)F</chem>	<chem>C33H40Cl2F6N4O8</chem>	805.589	AZ505 (ditrifluoroacetate)	
Express	HY-15226A					

Cayman						
Chemical	20389	CCC(=O)NCC[C@@H]1CCc2c1cCCOc1cc2	C16H21NO2	259.34	Ramelteon	
Cayman						
Chemical	11313	O[C@@H]1[C@@H](O)CN2[C@@H]([C@H]1O)[C@@H](O)CC2	C8H15NO4	189.21	Castanospermine	
Bide						
Pharmatec						
h	BD123889	O=C1NC(=O)CN(C1)C[C@@H](N1CC(=O)NC(=O)C1)C	C11H16N4O4	268.27	Dexrazoxane	
Maybridge	RH00511	CCCCc1ccc(c(c1)C)N/C=N/O	C12H18N2O	206.28	RH00511	
Specs	AQ-390/43364023	CCn1c2ccc(c3c2c(c1=O)ccc3)S(=O)(=O)Nc1cccc(c1)C(=O)C	C21H18N2O4S	394.44	AQ-390/43364023	
ChemDiv	K788-2368	Fc1ccc(cc1)S(=O)(=O)NCc1ccc(cc1)C(=O)NCc1ccncc1	C20H18FN3O3S	399.44	K788-2368	
Enamine						
Screening						
Compound						
s	Z26426477	O=C(C1CC(=O)N(C1)Cc1ccccc1)NCc1ccc(cc1)Cl	C19H18Cl2N2O2	377.26	Z26426477	
Maybridge	JFD01049	N#CCOC(=O)Cc1ccc(cc1)c1cc(=O)c2c(o1)cccc2	C18H11NO4	305.28	JFD01049	
Medchem						
Express	HY-10122	OCCCN1CCc2c1c(cc(c2)C[C@H](NCCOc1ccccc1OCC(F)(F)F)C)C(=O)N	C25H32F3N3O4	495.53	Silodosin	
Medchem						
Express	HY-12828	O=C(C(N1C)=C(/C(C#N)=C1N)C2=C1C(Cl)=C(Cl)C=C2)OCC	C15H13Cl2N3O2	338.189	KH-CB19	
Medchem		N#CC1=NN(C2=CC(Cl)=C(O)C(C=C3C(C)C)=NNC3=O)C(Cl)=C2)C(NC1=O				
Express	HY-12216)=O	C17H12Cl2N6O4	435.221	MGL-3196	
Medchem		O=C([C@H]1CC[C@]2([H])[C@]1(C)CC[C@]3([H])[C@@]4(C)C=CC(N[C				
Express	HY-13635	@]4([H])CC[C@]32[H])=O)NC(C)(C)C	C23H36N2O2	372.544	Finasteride	
Medchem		O=C1NN=C2C3=C1C=C(F)C=C3N[C@H](C4=CC=C(F)C=C4)[C@H]2C5=				
Express	HY-16106	NC=NN5C	C19H14F2N6O	380.351	BMN-673	
Medchem		FC1([C@H]2[C@@H]1C3=C([C@@H](C4=CC=CC=C4)N5CCN(CC5)C[C				
Express	HY-50671	@H](CO)C6=C7C=CC=NC7=CC=C6)O)C=CC=C3)F.Cl.Cl.Cl	C32H34Cl3F2N3O2	636.987	(trihydrochloride)	
Medchem		O=C1N(CC2=C(N1)C=CC=C2)C3CCN(C(N[C@@H](C(N[C@@H](C(N4CCN(
Express	HY-10095	C5=CC=NC=C5)CC4=O)CCCCN(=O)CC6=CC(Br)=C(C(Br)=C6)O)=O)CC	C38H47Br2N9O5	869.645	Olcegepant	
Medchem		OC1=C(O)[C@H]2C3=O)C([C@]2(C)[C@N@+](4(C)CC5CC5)[C@](CC3)(O)				
Express	HY-75766	[C@H]4C6)=C6C=C1.[Br-]	C21H26BrNO4	436.339	Methylnaltrexone (Bromide)	
Medchem		O=S(C1=CC(F)=CC2=C1N(C3=C2CC[C@H]3CC(O)=O)CC4=CC=C(Cl)				
Express	HY-50175	C=C4)(C)=O	C21H19ClFNO4S	435.896	Laropiprant	
Medchem		NC([C@H](CC1=CC=CC=C1)NC([C@H](CCCNC(N)=N)NC(C23C[C@H](C4				
Express	HY-107382)C[C@H](C[C@H]4C3)C2=O)=O)=O	C26H38N6O3	482.618	RF9	
Medchem						
Express	HY-108316	O=S(C1=CC=C(N(CCC2)S2=O)=O)C=C1)(N)=O	C10H14N2O4S2	290.359	Sultiame	
Medchem		CC(C)(C)C1=CC(SC(C)(C)SC2=CC(C(C)(C)C)=C(O)C(CCC(C)=O)=O)C(C(
Express	HY-14937	C)(C)C)=C2=CC(C(C)(C)C)=C1O	C35H52O5S2	616.914	Succinobucol	
Medchem						
Express	HY-16276	N#CC1=CC=C([C@H]2CCC3=CN=CN32)C(F)=C1	C13H10FN3	227.237	Osilodrostat	
Medchem		O=C(CC)O[C@@]([C@]([C@@]1([H])C2(C)C@H(O)[C@](F)([C@]3C=				
Express	HY-B0154	C4)C)[C@@]1([H])C[C@H](F)C3=CC4=O)C([C@H]2C)C(SCF)=O	C25H31F3O5S	500.571	Fluticasone (propionate)	
Medchem		CC1=CN=CC2=C1C(S(=O)N3[C@@H](C)CNC3C3)=O)=CC=C2.[H]Cl.[H]				
Express	HY-15720A	Cl	C16H23Cl2N3O2S	392.344	H-1152 (dihydrochloride)	
Medchem		O=C1[C@@H](C)[C@]2(O)[C@]3(C4=O)C(C5([C@@H](O)C(O6)=O)C				
Express	HY-B0355	6O3)([C@H](O4)C[C@H]5C(C)(C)C[C@]2([H])O1	C20H24O9	408.399	Ginkgolide A	
Medchem		CO)C1=C(O)C=C(CCO[C@H]2[C@H](N3CC[C@H](O)C3)CCCC2)C=C				
Express	HY-14183	1.Cl	C20H32ClNO4	385.925	Vernakalant (Hydrochloride)	
Medchem		NC1CCN(C2=C3N=C(C=CC3=CC=C2)N4C=NC5=CC(OCCO)C=CC=C54)C				
Express	HY-12050	C1	C24H27N5O2	417.504	CP-673451	
Medchem		O=S(CCC1=CC2=C(NC=C2C[C@H]3N(CCC3)C)C=C1)(C4=CC=CC=C4)				
Express	HY-A0010	=O.Br	C22H27BrN2O2S	463.431	Eletriptan (hydrobromide)	
Medchem						
Express	HY-107377	C12=C(C=C3)C=C(C=CC=C4)C4=C1C=CC5=CC=CC3=C25	C20H12	252.309	Benzo[a]pyrene	
Medchem		O=C(NC(C)(C)C)[C@@H](NC([C@H](CC(C)C)N)CC1=CC=C(C(C)(C)C)				
Express	HY-103318	C=C1)=O)CC2=CC=C(OCC3=CC=CC=C3)C=C2	C38H53N3O3	599.846	PD173212	
Medchem		C[C@@]12[C@](C(CO)C(=O)=O)(O)CC[C@]1([H])[C@]3([H])CCC4=				
Express	HY-B1383	CC(C=C[C@]4(C)[C@]3(C)[C@@H](Cl)C2)=O	C23H28Cl2O5	455.371	Dichlorisone acetate	
Medchem						
Express	HY-14929A	O[C@H]1[C@H](CO)NC[C@H](O)[C@H]1O.Cl	C6H14ClNO4	199.633	Migalastat (hydrochloride)	
Medchem		O=C(NCC(N[C@H](C(N[C@H](CC1=CC=CC=C1)C(N([C@H]2C(C)C)C)=O				
Express	HY-16141)=O)CC(O)=O)[C@H](CCCNC(N)=N)NC2=O	C27H40N8O7	588.656	Cilengitide	
Medchem		NC1=NC=NC2=C1C(Br)=CN2[C@H]3[C@H](O)[C@H](O)[C@@H](CN(CC				
Express	HY-15650	CNC(NC4=CC=C(C(C)(C)C)C=C4)=O)C(C)CO3	C28H40BrN7O4	618.566	SGC0946	
Medchem						
Express	HY-15449	O=C1C(O)=C(C2=CC=C(O)C)C=C2)OC3=CC(O)=CC(O)=C13	C16H12O6	300.263	Kaempferide	

Medchem		<chem>C1C1=CC(C2=CC=C(N=CC(C(C)=O)=C3N[C@H]4CC[C@H](CN(C)C)CC4)C3=N2)=CC(CI)=C1O.[H]Cl</chem>			OTSSP167
Express	HY-15512A		<chem>C25H29Cl3N4O2</chem>	523.882	(hydrochloride)
Medchem					
Express	HY-50855	<chem>O=C(C1=CC=C2C3=C(C(NC4=CC=CC(CI)=C4)=NC2=C1)C=CN=C3)O</chem>	<chem>C19H12ClN3O2</chem>	349.771	CX-4945
Medchem		<chem>O=C1C2=C(C(C=C(C([C@]3([H])[C@H](O)CN(C)CC3)=C2O)C(C4=CC=CC=C4C)=C1)O)O</chem>	<chem>C21H20ClNO5</chem>	401.84	Flavopiridol
Express	HY-10005				
Medchem		<chem>N[C@@H](CCCCNC(C)=N)C(O)=O</chem>	<chem>C8H17N3O2</chem>	187.24	L-NIL
Express	HY-12116				Phenethylamine, 2,6-
Medchem		<chem>NCCC1=C(C=C=C1Cl)Cl</chem>	<chem>C8H9Cl2N</chem>	190.07	dichloro-
Express	HY-107374				
Medchem		<chem>O=C([C@@H](N)C(C)C)N[C@H](C(O)=O)CC1=CC=CC=C1</chem>	<chem>C14H20N2O3</chem>	264.32	L-Valyl-L-phenylalanine
Express	HY-107378	<chem>C[C@@]12[C@@](C#CC)(O)CC[C@@]1([H])[C@]3([H])CCC4=CC(CCC4=C3[C@@H](C5=CC=C(N(C)C)C=C5)C2)=O</chem>	<chem>C29H35NO2</chem>	429.594	Mifepristone
Medchem	HY-13683	<chem>C1(C2=CC=CC(OCCN3CCCCC3)=C2)=NNC4=C1C=C(C=C4)C5=NC=NN5</chem>	<chem>C22H25ClN6O</chem>	424.927	CC-401 (hydrochloride)
Express	HY-13022	<chem>Cl</chem>			
Medchem		<chem>CC(C(C)[C@H](NCC1=CC=NC=C1)C(N2CC3=C(C=C(O)C(O)C=C3)CC2)=O</chem>	<chem>C23H31N3O3</chem>	397.511	TCS-OX2-29
Express	HY-100452				
Medchem		<chem>OC1=CC=C(C(C(C)=C(C)C)/C2=CC=C(O)C=C2)C=C1</chem>	<chem>C18H20O2</chem>	268.35	Diethylstilbestrol
Express	HY-14598				Dapiprazole
Medchem		<chem>CC1=CC=CC=C1N2CCN(CCC3=NN=C4CCCCN43)CC2.[H]Cl</chem>	<chem>C19H28ClN5</chem>	361.912	(hydrochloride)
Express	HY-A0142A	<chem>O[C@@H]1[C@H](C)[C@]2([H])CC[C@H](C)[C@]3([H])CC[C@@](O4)(C)O[C@]32[C@]4([H])O1</chem>	<chem>C15H24O5</chem>	284.348	Dihydroartemisinin
Medchem	HY-N0176				Roxatidine (Acetate
Express	HY-B0305A	<chem>O=C(NCCCOC1=CC=CC(CN2CCCCC2)=C1)CO(C)C=O.Cl</chem>	<chem>C19H29ClN2O4</chem>	384.898	Hydrochloride)
Medchem		<chem>O=C(NCC(N[C@H]1CN(CC2=CC=C(CI)C=C2)CC1)=O)C3=CC=CC(C(F)(F)F)=C3</chem>	<chem>C21H21ClF3N3O2</chem>	439.859	Teijin compound 1
Express	HY-108323	<chem>O[C@@H]1[C@H]([C@H]([C@H](N2C=NC3=C2N=C(N)N=C3SCC4=CC=C([N+])([O-])=O)C=C4)O1)O)O</chem>	<chem>C17H18N6O6S</chem>	434.426	NBTGR
Medchem	HY-108322	<chem>O=C(NC1=CC=C(N(C)[C@H](C(C)C)C(N[C@H](CO)C2=O)C2=C1)/C=C(C)C3=CC=C(C(F)(F)F)C=C3</chem>	<chem>C27H30F3N3O3</chem>	501.541	TPPB
Express	HY-12359	<chem>O=C(N(CCC1=CC=CC=C1O)C[C@H]2CNCC2)C3=CC=C(CN(CC)CC)C=C3.[H]Cl.[H]Cl</chem>	<chem>C25H37Cl2N3O2</chem>	482.486	PF429242
Medchem	HY-13447A				(dihydrochloride)
Express	HY-B0741A	<chem>O=C(N1CCN(C)CC1)O[C@@H]2N(C3=NC=C(CI)C=C3)C(C4=NC=CN=C42)=O</chem>	<chem>C17H17ClN6O3</chem>	388.808	Zopiclone (S-enantiomer)
Medchem		<chem>F C1=C(CN2CCOCC2)C(F)=CC(C3=C4N=C(C5=CN(C6CCNCC6)N=C5)C=NC4=CC=C3)=C1.Cl.Cl</chem>	<chem>C27H30Cl2F2N6O</chem>	563.47	NVP-BSK805
Express	HY-14722A				(dihydrochloride)
Medchem		<chem>O=C(O)CC1=CC=C(C(C2=C1)OCC3=CC=CC=C3CC2=C(CCN(C)C.Cl</chem>	<chem>C21H24ClNO3</chem>	373.873	Olopatadine
Express	HY-B0426A	<chem>N[C@@H](C1)CCCN1[C@@H]2CC3=CC=CC=C3[C@H]2O C4=C(CI)C=C(C#N)C=C4</chem>	<chem>C21H22ClN3O</chem>	367.872	(hydrochloride)
Medchem	HY-15699	<chem>O=C(N)C1=CC=CC=C1NC2=NC(C3=CC=C(C(O)C=C3)OC)=CC4=NC=CN</chem>	<chem>C20H20Cl2N6O3</chem>	463.317	SAR7334
Express	HY-14985	<chem>24.[H]Cl.[H]Cl</chem>			BAY 61-3606
Medchem		<chem>[H]Cl.[H]Cl.NCCCCN(CC1=NC2=CC=CC=C2N1)[C@@H]3C4=NC=CC=C4CCC3.[H]Cl</chem>	<chem>C21H30Cl3N5</chem>	458.855	(dihydrochloride)
Express	HY-50101A	<chem>O=C([C@@H](N1)CCC1=O)C[C@@H](CCCCN(C)=N)C(N2[C@H](CCC2)(N[C@H](CCNC(N)=N)C(N[C@H](CC(C)C)C(N[C@H](CO)C(N[C@H](C(N[C@H](CCCCN)C(NCC(N3[C@@H](CCC3)C(N[C@H](CCS)C(C)N4[C@H](CCC4)C(N[C@H](C(O)=O)CC5=CC=CC=C5)=O)=O)=O)=O)=O)CC6=CNC=N6)=O)=O)=O</chem>	<chem>C70H109N21O16S</chem>	1532.811	AMD-070 (hydrochloride)
Medchem	HY-P1033	<chem>O=C(N[C@H](C)C(N[C@H](C(C)C)C(NCC(N[C@H](C(N[C@H](CC(C)C)C(N[C@H](C(N)=O)CCSC)=O)=O)CC1=CN=CN1)=O)=O)[C@@H](NC([C@H](CCC(N)=O)NC([C@H](CC(N)=O)NC(CNC([C@H](CC(C)C)N C([C@H](CCCNC(N)=N)NC([C@H](CCC(N)=O)NC([C@H](N2)CCC2=O)=O)=O)=O)=O)=O)CC3=CNC4=CC=CC=C34</chem>	<chem>C71H110N24O18S</chem>	1619.848	[Pyr1]-Apelin-13
Express	HY-P0195				Bombesin
Medchem					
Express	HY-N1394	<chem>O=C(O)C1=CC=C(C(O)C)C=C1</chem>	<chem>C8H8O3</chem>	152.147	4-Methoxybenzoic acid
Medchem		<chem>C[C@H](CCC(O)=O)[C@H]1CC[C@]2([H])[C@]3([H])[C@@H](O)C[C@]4([H])C[C@H](O)CC[C@]4(C)[C@]3([H])CC[C@]12C</chem>	<chem>C24H40O4</chem>	392.572	UAMC00039
Express	HY-13771				(dihydrochloride)
Medchem		<chem>O=C(N1CCCCC1)[C@@H](N)CCNCC2=CC=C(CI)C=C2.[H]Cl.[H]Cl</chem>	<chem>C16H26Cl3N3O</chem>	382.756	Olaparib
Express	HY-101769	<chem>O=C(C1=CC(C2=CC(C3=CC=C2)=NNC3=O)=CC=C1F)N4CCN(C(C5CC5)=O)CC4</chem>	<chem>C24H23FN4O3</chem>	434.463	N6022
Medchem	HY-10162	<chem>OC(CCC1=CC=C(N1C2=CC=C(C(N)=O)C=C2)C(C=C3)=CC=C3N4C=CN=C4)=O</chem>	<chem>C24H22N4O3</chem>	414.457	Olodaterol
Express	HY-14984	<chem>O=C1NC2=CC(O)=CC([C@@H](O)CNC(C)(C)CC3=CC=C(C(O)C=C3)=C2</chem>	<chem>C21H26N2O5</chem>	386.442	
Medchem	HY-14301	<chem>OC1</chem>			

Medchem		<chem>O=C(CC1)O[C@@]21CC[C@@]3([H])[C@]4([H])[C@H](C(OC)=O)CC5=</chem>			
Express	HY-B0251	<chem>CC(C[C@]5(C)[C@@]46[C@H](O6)C[C@@]32C)=O</chem>	C24H30O6	414.491	Eplerenone
Medchem		<chem>C[C@]1([C@]([C@H](C)/C=C/[C@H](C)C(C)O)([H])CC1)(CC(2)[C@]1([H])C2=C1C=C3C[C@@H](O)C[C@H](O)C/3</chem>	C27H44O3	416.637	Paricalcitol
Express	HY-50919	<chem>O(C(CO C1=CC=CC2=C1C[C@]([C@@H](O)[C@@H]3CC[C@@H](O)C</chem>			
Medchem	HY-100441	<chem>CCCC)([H])[C@]3([H])C2)=O</chem>	C23H34O5	390.513	Treprostinil
Express	HY-108313	<chem>CC1=NC2=C(C3=CC=C(C(OC)C(OC)=C3)C(C)=NN2C(NCCN4CCOCC4)=C1</chem>	C22H29N5O3	411.497	T-00127_HEV1
Medchem					
Express	HY-A0070A	<chem>OC1=C(I)C=C(OC2=C(I)C=C(C[C@H](N)C(O)=O)C=C2)C=C1</chem>	C15H12I3NO4	650.974	3,3',5-Triodo-L-thyronine
Medchem		<chem>O=C1NC(C(C2=CN(C3=CC=CC=C3)CCO[C@H](CN(C)C)CC4)=C1C5=C</chem>			Ruboxistaurin
Express	HY-10195B	<chem>N4C6=CC=CC=C56)=O.[H]Cl</chem>	C28H29ClN4O3	505.008	(hydrochloride)
Medchem		<chem>3N(C([C@H](CO)NC([C@H](CC4=CC=CS4)NC(CNC([C@@H]5C[C@@H](</chem>			
Express	HY-17446	<chem>O)CN5C([C@H]6N(C([C@H](CCCNC(N)=N)NC([C@H](N)CCCNC(N)=N)=</chem>			
Medchem		<chem>O)=O)CC6)=O)=O)=O)=O)CC7=C(C=CC=C7)C3)=O)[C@]2([H])CC</chem>	C59H89N19O13S	1304.522	Icatibant
Express	HY-12588	<chem>CC1</chem>			
Medchem					
Express	HY-50759	<chem>O[C@H]1[C@H](O)[C@@]2([H])N=C(NCC)S[C@@]2([H])O[C@@H]1CO</chem>	C9H16N2O4S	248.299	Thiamet G
Medchem		<chem>O=C1N(CC2=CC=CC=C2)C([C@@H](C(C)N(CCCN)C(C3=CC=C(C)C=C</chem>			
Express	HY-10969	<chem>3)=O)=NC4=CC(CI)=CC=C14</chem>	C30H33ClN4O2	517.062	Ispinesib
Medchem		<chem>COC1=CC(C2=CC3=C(C=CC=C3)N2)=N/C1=C1C4=C(C=C(N4)C)C.CS(=</chem>			
Express	HY-B0600	<chem>O)(O)=O</chem>	C21H23N3O4S	413.49	Obatoclox
Medchem		<chem>O=C(O(C(C)CCC/C=C1C[C@@H]1[C@H](/C=C/C(F)(F)COC2=CC=C</chem>			
Express	HY-B1480	<chem>C=C2)[C@H](O)C[C@@H]1O</chem>	C25H34F2O5	452.531	Tafuprost
Medchem					
Express	HY-13755	<chem>O=S(C1=NC2=CC=C(C(OC)C=C2S1)(N)=O</chem>	C9H10N2O3S2	258.317	Ethoxzolamide
Medchem					
Express		<chem>O=S(CCCCN=C=S)C</chem>	C6H11NOS2	177.288	Sulforaphane
Medchem		<chem>O=C(N[C@@H](C(C)C)C(NCC(N[C@@H](CC(C)C)C(N[C@H](C(N)=O)CC</chem>			
Express	HY-P0197	<chem>SC)=O)=O)=O)[C@@H](NC([C@H](CO)NC([C@H](CC(O)=O)NC([C@@</chem>			
Medchem		<chem>])([C@H](O(C)[H])NC([C@H](CCCCN)NC([C@H](N)CC1=CN=CN1)=O)</chem>			
Express	HY-18077	<chem>=O)=O)=O)=O)CC2=CC=CC=C2</chem>	C50H80N14O14S	1133.321	Neurokinin A
Medchem					
Express	HY-13004	<chem>COC1=CC2=C(C=C1O)C=C(CN=C2CC3=CC=C(C(OC)C(OC)=C3</chem>	C20H21NO4	339.385	Papaverine
Medchem		<chem>O=C(C1CCC(F)(F)CC1)N[C@H](C2=CC=CC=C2)CCN3[C@H]4C[C@@H](</chem>			
Express	HY-15872A	<chem>N5(C)=NN=C5(C)C[C@@H]3CC4</chem>	C29H41F2N5O	513.666	Maraviroc
Medchem		<chem>CSCC[C@@H](C(OC)=O)NC(C1=CC=C(C(NC[C@@H](N)CS)C=C1C2=CC=</chem>			
Express	HY-14127	<chem>CC=C2)=O.[H]Cl</chem>	C22H30ClN3O3S2	484.075	FTI-277 (hydrochloride)
Medchem					
Express	HY-15292	<chem>CCCN(C1=CC(C)=NC2=C(C3=CN=C(N(C)C)C=C3C)C(C)=NN21)CCC</chem>	C22H32N6	380.53	R121919
Medchem					
Express	HY-17412	<chem>COC1=CC=C2C(CN(C)CCS2)=C1</chem>	C11H15NOS	209.308	S107
Medchem		<chem>OC1=C(C(N)=O)C([C@@]2(O)C(O)=C3C(C4=C(O)C=CC(N(C)C)=C4C[C</chem>			Minocycline
Express	HY-14992	<chem>@]3([H])C[C@@]2([H])[C@@H]1N(C)=O)=O.Cl</chem>	C23H28ClN3O7	493.937	(hydrochloride)
Medchem		<chem>O=C1N=C(CN2C1=C(N=C2[C@H])(CCCC3=CC=CC=C3)[C@@H](C(O)</chem>			
Express	HY-P0224	<chem>C)CC4=CC=C(C(OC)=C4)OC</chem>	C27H32N4O4	476.567	Bay 60-7550
Medchem		<chem>O=C(O)[C@H](CC1=CC=CC=C1)NC([C@H](CC(C)C)NC([C@H](CCSC)N</chem>			
Express	HY-B1334A	<chem>C=O)=O)=O</chem>	C21H31N3O5S	437.553	N-Formyl-Met-Leu-Phe
Medchem					
Express	HY-108321	<chem>O=C(O)/C=C1C(O)=O.C1(CC(C2CCCC2)C3CCCC3)NCCCC1</chem>	C23H39NO4	393.56	Perhexiline maleate
Medchem		<chem>O=C(O)[C@H]1N(C([C@H](C)CS(C2=CC=CC=C2)=O)=O)C[C@@H](S</chem>			
Express	HY-107372	<chem>C3=CC=CC=C3)C1</chem>	C22H23NO4S2	429.552	Zofenopril
Medchem		<chem>O[C@H]1[C@H](N2C(NC(C2)=O)=O)O[C@H](COP(OP(OP(O)=O)=O)</chem>			
Express	HY-B0374	<chem>(O)=O)(O)=O)[C@H]1O</chem>	C9H15N2O15P3	484.141	Uridine triphosphate
Medchem					
Express	HY-10234	<chem>CC1=NC(OC)=C(NC2=NCCN2)C(CI)=N1</chem>	C9H12ClN5O	241.678	Moxonidine
Medchem		<chem>Cl(C1=CC=C2C(OCO2)=C1NC3=C4C(OC5CCOCC5)=CC(OCN6CCN(C)C</chem>			
Express	HY-17368	<chem>C6)=CC4=NC=N3</chem>	C27H32ClN5O5	542.027	Saracatinib
Medchem					
Express	HY-13803	<chem>O=C(N(C)CC)OC1=CC=CC([C@H](C)N(C)C)=C1</chem>	C14H22N2O2	250.337	Rivastigmine
Medchem		<chem>O=C(C1=CC(C2=CC=C(CN3CCOCC3)C=C2)=CC(N(C)C)C4CCOCC4)=C1C</chem>			
Express	HY-15656	<chem>)NCC5=C(C)C=C(C)NC5=O</chem>	C34H44N4O4	572.738	EPZ-6438
Medchem		<chem>CC(C)OC1=CC(C2CCNCC2)=C(C)C=C1NC3=NC=C(CI)C(NC4=CC=CC=C4</chem>			
Express	HY-B0180	<chem>S(=O)(C(C)C)=O)=N3</chem>	C28H36ClN5O3S	558.135	LDK378
Medchem					
Express	HY-17040	<chem>NC1=NC2=CC=CC=C2C3=C1N=CN3CC(C)C</chem>	C14H16N4	240.304	Imiquimod
Medchem		<chem>O=C(O[C@@H]1[C@@]2([H])[C@@]([OCC2]([H])OC1)N[C@@H](CC3=C</chem>			
Express		<chem>C=CC=C3)[C@H](O)CN(S(=O)(C4=CC=C(N)C=C4)=O)CC(C)C</chem>	C27H37N3O7S	547.664	Darunavir

Medchem					
Express	HY-13677	S=C1NC=NC2=C1NC=N2	C5H4N4S	152.177	6-Mercaptopurine
Medchem		O=C(C1=C(C(=O)C=C(NC(C2=CC(F)=CC=C2C)=O)C=C1)N(C3)C4=CC=CC=C4CN5C3=CC=C5	C27H21ClFN3O2	473.926	Lixivaptan
Express	HY-14185	O=C1[C@@H](N(C2=C(N1C)C=NC(NC3=CC=C(C(NC4CCN(C)CC4)=O)C=C3O)C=N2)C5CCCC5)CC	C28H39N7O3	521.654	BI 2536
Medchem					Pramipexole
Express	HY-17355	NC(S1)=NC2=C1C[C@@H](NCCC)CC2.[H]Cl.[H]Cl	C10H19Cl2N3S	284.249	(dihydrochloride)
Medchem					
Express	HY-12787	OC1=CC(C2=C(C3=CC=NC=C3)N=C(C4=CC=CC=C4)N2)=CC=C1Cl	C20H14ClN3O	347.798	L-779450
Medchem		O=C(C1=CC2=C(N(C)C=N3)C3=C(C(NC4=NN(C)C(C)=C4)N=C2N1CC)N(C5CC5)C6CC6	C23H28N8O	432.521	BMS-911543
Express	HY-15270	O=C(C1=C(C(C=CC=C1)NC2=NC(NC3=C(C=C(C(C=C3)N4CCOCC4)O)C)=NC=C2C)N	C23H25ClN6O3	468.936	NVP-TAE 226
Medchem		NC1=NC=NC2=C1N=CN2[C@@H]3[C@@H](O)[C@H](O)[C@@H](CN([C@@H]4C[C@@H](CCC5=NC6=C(C(C=CC(C(C)C)C)C)C)C)O3	C30H42N8O3	562.706	EPZ-5676
Express	HY-15593	O=C1O[C@@H]([C@@H](N1CC2=CC(C(F)(F)F)=CC=C2C3=CC(C(C)C)=C(C=C3O)F)C4=CC(C(F)(F)F)=CC(C(F)(F)F)=C4	C30H25F10NO3	637.508	Anacetrapib
Medchem		O=C(C1=C(C(C)C2=CC=CC=C2)N3=C(C=C(C=C13)N[C@@H](C4=CC=C(C=C4)CC	C26H24N2O	380.482	SB-222200
Express	HY-15722				
Medchem					
Express	HY-13287	CN1CCC(CC1)CNC2=NN3C(C=C2)=NC=C3C4=CC=CC(OC(F)(F)F)=C4	C20H22F3N5O	405.417	SG1-1776
Medchem					
Express	HY-15388	O=C(C1=CC=C(C#CC2=CC=C3C(C(C)(C)CCS3)=C2)N=C1)OCC	C21H21NO2S	351.462	Tazarotene
Medchem					
Express	HY-14171	CC1(C2=C(C(C)(CC1)C)C=C(C(C(C3=CC=C(C(C=C3)C(O)=O)=C)=C2)C)C	C24H28O2	348.478	Bexarotene
Medchem					
Express	HY-B0246	O=C(N1C2=CC=CC=C2C=CC3=CC=CC=C3)N	C15H12N2O	236.269	Carbamazepine
Medchem		O=C(NC1=CC=CC(F)=C1)CC2=CC(CN3=C4C=CC(OC(CCN(CC)CCOP(O)(O)=O)=CC4=NC=N3)=NN2	C26H31FN7O6P	587.54	AZD1152
Express	HY-10127	O=C(C(C1=CN2CCN(C(N3CCCC3)=O)CC4=CC(F)=CC1=C42)=C5C6=C(N=C7C=CC=CN7)NC5=O	C28H25FN6O3	512.535	LY2090314
Medchem		BrC1=CN=C(C(OCOC2=C(C3=CC=C(Br)C=C3)C(NS(NCCC)(=O)=O)=NC=N2)N=C1	C19H20Br2N6O4S	588.273	Macitentan
Express	HY-14184				
Medchem					
Express	HY-16692	O=C(OC)CC1ON=C(C(C=C2)=CC=C2O)C1	C12H13NO4	235.236	ISO-1
Medchem					
Express	HY-12246	O=C(O)C1=C(C(C(F)(F)F)=CC=C1N2C[C@@H](OCC3=NC=CC=C3)CC2	C18H17F3N2O3	366.334	XEN445
Medchem					Guanfacine
Express	HY-17416	O=C(NC(N)=N)CC1=C(C(=O)C=CC=C1Cl.[H]Cl	C9H10Cl3N3O	282.554	(hydrochloride)
Medchem					
Express	HY-13734	CCC(SSC1=NC=CN1)C	C7H12N2S2	188.314	PX-12
Medchem					
Express	HY-15388	O=C(C1=CC=C(C#CC2=CC=C3C(C(C)(C)CCS3)=C2)N=C1)OCC	C21H21NO2S	351.462	Tazarotene
Medchem					
Express	HY-15433	O=C(C1=CN=C(N2CCC(CNCC3=NC(C)C4=C3C=CC=C4)CC2)N=C1)NO	C21H26N6O2	394.47	Quisinostat
Medchem					
Express	HY-13227	FC1=CC=C(C(=O)C=C1C2=NC3=NC=CN=C3(CN4=CC=NC=C4)=N2	C17H10ClFN6	352.753	SD-208
Medchem					
Express	HY-13688	O=C(NC(C=C1C2=C3C=CC=C2)=CC=C1NC3=O)CN(C)C.Cl	C17H18ClN3O2	331.797	PJ34 (hydrochloride)
Medchem					
Express	HY-13749	O=C(N1CC2=NN=C(C(F)(F)F)N2CC1)C[C@@H](N)CC3=CC(F)=C(F)C=C3F	C16H15F6N5O	407.314	Sitagliptin
Medchem					
Express	HY-15202	BrC1=CC=C(C(F)=C1)NC2=C(C3=C(C=C2C(NOCCO)=O)N(C=N3)C)F	C17H15BrF2N4O3	441.227	MEK162
Medchem		O=C(NC1=CC(C(C)(C)C)=NN1C2=CC=C(C(C)C=C2)NC3=C4C=CC=CC4=C(OCN5CCOCC5)C=C3	C31H37N5O3	527.657	Doramipimod
Express	HY-10320				
Medchem					
Express	HY-13104	S=C(NCCCCNC(NC1=CC(N=C=S)=CC=C1)=S)NC2=CC(N=C=S)=CC=C2	C20H20N6S4	472.673	MRS 2578
Medchem					Desvenlafaxine (succinate
Express	HY-B0602A	OC1=CC=C(C(C2(O)CCCCC2)CN(C)C)C=C1.O=C(O)CCC(O)=O.O	C20H33NO7	399.479	hydrate)
Medchem		O=C(C1=CC=CN(C2=CC=C(F)C(F)=C2)C1=O)N[C@@H](C3=CC=CC=C3)CO4=C(C=C(C(N5)C(NC5=O)=C4	C28H22F2N4O4	516.496	PDK1 inhibitor
Express	HY-14440	O=C(NC1=CC=C(C2=CC=C(C([C@@H]3CCCC[C@@H]3C(O)=O)=O)C=C2)C=C1)NC4=CC=CC=C4	C26H24N2O4	428.48	A 922500
Medchem					
Express	HY-15315	N#CCC1(N2N=CC(C3=C4C(NC=C4)=NC=N3)=C2)CN(S(=O)(CC)=O)C1	C16H17N7O2S	371.417	Baricitinib
Medchem		CC1=CC=C(C=C1NC2=NC(C3=CC=CN=C3)=NC4=C2C=NN4C)C(NC5=CC=CC(C(F)(F)F)=C5)=O	C26H20F3N7O	503.479	NVP-BHG712
Express	HY-13258				

Medchem		[H]Cl.COC1=C(O(C)C)=C(C(N[C@H]2[C@H](C(C)O)CNC2)=NC(C3=C(O			CCT241533
Express	HY-14715B)C=CC(F)=C3)=N4)C4=C1	C23H28ClFN4O4	478.944	(hydrochloride)
Medchem		CCCCNC1=NC(N[C@H]2CC[C@H](O)CC2)=C(C(NCC3=CC=C(N4C=NC			
Express	HY-15798	=C4)C=C3)=O)C=N1	C25H33N7O2	463.575	UNC2881
Medchem		O=C(C1=C2C(N=C(OCC)N2CC3=CC=C(C4=CC=CC=C4C(N5=NOC5=O)			
Express	HY-14914	C=C3)=CC=C1)O	C25H20N4O5	456.45	Azilsartan
Medchem		NC1=NC=C(C2=CC=C(S(=O)(C(C)C)=O)C=C2)N=C1C3=CC(C4=CC=C(C			
Express	HY-13902	NC)C=C4)=NO3	C24H25N5O3S	463.552	VE-822
Medchem		O=C(O)C1=CC=C(N(CC2=CC=C(C3CCCCC3)C=C2)C(CN(C)S(=O)(C4=C(
Express	HY-16975	F)C(F)=C(F)C(F)=C4F)=O)=O)C=C1	C29H27F5N2O5S	610.592	SH-4-54
Medchem		O=C(N([C@@H](C1=NC2=NC=CC=C2C(N1C3=CC=C(OCC)C=C3)=O)C)			
Express	HY-15320	CC4=CC=CN=C4)CC5=CC=C(F)C(C(F)(F)F)=C5	C32H27F4N5O3	605.582	NBI-74330
Medchem					
Express	HY-13075	CN(CC1)CCN1C2=CC=C(NC(C3=CC(C#N)=CN3)=O)C(N4CCC(C)CC4)=C2	C23H30N6O	406.524	c-FMS inhibitor
Medchem		O=C([C@H](CSSCCC(N[C@@H](C1=O)CC2=CC=C(OCC)C=C2)=O)NC([
Express	HY-17572	C@@H](NC(C(NC([C@](N1)([H])([C@@H](C)CC)=O)[C@H](O)C)=O)CC(C43H67N11O12S2	994.189	Atosiban
Medchem		N)=O)=O)N(CCC3)[C@@H]3C(N[C@@H](CCCN)C(NCC(N)=O)=O)=O			
Express	HY-50907	CN(CC[C@@H](NC1=CC=C(C=C1[N+])([O-			
Medchem))=O)S(NC(C2=CC=C(C=C2)N3CCN(CC3)CC4=CC=CC=C4C5=CC=C(C=	C42H45ClN6O5S2	813.427	ABT-737
Express	HY-10109	C5)Cl)=O)(=O)=O)CS C6=CC=CC=C6)C			
Medchem					
Express	HY-10109	O=C(NC(/=O)SC1=C/C2=CC=C3N=CC=NC3=C2	C12H7N3O2S	257.268	AS-605240
Medchem		F(C1=C1N=C(C(NC2=C(C1)N([C@@H]3[C@@H](F)CN(C4CO C4)CC3)N=C2)			
Express	HY-12282	N=C1NC)(F)F	C17H20ClF4N7O	449.834	GN-9605
Medchem		CCC1=CN=C(N2CCC(C3=NC(CO C4=CC=C(N5N=NN=C5)C=C4)=CS3)CC			
Express	HY-15291	2)N=C1	C22H24N8O S	448.544	MBX-2982
Medchem					
Express	HY-19351	O=C1C=C(C2=CC=C(C(C)C)C=C2)OC3=CC=CC=C13	C18H16O2	264.319	MN-64
Medchem		O=C1C(C2=NC3=CC(N4CCOCC4)=CC(C)=C3N2)=C(C=CN1)N[C@@H](
Express	HY-10262	O)C5=CC=CC(C1)=C5	C25H26ClN5O3	479.959	BMS-536924
Medchem		ClC1=CC2=C(C=C1)C=CC(/C=C/C3=CC([C@H](SCC4(C([O-			
Express	HY-13315))=O)CC4)CCC5=CC=CC=C5C(C)(O)C)=CC=C3)=N2.[Na+]	C35H35ClNNaO3S	608.165	Montelukast (sodium)
Medchem					
Express	HY-15224	COC(C=C1)=CC=C1CN2C3=CC(C(NO)=O)=CC=C3C=C2	C17H16N2O3	296.321	PCI-34051
Medchem					
Express	HY-13340	CC1=C2C(SC(C(NCC3=CC=C(O(C)C=C3)=O)=C2N)=NC(C)=C1	C18H19N3O2S	341.427	VU0152100
Medchem		O=C1N(C[C@@]([H])(CCC2)C3=C2C=CC=C13)[C@@H]4CN5CCC4CC5.[
Express	HY-A0021	H]Cl	C19H25ClN2O	332.868	Palonosetron (Hydrochloride)
Medchem					
Express	HY-14397	COC1=CC=C(N(C(C2=CC=C(C1)C=C2)=O)C(C)=C3CC(O)=O)C3=C1	C19H16ClNO4	357.788	Indomethacin
Medchem					
Express	HY-18314	O=C1/C(C2=NC=CC=C2N1)=C\C3=CN(C)C4=C3C=CC=C4	C17H13N3O	275.305	GW 441756
Medchem					
Express	HY-15452	O=C(C1C(NC2=C3C=C(C1)C=C2)=C3CCC1)N	C13H13ClN2O	248.708	EX-527
Medchem		O=C(C1=CC=CC=C1)N(C)[C@H]2[C@@H](O(C)[C@@]3(C)N(C4=C5C=C			
Express	HY-10230	C=C4)C6=C5C7=C(C(NC7)=O)C8=C6N(C9=CC=CC=C9)[C@@](O3)([H])	C35H30N4O4	570.637	PKC412
Medchem		CC1=CC=CC(C(C(N2CCC3=C2C=CC(C4=CN(C)C5=NC=NC(N)=C54)=C3F)			
Express	HY-13820	=O)=N1	C23H21FN6O	416.451	GSK2656157
Medchem					
Express	HY-13805	NC1=C2C(N(C(C)C)N=C2C3=CC=C(C1)C=C3)=NC=N1	C15H16ClN5	301.774	PP2
Medchem		O=C(C1=CC=C([C@@H](C)N)C=C1)NC2=C3C(NC=C3)=NC=C2.[H]Cl.[H]			
Express	HY-10069	Cl	C16H18Cl2N4O	353.246	Y-33075 (dihydrochloride)
Medchem		O=C(C[C@H]1C2=NN=C(N2C3=C(C(C4=CC=C(C=C4)Cl)=N1)C(C)=C(S3)			
Express	HY-13030	C)C)OC(C)C)C	C23H25ClN4O2S	456.988	(+)-JQ-1
Medchem					
Express	HY-16425	O=C(NCCCCC(NC1=CC=CC=C1N)=O)C2=CC=C(C)C=C2	C20H25N3O2	339.431	RG2833
Medchem					
Express	HY-12041	O=C1C2=C3C(NN=C3C4=C1C=CC=C4)=CC=C2	C14H8N2O	220.226	SP600125
Medchem					
Express	HY-14711	C1(NC2=CC=C(N3CCOCC3)C=C2)=NC(NC4CCCCC4)=C5C(NC=N5)=N1	C21H27N7O	393.485	Reversine
Medchem		OC(C(/C=N1CCN(C)CC1)=C(NC(/C)=Cl)C=C[C@@H]([C@@H]([C@			
Express	HY-B0272	@H)(C)[C@H]2O)O)C)=O)C(O)=C3C(O)=C4C)=C3C5=C4O[C@](C)(O/C	C43H58N4O12	822.94	Rifampicin
Medchem		=C/[C@@H]([C@H]([C@@]([C@@H]2C)([H])O(C)=O)C)OC)C5=O			
Express	HY-12529	O=C1N=C(NCC2=CC=CS2)S/C1=C\C3=CC=C4N=CC=C4=C3	C18H13N3O S2	351.445	Ro-3306
Medchem		NC(C1=CN=C(N[C@H]2[C@@H](N)CCCC2)N=C1NC3=CC=CC(N4N=CC=			
Express	HY-15323	N4)=C3)=O.[H]Cl	C19H24ClN9O	429.907	(Hydrochloride)

Medchem					
Express	HY-B0553	CC(/N=C1SC(S(=O)(N)=O)=NN/1C)=O	C5H8N4O3S2	236.272	Methazolamide
Medchem		C1C1=CC=C(C(C@H)(C2=CC=CC(C#N)=C2)[C@@H](NC(C(C)(OC3=CC			
Express	HY-10013	=C(C=N3)C(F)(F)C)=O)C)C=C1	C27H25ClF3N3O2	515.955	Taranabant
Medchem		N#CC1(NC([C@@H](N[C@H](C(F)(F)F)C2=CC=C(C3=CC=C(S(=O)(C)=			
Express	HY-10042	O)C=C3)C=C2)CC(C)(F)C)=O)CC1	C25H27F4N3O3S	525.559	Odanacatib
		O=C([C@@](CCCC1)([H])N1C(C([C@@]2(O)[C@H](C)C[C@H](OC)[C@			
Medchem		@)(O2)([H])[C@@H](OC)C[C@@H](C)C(C)=C/[C@H]3CC=C)=O)=O)			
Express	HY-13756	O[C@H](/C(C)=C/[C@H]4C[C@@H](OC)[C@H](O)CC4)[C@H](C)[C@@H	C44H69NO12	804.018	Tacrolimus
Medchem		H)(O)CC3=O			
Express	HY-B0121	O=C(O)CCC(O)=O.O.O=S(CCC1=CC2=C(NC=C2CCN(C)C)C=C1)(NC)=O	C18H27N3O6S	413.489	Sumatriptan (succinate)
Medchem		O=C(O)C(C)CC1=C(SC(C)(C)C)C2=C(C=CC(OCC3=NC4=CC=CC=C4			
Express	HY-10037	C=C3)=C2)N1CC5=CC=C(C)C=C5	C34H35ClN2O3S	587.171	MK-0591
Medchem		O=C1C2(NC[C@@H](C3=CC(F)=CC(F)=C3)N1CC(NC4=CC5=C(C[C@@]			
Express	HY-10302	6(C(NC7=C6C=CC=N7)=O)C5)C=C4)=O)CCCC2.Cl	C31H30ClF2N5O3	594.051	MK-3207 (Hydrochloride)
Medchem		O[C@@H]1[C@H]([C@H]([C@H](N2C=NC3=C2N=CN=C3N[C@@H]4[C			
Express	HY-18978	@H)(O)CCCC(O1)O)O	C15H21N5O5	351.358	GR79236
Medchem		[H]Cl.O=C1N(CCN)C2=CC(OC)=CC=C2N1C([C@H]3[C@H](C(C)C)CC[C			
Express	HY-16162A	@H)(C)C3)=O	C21H32ClN3O3	409.95	D-3263 (hydrochloride)
Medchem		C[C@]1([C@](CC2)([H])(C@]3[H])CCCC=C(O)C)CC[C@]4(C)[C@@]3([H]			
Express	HY-B0697)CC1)=O)C2=O	C19H26O3	302.408	Formestane
Medchem		CO C1=CC2=C(NC3CCN(CC4CCCC4)CC3)N=C(N5CCN(C(C)C)CCC5)N=C			
Express	HY-13808	2C=C1O CCCN6CCCC6	C37H61N7O2	635.926	UNC 0631
Medchem					
Express	HY-13812	NC1=CC2=C(NCCC3=CC=C(O)C4=CC=CC=C4)C=C3)N=CN=C2C=C1	C22H20N4O	356.42	QNZ
Medchem		C[C@@]12[C@](C[C@H](C)[C@]2(O)C(CO)=O)([H])(C@]3[H])CCCC=C			
Express	HY-13570	C(C=C[C@]4(C)[C@@]3F)[C@H](O)C1)=O	C22H29FO5	392.461	Betamethasone
Medchem		O=C1NC([C@H]2[C@@H](CN(C2)CC3=CC=CC=C3)C)=NC4=C1C=NN4C			
Express	HY-50865	5CCOCC5	C22H27N5O2	393.482	PDE-9 inhibitor
Medchem		O=C1C=C(N2CCOCC2)OC3=C1C=CC=C3C4=CC=CC5=C4SC6=C5C=CC			
Express	HY-11006	=C6	C25H19NO3S	413.488	KU-57788
Medchem		O=C(NCCN1CCCC1)C2=C(NC(/C=C3C(NC4=C1.3C=C(C=C4)F)=O)=C2C)			
Express	HY-10330	C	C22H25FN4O2	396.458	Toceranib
Medchem		O=C(NC1=CC=C(NC2=NC(N)=NC(C)=C2)C=C1)C3=CC=C(C(NC4=CC=NC5			
Express	HY-13962	=CC=CC=C45)C=C3	C27H23N7O	461.518	SGI-1027
Medchem		O[C@H]([C@@H]1O)[C@@H](O[C@@H]1C(NC)=O)N2C3=NC(CI)=NC(N			
Express	HY-12365	CC4=CC(I)=CC=C4)=C3N=C2	C18H18ClIN6O4	544.731	2-CHB-MECA
Medchem		NC(C(NC(C)NC(C)NC(C)C1=CN2=C1C=CC=C2)C3=O)=O)CC4=CC=CC=			
Express	HY-17365	C4)=O)CSSCC(C(NC(CO)C(O)C)=O)NC(C(NC(C(CCCCN)N3)=O)C(O)C)=	C51H70N10O12S2	1079.291	Octreotide (acetate)
Medchem		O)=O)CC5=CC=CC=C5.CC(O)=O			
Express	HY-B1227	O=C(O)C(C)C1=CC(NC2=C3C=C(C(C)C=C2)=C3C=C1	C15H12ClNO2	273.714	Carprofen
Medchem		O=C(C1=C2SC(C)C3=C(NN=C3C)C)=C1C(N4C[C@@H](CO4)O)=O)N(C(N			
Express	HY-13248	2CC(C)C)=O)C	C21H27N5O5S	461.535	AR-C155858
Medchem		OC(C1=CC=C(O)CO2)C2=C1)(C3CCN(C(CO4=CC=C([N+])([O-			
Express	HY-15249))=O)C=C4)=O)CC3)C5=CC(O)CO6)=C6=C5	C27H24N2O9	520.487	JZL 184
Medchem		O=C(O)/C=C1C(O)=O.CC(C)(C)C#C/C=C/CC(C)CC1=CC(OCC2=CC(C3			
Express	HY-16343C	=CSC=C3)=CS2)=CC=C1	C31H35NO5S2	565.743	NB-598 (Maleate)
Medchem					
Express	HY-14111	O=C(NC)C(C=N1)=CC=C1O C2=CC(C)C3=C(C=C2)CCN3C4CCCC4	C21H25N3O2	351.442	GSK189254A
Medchem		NS(O[C@]1(O(C(C)(O)O2)[C@@H]2[C@H](O(C(C)(O)O3)[C@H]3CO1)(=			
Express	HY-B0122	O)=O	C12H21NO8S	339.362	Topiramate
Medchem					
Express	HY-15455	O=C(NC1=C(C)C=NC=C1C)C2=CC=C(O(C(F)F)C(C)OCC3CC3)=C2	C17H14Cl2F2N2O3	403.208	Roflumilast
Medchem					
Express	HY-B0134	CC(C)C[C@@H](C(O)=O)NC([C@@H](O)[C@H](N)CC1=CC=CC=C1)=O	C16H24N2O4	308.373	Bestatin
Medchem		O=C(C1=C(N(C)C2=C1C=CC=C2)=C3C4=CN(C5CCN(CO6=NC=CC=C6)			
Express	HY-10342	CC5)C7=C4C=CC=C7)NC3=O	C32H29N5O2	515.605	Enzastaurin
Medchem		CS(=O)(NC1=CC=C(NC2=C(C=CC=C3)C3=NC4=CC=CC=C42)C(O)C)=C1			
Express	HY-13551)=O	C21H19N3O3S	393.459	Amsacrine
Medchem		O=C(NCC(N[C@H]1CN([C@@H]2CC[C@])(C3=CC=C(O)C)N=C3)(O)CC2)			
Express	HY-15450C	CC1)=O)C4=CC=CC(C(F)(F)F)=C4	C26H31F3N4O4	520.544	INCB 3284 enantiomer 1
Medchem					
Express	HY-B0188A	CN(CC1)CC2N1C3=CC=CC=C3CC4=CC=CC=C24.Cl	C18H21ClN2	300.826	Mianserin (hydrochloride)
Medchem		O=C(NC1=CC(C(F)(F)F)=CC(N2C=NC(C)=C2)=C1)C3=CC=C(C(C)C(NC4=N			
Express	HY-10159	C=CC(C5=CC=CN=C5)=N4)=C3	C28H22F3N7O	529.516	Nilotinib

Medchem						
Express	HY-16114	<chem>COC1=CC(C(C2=C(C(C)OC3=C(O)C(C)OC=CC23)=O)=CC(OC)=C1OC</chem>	C20H20O7	372.369	BNC105	
Medchem		<chem>O=C(O)CN(CCOCC1=CC=C(C(C2=CC=C(C(OCO3)C3=C2)C=C1C(C)(C)C)C.C.[Cl</chem>			LY2365109	
Express	HY-100416A	<chem>H]</chem>	C22H28ClNO5	421.914	(hydrochloride)	
Medchem		<chem>ClC1=C(C(C=CC(NC2=NC=NC3=C2C=C(C(C(OC)=C3)OCCCN4CCOCC4)=C1)</chem>				
Express	HY-50895	<chem>F</chem>	C22H24ClFN4O3	446.902	Gefitinib	
Medchem		<chem>C[C@@@]12[C@](OC3=O)(CC3)CC[C@@@]1([H])[C@@@]([C@@@H](CC4=C</chem>				
Express	HY-B0561	<chem>C5=O)SC(C)=O)([H])[C@]([C@]4(CC5C)([H])CC2</chem>	C24H32O4S	416.574	Spironolactone	
Medchem		<chem>O=C1N(C2=C(C(C3=CC=CC(C)=C3)=C1)C=C(C=C2)[C@@@](N)(C4=CN=</chem>				
Express	HY-10502	<chem>CN4C)C5=CC=C(C(C=C5)Cl)C</chem>	C27H22Cl2N4O	489.396	Tipifarnib	
Medchem		<chem>O=C([C@@@H](NC([C@H]([C@@@H](C)O)NC([C@@@H](NC([C@H]([C@@@</chem>				
Express	HY-13821	<chem>H])(C)CC)N(C)C(C)=O)=O)[C@@@H](C)CC)=O)=O)CC(C)C)[C@@@]1(C)CO</chem>	C28H50N4O7	554.719	Epoxomicin	
Medchem		<chem>ClC1=C(CN2N=C(C(C(F)(F)F)=CC=C3)C3=C2C4=CC=C(C(F)=C4)C=CC(F</chem>				
Express	HY-10629	<chem>)=C1</chem>	C21H12ClF5N2	422.778	LXR-623	
Medchem						
Express	HY-15640	<chem>S=C(N1CCCC2=CC(O)=C(O)C=C2C1)NCCC3=CC=C(C)C=C3</chem>	C19H21ClN2O2S	376.9	Capsazepine	
Medchem		<chem>O=C(N1CCC[C@@@H]([C@@@H](OCCNC(OC)=O)C2=CC=CC(C)=C2)C1)N</chem>			VTP-27999 (2,2,2-	
Express	HY-50769	<chem>C[C@@@H](NC)C[C@@@H]3COCCC3.O=C(C(F)(F)F)O</chem>	C28H42ClF3N4O7	639.104	trifluoroacetate)	
Medchem		<chem>O=C(O)CC1=CC=C(C(C2=CC=C(C3=C(NC(O[C@@@H](C4=CC=CC=C4)C)=</chem>				
Express	HY-16040	<chem>O)C(C)=NO3)C=C2)C=C1</chem>	C27H24N2O5	456.49	AM095 (free acid)	
Medchem						
Express	HY-B0422	<chem>O=C(O)[C@@@H](CC1=CC=CC=C1)NC([C@H]2CC[C@@H](C(C)C)CC2)=O</chem>	C19H27NO3	317.423	Nateglinide	
Medchem		<chem>F C1=CC=C(C(F)=C1C(C2=CC=CC=C2)C=C(C(C=C3)C4=CC=C(C(C=C4)Cl)=O)</chem>				
Express	HY-12057	<chem>NS(CCC)(=O)=O</chem>	C23H18ClF2N3O3S	489.922	Vemurafenib	
Medchem		<chem>C[C@@@]12C(C3=CN=CC=C3)=CC[C@@]1([C@@@]4(CC=C5[C@@@](C)([C@</chem>				
Express	HY-70013	<chem>]4(CC2[H])CC[C@@@H](C5O)[H])[H]</chem>	C24H31NO	349.509	Abiraterone	
Medchem						
Express	HY-B0101	<chem>F C1=CC=C(C(C)O)(CN2C=NC=N2)CN3C=NC=N3)C(F)=C1</chem>	C13H12F2N6O	306.271	Fluconazole	
Medchem						
Express	HY-18008	<chem>O=C(C1=CC=CN=C1)NC2=CC(C)=CC3=C2NC4=C3C=CN=C4</chem>	C17H11ClN4O	322.748	PS-1145	
Medchem						
Express	HY-15416	<chem>O=C1NC2=C(C=CC(C)C2Cl)/C1=N/O</chem>	C8H4Cl2N2O2	231.036	NS309	
Medchem						
Express	HY-13822	<chem>OC1=CC=C(CNC2=NC(C3=CC=C(C(C)C)=C3)=CS2)C=C1</chem>	C15H11ClN2OS	302.779	SKI II	
Medchem						
Express	HY-19533	<chem>NC1=NC(N(CCC2=CC=CC=C2)N=C3)=C3C4=NC(C5=CC=CO5)=NN14</chem>	C18H15N7O	345.358	SCH 58261	
Medchem						
Express	HY-15471	<chem>O=C(OC)NC1=CC=C(NCC2=CC=C(F)C2)C=C1N</chem>	C16H18FN3O2	303.331	Retigabine	
Medchem		<chem>O=C([C@H]1CC[C@H](C2=NC(C(N3)=CC4=C3C(OC)=CC=C4)=C5C(N)=</chem>				
Express	HY-10423	<chem>NC=NN52)CC1)O</chem>	C21H22N6O3	406.438	OSI-027	
Medchem						
Express	HY-B0774	<chem>CC(C1=O)=C(C(C(C)=C1C)=O)C(C2=CC=CC=C2)CCCCC(O)=O</chem>	C22H26O4	354.44	Seratrodast	
Medchem		<chem>C[N+](C)(OC1=CC=C(NC(C2=CC3=CC(C4=CC=C(C(C)C=C4)=CC=C3CCC2)</chem>				
Express	HY-13406	<chem>=O)C=C1)C5CCOC5.[Cl-]</chem>	C33H39ClN2O2	531.128	TAK-779	
Medchem		<chem>O=C(C1=NC=CC=C1)NC2=CC=C(S(=O)(NC3=CC=CC=C3Cl)=O)C(Cl)=C</chem>				
Express	HY-15476	<chem>2</chem>	C18H13Cl2N3O3S	422.285	VU 0364439	
Medchem						
Express	HY-15472	<chem>N#CC1=CC(CN2CCC(NC3=C(C=C(Cl)S4)C4=NC=N3)CC2)=CC=C1F</chem>	C19H17ClFN5S	401.888	PRX-08066	
Medchem					4-[(4-chlorophenyl)methyl]-	
Express	HY-76859	<chem>O=S(C1=CC(F)=CC2=C1N(C(C(C3)=CC=C3Cl)C4=C2CCC4CC(O)=O)(</chem>	C21H19ClFN4S	435.896	7-fluoro-1,2,3,4-	
Medchem		<chem>C)=O</chem>			tetrahydro-5-	
Express	HY-16508	<chem>O=C1CCC2=C3[C@@@H](C4=CC=C(N(C)C)C=C4)C[C@@@]5(C)[C@](CC[C</chem>	C30H37NO4	475.619	(methylsulfonyl)-	
Medchem		<chem>@]5(OC(C)=O)C(C)=O)([H])[C@]3([H])CCC2=C1</chem>			Cyclopent[b]indole-3-	
Express	HY-B0259	<chem>O=C(NN1(C)C)CC2=C1C=CC=C2)C3=CC=C(C)C(S(=O)(N)=O)=C3</chem>	C16H16ClN3O3S	365.835	acetic acid	
Medchem		<chem>C[C@]([C@@@]1([H])[C@]2(CC[C@@@H]3O)C(C[C@@@]2([H])C3(C)C)[C</chem>				
Express	HY-N0156	<chem>@@]([C4=CC1)(CC[C@@]5(C)O)=O)[C@@@]4([H])C(C)C(C)CC5)C</chem>	C30H48O3	456.7	Ulipristal (acetate)	
Medchem						
Express	HY-15685	<chem>F C1=CN=CC2=C1C(S(N3CCNC[C@@@H]3C)(=O)=O)=CC=C2.[H]Cl.O.O</chem>	C15H23ClFN3O4S	395.877	Indapamide	
Medchem		<chem>O=C(O)C1=CC(OC)=C(NC([C@H]2[C@H](C3=C(F)C(Cl)=CC=C3)[C@](C</chem>			K-115	
Express	HY-15676	<chem>4=CC=C(C)C=C4F)(C#N)[C@H](CC(C)(C)C)N2)=O)C=C1</chem>	C31H29Cl2F2N3O4	616.482	RG 7388	
Medchem		<chem>O=C(C1=C(N)N(C2=CC=C3N=C(C)NC3=C2)N=C1)C(N4)=CC5=C4C=CC=</chem>				
Express	HY-19957	<chem>C5</chem>	C20H16N6O	356.381	CH5183284	
Medchem						
Express	HY-70068	<chem>O=C(NC1=CC(C)=NC2=C(C(C=C2)F)F)NC3=CC=C(C=C3)N(C)C</chem>	C19H18F2N4O	356.369	SB-408124	

Medchem		CC(C)(O/N=C(C1=CSC(N)=N1)\C(N[C@H]2[C@H](C)N(S(=O)(O)=O)C2=O)=O)C(O)=O	C13H17N5O8S2	435.433	Aztreonam
Express	HY-B0129				
Medchem		CCC(C)(C)C(O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(O3)=O)[C@@]12[H])=O	C25H38O5	418.566	Simvastatin
Express	HY-17502				
Medchem		O=C1N(C2=CC=CC=C2)C([C@H](NC3=C4N=CNC4=NC=N3)C)=CC5=C1C(O)=CC=C5	C22H17ClN6O	416.863	Duvelisib
Express	HY-17044				
Medchem		ClCC/C(C1=CC=CC=C1)=C(C2=CC=C(OCCO)C=C2)\C3=CC=CC=C3	C24H23ClO2	378.891	Ospemifene
Express	HY-B0723				
Medchem		O=C(N(C)C)C(N1C2CCCC2)=CC(C1=N3)=CN=C3NC(N=C4)=CC=C4N5CCCNC5	C23H30N8O	434.537	LEE011
Express	HY-15777				
Medchem		F C(F)(C(O)=O)F.F C(F)(C(O)=O)F.O=C([C@@H]1CC2=C(N=CN2CC3=C(C(N(C)C)C(C)=C3)CN1C(C4=CC=CC=C4)C5=CC=CC=C5)=O)O	C35H34F6N4O7	736.657	PD 123319 (ditrifluoroacetate)
Express	HY-10259A				
Medchem		ClC1=C(N)C(CCO2)=C2C(C(NC3CCN(CCCO)CC3)=O)=C1	C18H26ClN3O3	367.87	Prucalopride
Express	HY-14151				
Medchem		CN(C1CCN(C(C2=CC=C(NC(NC3=CC=C(C4=NC(N5CCOCC5)=NC(N6CCOCC6)=N4)C=C3)=O)C=C2)=O)CC1)C	C32H41N9O4	615.726	PKI-587
Express	HY-10681				
Medchem		O=C(O)CSC1=CC(NS(=O)(C2=CC=C(Br)C=C2)=O)=C3C=CC=CC3=C1O	C18H14BrNO5S2	468.342	UMI-77
Express	HY-18628				
Medchem		O=C1[C@@H](C(C)C)[C@@](N(C/C=C/C/N2CCCC2)=O)CC3([H])[C@]3([H])N1S(=O)(C)=O	C19H31N3O4S	397.532	GW311616
Express	HY-15891				
Medchem		O=C(NC1=NC=CS1)[C@H](CC2CCCC2)C3=CC=C(S(=O)(C)=O)C=C3	C18H22N2O3S2	378.509	Ro 28-1675 BCX 1470
Express	HY-10595				
Medchem		N=C(C1=CC2=CC=C(O(C(C3=CC=CS3)=O)C=C2S1)N.O=S(O)(C)=O	C15H14N2O5S3	398.477	(methanesulfonate)
Express	HY-50875				
Medchem		ClC1=CC=CC=C1C(N2N=CC=C2)(C3=CC=CC=C3)C4=CC=CC=C4	C22H17ClN2	344.837	TRAM-34
Express	HY-13519				
Medchem		O=C(O)CCC1=CC=C(NCC2=CC=CC(O C3=CC=CC=C3)=C2)C=C1	C22H21NO3	347.407	GW9508
Express	HY-15589				
Medchem		O=C(C1(C2=CC=C(O C(F)(F)O3)C3=C2)CC1)NC4=CC5=C(N(C[C@@H](O)CO)C(C(C)CO)=C5)C=C4F	C26H27F3N2O6	520.498	VX-661
Express	HY-15448				
Medchem		ClC1=C(C)C(C2=NN=NN2CC3=CC=CN=C3)=CC=C1	C13H9Cl2N5	306.15	A 438079
Express	HY-15488				
Medchem		C[C@@H]1O[C@@H](CN(CC(NC2=CC3=C(C=C2)SC4=C(C3)C=CC=C4C5=CC(C=C(O5)N6CCOCC6)=O)=O)C1)C	C30H33N3O5S	547.665	KU-60019
Express	HY-12061				
Medchem		O=C(O)CN1C(C)=C(C C2=NC3=CC=CC=C3C=C2)C4=C1C=CC(F)=C4	C21H17FN2O2	348.37	OC000459
Express	HY-15342				
Medchem		OC(COCCCN(C(C)C)C1=NC(C2=CC=CC=C2)=C(C3=CC=CC=C3)N=C1)=O	C25H29N3O3	419.516	MRE-269
Express	HY-79593				
Medchem		O=C1N(CCCN(C[C@@H]2C3=CC(O C)=C(O C)C=C3C2)C)CCC4=CC(O C)=C(O C)C=C4C1.Cl	C27H37ClN2O5	505.046	Ivabradine (hydrochloride)
Express	HY-B0162A				
Medchem		O=C(C(C1=CC=CC=C1)C2=CC=CC=C2)N3CCN(C(C4=CC=CC=C4)C5=CC=CC=C5)CC3	C32H32N2O	460.609	NP118809
Express	HY-14462				
Medchem		O=C(NC1=C2N=CC=CC=C1)C3=CC=C(N(C([C@]4([H])[C@]([C5]([H])C=C[C@]5([H])[C@]64[H])=O)C6=O)C=C3	C25H19N3O3	409.437	IWR-1
Express	HY-12238				
Medchem		O=C(C1=C(C)NC(C)=C(C(O C)=O)C1C2=CC=CC=C2[N+](O-)=O)OC	C17H18N2O6	346.335	Nifedipine
Express	HY-B0284				
Medchem		O=C1C2=C(NC(N)=N1)NCC(C(O)C(O)C)N2	C9H15N5O3	241.247	Tetrahydrobiopterin
Express	HY-107383				
Medchem		O=C([C@H]1N(C([C@@H](N[C@H](C(OCC)=O)CCC)=O)[C@@]2([H])CCC[C@@]2([H])C1)O.CC(C)(C)N	C23H43N3O5	441.605	Perindopril (erbumine)
Express	HY-B0130A				
Medchem		C1(C2=NC3=CC=CC=C3C=C2)=NC4=CC=CC=C4C=C1	C18H12N2	256.308	2,2'-Biquinoline
Express	HY-W011846				
Medchem		O=C(N1[C@@H](CCC1)C(O)=O)[C@@]([C@@H](C)CC)([H])NC([C@@H]2[C@@H](C(NCCC)=O)O2)=O	C18H29N3O6	383.439	CA-074
Express	HY-103350				
Medchem		OC(P(O)(O)=O)(P(O)(O)=O)CCN	C3H11NO7P2	235.07	Pamidronic acid
Express	HY-B0012				
Medchem		OC(CCC/C=C/C[C@H]1[C@H]([C@H](O)C[C@H]1O)/C=C/[C@H](O)CO C2=CC(Cl)=CC=C2)=O	C22H29ClO6	424.915	(+)-Cloprostamol
Express	HY-107381				
Medchem		OC([C@@H](N)CCl)=O	C3H6ClNO2	123.538	β-Chloro-L-alanine
Express	HY-107373				
Medchem		O=C(NC[C@@H]1[C@@]2([H])CN(CCC(C)(C)C[C@@]12[H])C3=CC(Cl)=CC(Cl)=C3	C19H26Cl2N2O	369.329	ML218
Express	HY-103309				
Medchem		CC(NCCN1C2=C(C3=C1C=CC(C(C)=O)=C3)C=C(C(C)=O)C=C2)C.[H]Cl	C21H25ClN2O2	372.89	CB0137 HCl
Express	HY-18935A				
Medchem		NC1=NC=C(C C2=C3C=CC(C4CC4)OC3=C(O C)C(O C)=C2)C(N)=N1	C19H22N4O3	354.4	Iclaprim
Express	HY-101479				
Medchem		O=C1[C@](O)(CC)C2=C(CO1)C(N3CC4=CC5=C(N)C=CC=C5N=C4C3=C2)=O	C20H17N3O4	363.367	9-Aminocamptothecin
Express	HY-100309				

Medchem		O=S([N-				
Express	HY-11103]C1=C(C(C)=NO1)Cl)(C2=C(SC=C2)C(C3=C(C=C4OCO4=C3)C)=O)=	C18H14ClN2NaO6S2	476.886	Sitaxsentan (sodium)	
Medchem		O.[Na+]				
Express	HY-101105A	O=C(C1=CC=C(C2=CC=C(C3=NO(C)C)=N3)C=C2C)C=C1)N4CCC5=C4C=	C32H33ClN4O3	557.082	SB-224289 hydrochloride	
Medchem		C6C(OC67CCN(C)CC7)=C5.Cl				
Express	HY-19334	O=S(C1=CC=C(C(NC(CCCCC)=O)C=C1)(NC2=CC=C(C(CNC[C@H](O)C	C30H40N4O6S	584.727	L755507	
Medchem		OC3=CC=C(O)C=C3)C=C2)=O				
Express	HY-107371	O=CC1=C(C(C(OC)=CC=C1Br)O	C8H7BrO3	231.043	NSC95682	
Medchem						
Express	HY-22024	O=C1C=C(C2=CC=CC=C2)OC3=CC=CC(O)=C13	C15H10O3	238.238	5-Hydroxyflavone	
Medchem						
Express	HY-13455	NCCCC1=C(C=C(C(OC)C=C2)C2=NC3=CC=C(C(OC)C=C31	C18H20N2O2S	328.429	LDN-192960	
Medchem		O[C@H]1CCN(C1)C[C@H](C2=CC=CC=C2)N(C)C(C3=CC=CC=C3)C4=				
Express	HY-107384	CC=CC=C4)=O	C27H30N2O2	414.539	Asimadoline	
Medchem						
Express	HY-108314A	NC(NCCCCCCN)=N.O=S(O)(O)=O	C8H22N4O4S	270.348	GC7 Sulfate	
Medchem		N=C(N)NCCC[C@H](C(O)=O)NC(COCC(C1=CC=CC=C1)C2=CC=CC=			SB290157	
Express	HY-101502A	C2)=O.O.C(C(F)(F)F)=O	C24H29F3N4O6	526.51	(trifluoroacetate)	
Medchem						
Express	HY-12336	O=C(N1CCN(C(C2=CC=C(C(OC)C=C2)=O)CC1)/C=C/C3=CC=C(Br)C=C3	C21H21BrN2O3	429.307	NI8R189	
Medchem						
Express	HY-10992	O=C(N[C@@H]1CNCCC1)C2=C(C=C(C(S2)C3=CC=CC(F)=C3)NC(N)=O	C17H19FN4O2S	362.422	AZD-7762	
Medchem						
Express	HY-N0170	OCC1=CNC2=C1C=CC=C2	C9H9NO	147.174	Indole-3-carbinol	
Medchem					GSK-LSD1	
Express	HY-100546A	C1(N[C@H]2[C@H](C3=CC=CC=C3)C2)CCNCC1.Cl.Cl	C14H22Cl2N2	289.244	Dihydrochloride	
Medchem						
Express	HY-18260	CC(C1=CC=C(O)C=C1)(C2=CC=C(O)C=C2)C	C15H16O2	228.286	Bisphenol A	
Medchem						
Express	HY-14167	ClC1=CC(Cl)=C(NC2=NC=C(C(NCC3CCOCC3)=O)C(C(F)(F)F)=N2)C=C1	C18H17Cl2F3N4O2	449.254	GW842166X	
Medchem		C[C@@]12[C@](C(C[C@@H]2C(NC(C)C)=O)([H])(C@@)3([H])(C@)([C				
Express	HY-107385	@@]4(C=C(C(O)=O)CC4)=CC3C)([H])CC1	C25H37NO3	399.566	Epristeride	
Medchem					4-[(Piperidin-4-yl)oxy]piperidine-1-carboxylic acid tert-butyl ester	
Express	HY-22026	CC(C)(C)OC(N(CC1CCC1OC2CCNCC2)=O	C15H28N2O3	284.394		
Medchem		O=C(O)C1=CC=C(NC2=C3N=CN(C(C)C)C3=NC(N[C@@H](CO)C(C)C)=N				
Express	HY-18299	2)C=C1Cl	C20H25ClN6O3	432.9	Purvalanol	
Medchem		O=C([C@]1([H])CC2=C([C@H](/C=C(C)C)N13)NC4=C2C=CC(OC)=C4)N				
Express	HY-N2143	5[C@]([CC5])([H])C3=O	C22H25N3O3	379.45	Fumitremorgin C	
Medchem		O=S(C1=C(C(S(=O))(C2=CC=CC=C2)=O)=CC=C1C(F)(F)F)(NC3CCNCC3)				
Express	HY-10858	=O	C18H19F3N2O4S2	448.48	WAY 316606	
Medchem		ClC1=C(F)C=CC(Cl)=C1[C@H](OC2=CC(C3=CN(N=C3)C4CCNCC4)=CN=				
Express	HY-50878	C2N)C	C21H22Cl2FN5O	450.337	Crizotinib	
Medchem						
Express	HY-107379	O=S(N1CC2=CC=CC=C2CC1)(C3=CC(C(O)=O)=CC=C3)=O	C16H15NO4S	317.36	AKR1C3-IN-1	
Medchem		OC1=C(OC)C(O)=C([C@@]2([H])(C@@)(OC3=O)([H])(C@@H)(O)(C@H				
Express	HY-N0017)(O)(C@@H)(CO)O2)C3=C1	C14H16O9	328.272	Bergenin	
Medchem						
Express	HY-N0085	O=C1C=CC2=CC(OC)=C(OC)C(OC)=C2O1	C12H12O5	236.221	Dimethylfraxetin	
Medchem		N[C@@H](CC1=CC=C(C2=NC(N)=NC(OC)C3=CC=C(C4=CC=CC(F)=C4)				
Express	HY-15849	C=C3)C(F)(F)F)=C2)C=C1)C(O)=O	C27H22F4N4O3	526.482	LP-533401	
Medchem		C[C@H]([C@](O(C@@H)1C(C)C)(C[C@@H](O)(C@@H)1C)O)(C@H)(O)				
Express	HY-100558	[C@@H]([C@](OC(C(C)C)=C(C)C)=C[C@@H](C)[C@@H](O)(C@H)(
Medchem		C)C2)=O)([H])(C@H)(/C=C/C=C2)OC)C	C35H58O9	622.83	Bafilomycin A1	
Express	HY-108318	NC1=C2C(N(C3CCCC3)C=C2C4=CC=C(OC5=CC=CC=C5)C=C4)=NC=N1	C23H22N4O	370.447	RK-24466	
Medchem		CCCCC1=C(C2=C(C=C(CS(C)=O)=O)=C2)O1)C(C3=CC=C(C=C3)OCC				
Express	HY-A0016	CN(CCCC)CCC)=O	C31H44N2O5S	556.76	Dronedaron	
Medchem		O=C1C=C(CSC2=NC=CC=C2)OC=C1OC(C3=CC=C([N+])([O-				
Express	HY-103254))=O)C=C3)=O	C17H11N3O6S	385.35	ML221	
Medchem		O=C(C1=CC=C2C=CC=CC=C1O)O.O.C3=C(CO)C=C(C(CNCCCCCO				
Express	HY-17453	CCCC4=CC=CC=C4)O)C=C3	C36H45NO7	603.745	Salmeterol (xinafoate)	
Medchem						
Express	HY-B0192	O=C(C1CCCC1)NCCCN(C2=NC(N)=C3C=C(C(OC)C(OC)=CC3=N2)C	C19H27N5O4	389.449	Alfuzosin	
Medchem		C[C@@]12[C@@](C)(O)CC[C@@]1([H])(C@@)3([H])CCC4=CC(C[C@]4(
Express	HY-B2159	C)[C@@]3(F)[C@H](O)C2)=O	C20H29FO3	336.441	Fluoxymesterone	

Medchem					
Express	HY-103392	<chem>CC(C)(C)C(O)/C=C/C1=CC=C(C(=O)CO)C2=C1</chem>	C14H18O3	234.291	Stiripentol
Medchem					
Express	HY-103609	<chem>C12=CC=C3C=CC=C4C=CC(C2=C34)=CC=C1</chem>	C16H10	202.251	Pyrene
Medchem					
Express	HY-W008613	<chem>O=C(O)C1=C(O)C(CC2=C3C=CC=CC3=CC(C(O)=O)=C2O)=C4C=CC=C4=C1</chem>	C23H16O6	388.375	4,4'-Methylenebis(3-hydroxy-2-naphthoic acid)
Medchem					
Express	HY-59047	<chem>O=C1N=CC(O)C2=CC=CC(C)=C2)CN1</chem>	C11H10N2O2	202.209	Tolimidone
Medchem					
Express	HY-100737	<chem>CO C1=CC=C(C(N2CCN(C(C3=CC4=C(C(C=C5)C5S(C4)(=O)=O)S3)=O)CC2)C=C1</chem>	C23H22N2O4S2	454.562	ML349
Medchem					
Express	HY-12956A	<chem>CCCCC[C@H](O)/C=C/[C@H]1[C@H](O)C[C@H](O)[C@@H]1C/C=C/C(CC(CO)=O.OCC(CO)(N)CO</chem>	C24H45NO8	475.62	Dinoprost (tromethamine salt)
Medchem					
Express	HY-108319	<chem>O=C(O)CC1=CC=C([N+])([O-])=O)C=C1)NCCCC[C@H](N)C(N2CCCC2)=O</chem>	C18H26N4O5	378.42	DPP-IV-IN-2
Medchem					
Express	HY-10797	<chem>ClC1=CC=C(C(O)C2=CC=C(F)C=C2)C(C(N[C@H](C3=CC=C(C(O)=O)C=C3)C)=O)=C1</chem>	C22H17ClFNO4	413.826	CJ-42794
Medchem					
Express	HY-10997A	<chem>C=CC(N1CC(N2N=C(C3=CC=C(C(O)C4=CC=CC=C4)C=C3)C5=C(N)N=CN=C52)CCC1)=O</chem>	C25H24N6O2	440.497	PCI-32765 (Racemate)
Medchem					
Express	HY-22023	<chem>C1(CC2=CC=CC=C2)=CC=NC=C1</chem>	C12H11N	169.222	4-Benzylpyridine
Medchem					
Express	HY-107369	<chem>CCCCC1=C(C=C(C(O)C=C1)O</chem>	C10H14O2	166.217	4-Butylresorcinol
Medchem					
Express	HY-107368	<chem>O=C(C1C(CCCC1=O)=O)C2=C(C=C(C(S(C)=O)=O)C=C2)Cl</chem>	C14H13ClO5S	328.768	Sulcotrione
Medchem					
Express	HY-100578	<chem>O=C(NC1=C2C=CC=NC2=C1)/C(C#N)=C/C3=CC=C(C4=CC(Cl)=CC=C4Cl)O3</chem>	C23H13Cl2N3O2	434.274	AGK2
Medchem					
Express	HY-W016403	<chem>O=C1C(C2=C3C1=CC=CC3=CC=C2)=O</chem>	C12H6O2	182.178	Acenaphthylene-1,2-dione
Medchem					
Express	HY-12170	<chem>O=C([C@@H]1N(S(=O))(C2=CC=C(C(O)C3=CC=NC3)C=C2)=O)CCSC1(C)C)NO</chem>	C18H21N3O5S2	423.506	Prinomastat
Medchem					
Express	HY-14861A	<chem>O=C(NC1=NC(C2CCN(C)CC2)=O)=CC=C1)C3=C(F)C=C(F)C=C3F.[H]Cl</chem>	C19H19ClF3N3O2	413.82	Lasmiditan (hydrochloride)
Medchem					
Express	HY-13861	<chem>CC(C)(SC1=CC=C(CCN(C(NC2CCCC2)=O)CCCC3CCCC3)C=C1)C(O)=O</chem>	C29H46N2O3S	502.75	GW7647
Medchem					
Express	HY-90009A	<chem>O=C([C@@]1([H])CC2=C([C@@H](C3=CC=C(C(O)CO)C4=C3)N15)NC6=C2C=CC=C6)N(C)CC5=O</chem>	C22H19N3O4	389.404	Tadalafil
Medchem					
Express	HY-12222	<chem>C([C@@]1([C@]2([H])([H])(C@@H)(CC)[C@H]2O)(CC[C@H](O)C1)[C@]3([H])([C@]2([H])([C@@])(CC[C@]4([H])([C@H](C)CCC(O)=O)([H])(C@]4(C)CC</chem>	C26H44O4	420.625	INT-747
Medchem					
Express	HY-108325	<chem>O=C(C1=C(C(C)C2=CC=C(C3=CC=CC=C3F)C=C2)=NC4=CC=C(F)C=C14)O</chem>	C23H15F2NO2	375.368	Brequinar
Medchem					
Express	HY-106441A	<chem>O=C(N1C[C@@H](F)[C@@H](CNC2=NC=CC=N2)CC1)OCC3=CC=C(C)C=C3</chem>	C19H23FN4O2	358.41	Rislenemdaz
Medchem					
Express	HY-B1751	<chem>C=C[C@H]1C[N@](CC[C@H]1C2)[C@@]2([H])([C@@H](O)C3=CC=NC4=CC=C(O)C=C34</chem>	C20H24N2O2	324.417	Quinidine
Medchem					
Express	HY-100788	<chem>O=C(O)C(CP(O)(O)=O)CCC(O)=O</chem>	C6H11O7P	226.121	2-PMPA
Medchem					
Express	HY-108324	<chem>O=S(C1=CC(/C2=C(CCN3CCN(C)CC3)=C(SC4=C2C=CC=C4)C=C1)(N(C)C)=O</chem>	C23H29N3O2S2	443.625	(Z)-Thiothixene
Medchem					
Express	HY-Y0355	<chem>ClC1=NC(Cl)=NC(Cl)=N1</chem>	C3Cl3N3	184.411	Cyanuric chloride
Medchem					
Express	HY-50108	<chem>O=C(C1=CC=CC(/C=C/C2=CC=C(C=C2)OCC3=C(ON=C3C4=C(C)C=C4C4Cl)C(C)C=C1)O</chem>	C28H22Cl3NO4	542.84	GW 4064
Medchem					
Express	HY-103107	<chem>O=C(C1=CC=C(F)C=C1)NC2=CC3=C(C=C2)NC=C3C4CCN(C)CC4</chem>	C21H22FN3O	351.42	LY334370
Medchem					
Express	HY-15245	<chem>CC1=NC2=C(C(O)=O)C=C(C(C=C2N1CC3=CC=CC(C(F)(F)F)=C3)N4CCOCC4</chem>	C22H22F3N3O3	433.424	GSK2636771
Medchem					
Express	HY-103610	<chem>O=C(C1=CC=C(C(O)C=C1)C(C2=CC=C(C(O)C=C2)=O</chem>	C16H14O4	270.28	4,4'-Dimethoxybenzil
Medchem					
Express	HY-W012484	<chem>NCCC1=CC=CC=C1Br</chem>	C8H10BrN	200.079	2-Bromophenethylamine
Medchem					
Express	HY-20891	<chem>CCC(/C(C)=C/C1=CC=C(F)C=C1)=N.O</chem>	C12H14FNO	207.244	2-Bromophenethylamine 1-Penten-3-one, 1-(4-fluorophenyl)-2-methyl-, oxime
Medchem					
Express	HY-17385	<chem>CC1=CC=CC=C1O[C@@H](C2=CC=CC=C2)CCNC.[H]Cl</chem>	C17H22ClNO	291.816	Atomoxetine (hydrochloride)
Medchem					
Express	HY-17042A	<chem>O=C(O)COCCN1CCN(C2=CC=C(C)C=C2)C3=CC=CC=C3)CC1.Cl.Cl</chem>	C21H27Cl3N2O3	461.81	Cetirizine (dihydrochloride)

Medchem	Express	HY-108315	NC1=C2C=CC=CC2=C3C(C4=CC=CC=C4C=C3)=C1	C18H13N	243.303	6-Aminochrysene
Medchem	Express	HY-108317	O=C(N1N(C(OC)=O)[C@@](C2=CC=CC=C2)(C3CCCC3)C1=O)OC	C17H20N2O5	332.351	ABL127
Medchem	Express	HY-B0800	NC(NCCN1CCCCCCC1)=N.O=S(O)(O)=O	C10H24N4O4S	296.39	Guanethidine (sulfate)
Medchem	Express	HY-101932	C[C@]1([C@@H](C/C=C(C)/C)O1)[C@]([C@@H]2OC([H])[C@]3(CC[C@@H]2OC(NC(C)=O)=O)CO3	C19H28ClNO6	401.88	TNP-470
Medchem	Express	HY-18234A	O=S(O)(O)=O.O=C(N[C@H](C(N[C@H](C([H])=O)CCNC(N)=N)=O)CC(C)C)[C@@H](NC(C)=O)CC(C)C.O=C(N[C@H](C(N[C@H](C([H])=O)CCCNC(N)=N)=O)CC(C)C)[C@@H](NC(C)=O)CC(C)C	C40H78N12O12S	475.59	Leupeptin (hemisulfate)
Medchem	Express	HY-10358	O=C1N2C(C3=CC(C4=CC=CC=C4)=C(N=C3C=C2)C5=CC=C(C6(N)CCC6)C=C5)=NN1.Cl.Cl	C25H23Cl2N5O	480.39	MK 2206 (dihydrochloride)
Medchem	Express	HY-N0700	C/C=C/C1=C(C(OC)C=C(C(OC)C(OC)=C1	C12H16O3	208.25	alpha-Asarone
Medchem	Express	HY-12355	O=C(C1CN(CC2=CC=C(C/C(C)=N/OCC3=CC=C(C4CCCC4)C(C(F)F)F)=C3)C=C2CC)C1)O	C29H35F3N2O3	516.6	Siponimod
Medchem	Express	HY-10029	O=C(N1C(C2=C(C=C(C2)OC)OC(C)C)=N[C@H]([C@H]1C3=CC=C(C=C3)Cl)C4=CC=C(C=C4)Cl)N5CC(NCC5)=O	C30H30Cl2N4O4	581.49	Nutlin (3a)
Medchem	Express	HY-A0013	O=S(NC1=NC(C2=NC=CC=N2)=NC(OCO)=C1OC3=CC=CC=C3OC)/C4=CC=C(C(C)(C)C)C=C4)=O	C27H29N5O6S	551.61	Bosentan
Medchem	Express	HY-15187	O=C(N1[C@@]([C2=CC=CC=C2](CCCN)SC(C3=CC(F)=CC=C3F)=N1)N(OC)C	C20H22F2N4O2S	420.48	ARRY-520
Medchem	Express	HY-76948	O=C(O[C@@H]1CNC(C2=CC=C(C)S2)=O)N(C1)C(C=C3)=CC=C3N4C(C(OC)C4)=O	C19H18ClN3O5S	435.88	5-R-Rivaroxaban
Medchem	Express	HY-13327	O=C([C@H]1CC[C@H](CN2CCC[C@H](N(CC3=CC(C(F)F)=CC(C(F)F)F)=C3)C4=NN(C)N=N4)C5=CC(C)=CC(C)=C52)CC1)O	C31H36F6N6O2	638.65	Evacetrapib
Medchem	Express	HY-10001	C=C1[C@H](C[C@H](C/C1=C/C=C2[C@]3([C@@]([C@H](CC3)[C@@H]//C=C/[C@H](C4CC4)O)C)CCC2[H])O)O	C27H40O3	412.6	Calcipotriol
Medchem	Express	HY-B1017	O=C1C2=C(NC(C)=C2CC)CCC1CN3CCOCC3.[H]Cl	C16H25ClN2O2	312.83	Molindone (hydrochloride)
Medchem	Express	HY-12424	CO[C@H]1[C@@H](N2C=NN=N2)CC[C@H](C[C@H]([C@@](CC([C@@H]//C=C([C@H]([C@H](C([C@H](C[C@@H]3C)C)=O)O(C)O)C)C)=O)([H])O(C([C@@](CCCC4)([H])N4C(C([C@](O)C@]5([H])C[C@@H]//C(C)=C/C=C/C3)OC)([C@H](CC5)C)O)=O)=O)O)C1	C52H79N5O12	966.21	Zotatarlimus
Medchem	Express	HY-17377	CC1(N2C[C@H](C)N([C@H](C3=CC=C(C(F)F)F)C=C3)CO(C)CC2)CCN(C(C4=C(C)N=CN=C4C)=O)CC1.O=C(C)O/C=C(Cl)O)=O	C32H42F3N5O6	649.7	Vicriviroc (maleate)
Medchem	Express	HY-10801	O=C(CN1C(C=CC(C(O)=O)=C2)=C2C(C(C(C)C)=O)=C1)CO(C(C=C3)=CC=C3O)C4=CC=CC=C4	C28H25NO6	471.5	CAY10650
Medchem	Express	HY-11093	C[C@H]1CNCCC2=CC=C(C)C=C12	C11H14ClN	195.69	Lorcaserin
Medchem	Express	HY-13511A	CC1=CN=CC(CN2CC(C(C2)=C3C4=CC=C(C)C)C=C4CCC5=CC=CN=C5)3)=C1.O=C(C)O/C=C(C)O)=O	C30H30ClN3O4	532.03	Rupatadine (Fumarate)
Medchem	Express	HY-15478	C1(CNC2=NC=CC=C2)=CC=C(CNC3=NC=CC=C3)C=C1	C18H18N4	290.36	WZ811
Medchem	Express	HY-50844	CC(N)(C(N[C@H](C1NCCC2(CN(C3=C2C=CC=C3)S(=O)(O)C)=O)CC1)=O)COCC4=CC=CC=C4)O.C.S(=O)(O)=O	C28H40N4O8S2	624.77	Ibutamoren (Mesylate)
Medchem	Express	HY-10997	C=CC(N1C[C@H](N2N=C(C3=CC=C(C)O)C4=CC=CC=C4)C=C3)C5=C(N)N=CN=C52)CCC1)=O	C25H24N6O2	440.5	PCI-32765
Medchem	Express	HY-11000	O=C(C(C(C1=CC=C(C(F)F)C=C1)C2)=C(C)NC2=O)NC3=CC4=C(NN=C4)C=C3F	C21H16F4N4O2	432.37	GSK429286A
Medchem	Express	HY-A0096	O=C(O)CCC/C=C1C[C@@]2([H])C[C@@H](O)[C@H]//C=C/[C@@H](O)C(C)CC#CC[C@@]2([H])C1	C22H32O4	360.49	Iloprost
Medchem	Express	HY-19329	O=C1N(CC2=CC=C(F)C=C2)C(S/C1=C)C3=CC=C(C(OC4=CC(B(O)O)=C=C4)C=C3)=O	C24H19BFNO5S	463.29	HA130
Medchem	Express	HY-12684	O=C(C1=CC=NN1C)NC2=CC=C(C/N=N/C3=CC=CC=C3)C=C2C	C19H19N5O	333.39	CH-223191
Medchem	Express	HY-12299	O=C(OC1=C(C)C=CC=C1C)N(C2=CC=C(C(OC)C=C2O)C3=NC(NC4=CC=C(N5CCN(C)CC5)C=C4)=NC=C3	C32H36N6O4	568.67	WH-4-023
Medchem	Express	HY-10460	CS(=O)(N(C)C1=CC=CC=C1CNC2=NC(NC3=CC4=C(C=C3)NC(C4)=O)=N=C2C(F)F)F)=O	C22H21F3N6O3S	506.5	PF-431396
Medchem	Express	HY-15968	C12=NC=CN1C=C(C3=CC4=C(C=C3)C=NN4)N=C2NC5=CC=C(N6CCOCC6)C=C5	C23H21N7O	411.46	GS-9973
Medchem	Express	HY-13343	O=C(NC1=CC=C(C)C(NC(C2=CC=C(O)C=C2)=O)=C1)C3=CC=CC(N(C)C)=C3	C23H23N3O3	389.45	ZM 336372
Medchem	Express	HY-15196	ClC(C=C(NC1=NC=NC2=C1N(CCN(C(C(C)O)=O)C=C2)C=C3)=C3O)C4=CC=CC(C(F)F)F)=C4	C26H25ClF3N5O3	547.96	TAK-285

Medchem		O=C(C1=CC=CC=C1C2=CC=C(CN3C4=CC(C5=NC6=CC=CC=C6N5C)=C			
Express	HY-13955	C(C)=C4N=C3CCC(C)=C2)O	C33H30N4O2	514.62	Telmisartan
Medchem		O=C(C1=CC(C2=CC=C(N3CCNCC3)N=C2)=CC4=C1C(C)=CN4[C@@H](C			
Express	HY-13470)CC)NCC5=C(C(C)=C(C)NC5=O	C31H38N6O2	526.67	GSK126
Medchem		O=C(NC1=CC=CN=C1)C2=CC=C(CNS(=O)(C3=CC=C(C(C)(C)C)=C3)=			
Express	HY-18728	O)C=C2	C23H25N3O3S	423.53	STF-31
Medchem		O=C(C1=CC=C(C(C(F)(F)F)=C1)CN2C[C@@H](N(C)C)CC2)NC3=CC=C(C			
Express	HY-50868	C(C)(NC4=NC=CC(C5=CN=CN=C5)=N4)=C3	C30H31F3N8O	576.62	Bafetinib
Medchem		O=C1N(C2=C(C(N1CC3=NC(C)=C4C=CC=C4=N3)=O)N(CC#CC)C(N5CC			
Express	HY-10284	C[C@@H](N)C5=N2)C	C25H28N8O2	472.54	Linagliptin
Medchem		CS(=O)(NC1=CC=CC=C1NC2=NC(NC3=CC=C(N4CCOCC4)C=C3OC)=N			
Express	HY-15800A	C=C2F)=O	C22H25FN6O4S	488.54	CZC-25146
Medchem		O=C1N2C(C([C@H](NC3=CC=CC=C3C(O)=O)C)=CC(C)=C2)=NC(N4CC			
Express	HY-10344	OCC4)=C1	C22H24N4O4	408.45	AZD 6482
Medchem		O=C1C(C(NC2=CC=CC(C(N(C)C)=O)=C2O)=C1N[C@H](CC)C3=CC=C(C(O			
Express	HY-10198	3)C)=O	C21H23N3O5	397.42	SCH 527123
Medchem		O=C(CN)NC1=CC=C(C=C1)N2N=C(C=C2C3=CC=C4C5=CC=CC=C5C=C			
Express	HY-10547	C4=C3)C(F)(F)F	C26H19F3N4O	460.45	OSU-03012
Medchem					
Express	HY-20019	O=C(O)CO(C(C=C1)=CC=C1OCCOC2=CC=C(C(C)=O)C(O)=C2CCC	C22H26O7	402.44	L-165041
Medchem		O=C1N(C(CN2C3=C(C(N)=NC=N3)N=C2)=NC4=CC=CC(C)=C14)C5=C(C(C			
Express	HY-10110	C=CC=C5	C22H19N7O	397.43	IC-87114
Medchem					
Express	HY-106150B	CS(=O)(C1=C(N2C=CC=C2)C=C(C)C(C(NC(N)=O)=O)=C1)O.[H]Cl	C14H17ClN4O3S	356.83	Eniporide hydrochloride
Medchem					
Express	HY-15601	O=C1NC2=C(N)N=C(OCCCC)N=C2N(CC3=CC=CC(CN4CCCC4)=C3)C1	C22H30N6O2	410.51	GS-9620
Medchem					
Express	HY-14289	CC1=C(CSCC/N=C(NC)/NC#N)NC=N1	C10H16N6S	252.34	Cimetidine
Medchem					
Express	HY-12043	CC(C)(C1=NC(C2=CC=CC(C)=N2)=C(C3=CC=C4N=CC=NC4=C3)N1)C	C21H21N5	343.42	SB 525334
Medchem		CC1=NNC(NC2=NN3C(C(CN4CCOCC4)=C2)=NC(C)=C3CC5=CC=C(C=C5			
Express	HY-13034	F)Cl)=C1	C23H25ClFN7O	469.94	LY2784544
Medchem		F(C(F)(C1=NN=C2C=CC(C3=CN(C)N=C3)=NN21)C4=CC5=C(N=CC=C5)C			
Express	HY-50683	=C4	C19H13F2N7	377.35	JNJ-38877605
Medchem					
Express	HY-10505	O=C(C1=CC=C2C=C(C([C@@]3(O)CCN4C=NC=C43)C=CC2=C1)NC	C18H17N3O2	307.35	Orteronel
Medchem					
Express	HY-B0006	OC(CNCCOC1=CC=CC=C1O)CO C2=CC=CC(N3)=C2C4=C3C=CC=C4	C24H26N2O4	406.47	Carvedilol
Medchem					
Express	HY-17372	O=C1OCC(C2=CC=C(S(=O)(C)=O)C=C2)=C1C3=CC=CC=C3	C17H14O4S	314.36	Rofecoxib
Medchem					
Express	HY-15466	NC1=NC=C(C2=C3C(N(S(=O)(C)=O)CC3)=NC(N4CCOCC4)=N2)C=N1	C15H19N7O3S	377.42	CH5132799
Medchem		C[C@@](C1=CC(C(F)(F)F)=CC(C(F)(F)F)=C1)([H])OC[C@@]2(C3=CC=			
Express	HY-14751	CC=C3)CC[C@@](CCC4=O)(N4)CN2	C25H26F6N2O2	500.48	Rolapitant
Medchem		CCCC[C@H](C([O-			
Express	HY-15894])=O)NC([C@H](CC1=CN(C(O)C)=O)C2=CC=CC=C12)NC([C@H](CC(C)	C34H50N5NaO7	663.78	BQ-788 (sodium salt)
Medchem		(C)C)NC(N3[C@H](C)CCC[C@@H]3C)=O)=O.[Na+]			
Express	HY-70044	O=C(NC1=CC=C(C2=NN(C=C2C3=C4C(NC(C5=CC=CC(CN(C)C)=C5)=C4	C30H33N7O	507.63	GSK-1070916
Medchem)=NC=C3)CC(C=C1)N(C)C			
Express	HY-15227	NC1=C2C(N([C@H]3[C@H](O)[C@H](O)[C@H](CN(C(C)C)CCNC(NC4	C28H41N7O4	539.67	EPZ004777
Medchem		=CC=C(C(C)(C)C)=C4)=O)O3)C=C2)=NC=N1			
Express	HY-50098	CN(N=C1C2=CC=C(OCC3=NC4=CC=CC=C4C=C3)C=C2)C=C1C5=CC=N	C25H20N4O	392.45	PF-2545920
Medchem		C=C5			
Express	HY-51424	O=S(NC1=CC=C(C(C(C2=CNC3=NC=C(C=C23)Cl)=O)=C1F)F)(CCC)=O	C17H14ClF2N3O3S	413.83	PLX-4720
Medchem		O=C(NC1=CC=C(O)C=C1)C[C@H]2C3=NN=C(C)N3C4=C(C(C)=C(C)S4)C			
Express	HY-15743	(C5=CC=C(C)C=C5)=N2	C25H22ClN5O2S	491.99	OTX-015
Medchem					
Express	HY-10012	O=S(C1=CC=C(NC2=NC(C3=CN=C(N3C(C)C)C)=CC=N2)C=C1)(C)=O	C18H21N5O2S	371.46	AZD-5438
Medchem		O=S(C1(C2=CC(N3[C@H](C)COC3)=NC(C4=CC=CC=C4C=CN5)=N2)C	C21H24N4O3S	412.51	AZ20
Express	HY-15557	C1(C)=O			
Medchem					
Express	HY-12152	O=C(NC1=CC(Cl)=C(C=C1O)C)NC2=NO(C)C=C2	C13H14ClN3O4	311.72	PNU-120596
Medchem					
Express	HY-14197A	C#CCN(CCCOC1=CC=C(Cl)C=C1Cl)C.[H]Cl	C13H16Cl3NO	308.63	Clorgiline (hydrochloride)
Medchem					
Express	HY-19975	O=S(C1=CC=C(Cl)C=C1Cl)(N(C(C)C)CCNC(C)C)=O	C14H22Cl2N2O2S	353.31	RN-1734

Medchem		<chem>CC([C@H]1CC[C@@]2([H])[C@]3([H])CCC4=CC(CC[C@]4(C)[C@@]3([H])CC[C@]12C)=O)=O</chem>	C21H30O2	314.46	Progesterone
Express	HY-N0437				
Medchem		<chem>O=C1=CC=C2C(CC[C@]3([H])[C@]2([H])CC[C@@]4(C)[C@]3([H])CC[C@]4(C#C)O)=C1</chem>	C20H24O2	296.4	Ethinyl Estradiol
Express	HY-B0216				
Medchem		<chem>O=C([C@H]1CN(CC/C=C(C2=C(C)C=CS2)/C3=C(C)C=CS3)CCC1)O.[H]Cl</chem>	C20H26ClNO2S2	412.01	Tiagabine (hydrochloride)
Express	HY-B0696A				
Medchem		<chem>O=C(NO)C1=CC=C(CN(CCCC)C(NC2=CC=CC=C2)=O)C=C1</chem>	C19H23N3O3	341.4	Nexturastat A
Express	HY-16699				
Medchem		<chem>O=C(O)/C=C/C1=CC=C(CN2C=CN=C2)C=C1</chem>	C13H12N2O2	228.25	Ozagrel
Express	HY-B0428				
Medchem		<chem>ClC1=CC=C(C(C)C(C(NN3CCCC3)=O)=NN2C4=CC=C(C(C)C=C4Cl)C=C1.Cl</chem>	C22H22Cl4N4O	500.25	Rimonabant (Hydrochloride)
Express	HY-14137				
Medchem		<chem>O=C([C@H]1N(C(CSC2=NC3=CC=CC=C3N2C)=O)CCC1)NC4=CC=CC=C4C5=CC=CC=C5</chem>	C27H26N4O2S	470.59	TCS 1102
Express	HY-10900				
Medchem		<chem>CC(N1C2=CC(C3=NC(NC4=NC=C(CN5CCN(CC)CC5)C=C4)=NC=C3F)=C(C(F)=C2N=C1C)C.CS(=O)(O)=O</chem>	C28H36F2N8O3S	602.7	LY2835219
Express	HY-16297				
Medchem		<chem>OC1=C(C(C)(C)C)C=C(C(C)C=C1C(C)(C)C</chem>	C15H24O	220.35	2,6-Di-tert-butyl-4-methylphenol
Express	HY-Y0172				
Medchem		<chem>O=C(N(CCCCN1CCN(C2=NC=CC=N2)CC1)C(C3)=O)CC43CCCC4.[H]Cl</chem>	C21H32ClN5O2	421.96	Buspirone (hydrochloride)
Express	HY-B1115				
Medchem		<chem>F=C1=CC2=C(N=CN=C2C=C1)NCC3=CC=C(F)C=C3</chem>	C15H11F2N3	271.26	Spautin-1
Express	HY-12990				
Medchem		<chem>O=C1CC[C@]2([H])[C@@]([C]1C)[C@]3([H])[C@@]4(C)C=CC(C=C4CC[C@]32[H])=O)(C)O1</chem>	C19H24O3	300.39	Testolactone
Express	HY-13763				
Medchem		<chem>C#CC1=CC(NC2=C(C=C(C(OCOCOCOCOC3)C3=C4)C4=NC=N2)=CC=C1.[H]Cl</chem>	C22H22ClN3O4	427.88	Icotinib (Hydrochloride)
Express	HY-15164				
Medchem		<chem>F=C1=C(C2=C(C(N3[C@H](CC4=NN=C(C5=CC=CC=C5)O4)CCC3)=O)N=C(C)S2)C=CC=C1</chem>	C24H21FN4O2S	448.51	SB-674042
Express	HY-10898				
Medchem		<chem>ClC1=CC=C(C=C1)CC2(CCN(CC2)C3=NC=NC4=C3C=CN4)N</chem>	C18H20ClN5	341.84	CCT128930
Express	HY-13260				
Medchem		<chem>OC(C=C1)=CN=C1C2=NO(C(C(C)C(C(NC3=C(C(O)=O)CCCC3)=O)=N2O=C1O[C@]2([H])[C@@H](O)C3=C(C=C4OCOC4=C3)[C@@H](C5=C(C(O)C=C(O)C(C)C5)=C5)[C@@]21[H]</chem>	C19H22N4O5	386.4	MK-6892
Express	HY-10680				
Medchem		<chem>CC1=CC(NC2=NC(SC3=CC=C(C=C3)NC(C4CC4)=O)=NC(N5CCN(CC5)C)=C2)=NN1</chem>	C22H22O8	414.41	AXL1717
Express	HY-15494				
Medchem		<chem>F=C1=CC2=C3C(CCN2=O)=C(C4=CC=C(CNC)C=C4)NC3=C1.O=S(C[C@@]5(C6(C)C)C(C[C@@]6([H])CC5)=O)(O)=O</chem>	C23H28N8OS	464.59	Tozasertib
Express	HY-10161				
Medchem			C29H34FN3O5S	555.66	Rucaparib (Camsylate)
Express	HY-102003				