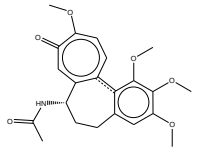
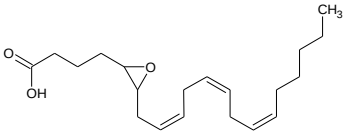
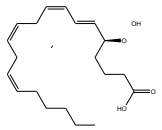
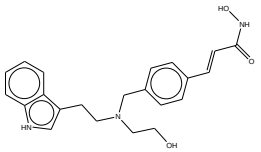
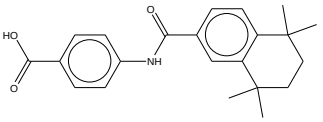
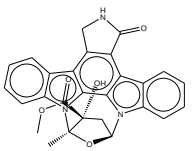
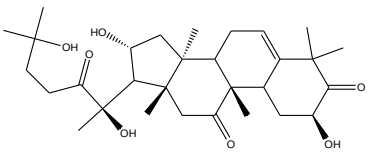
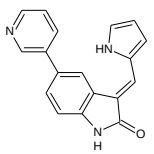
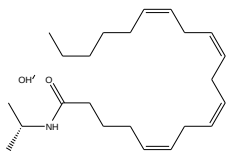
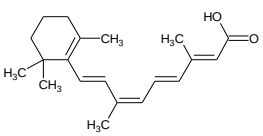
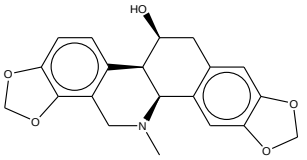
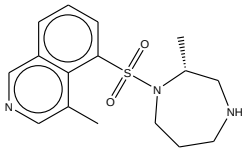
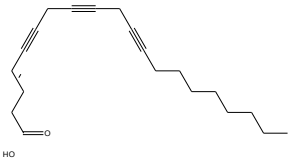
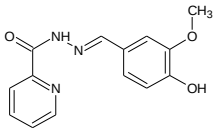
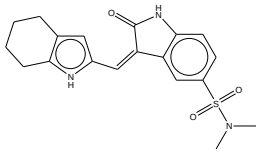
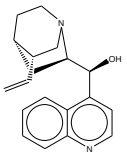
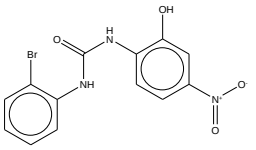
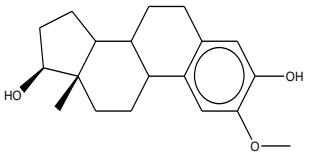
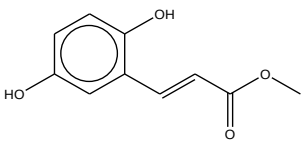
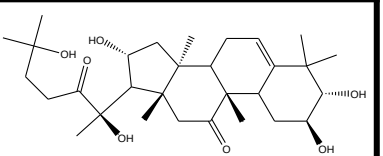
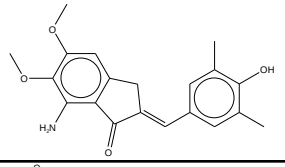
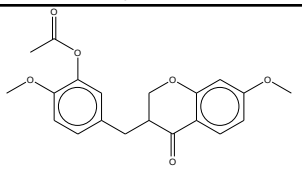
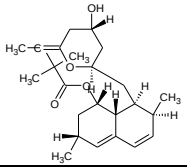
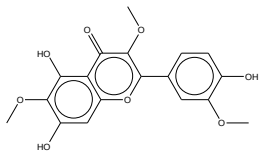
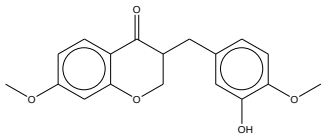
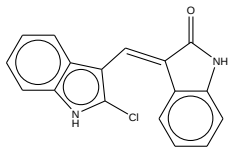
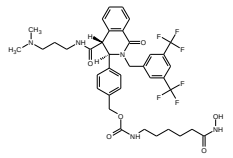
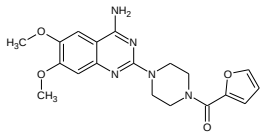
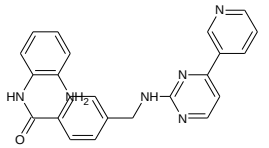
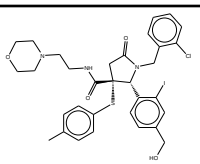
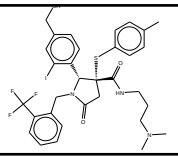
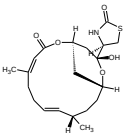
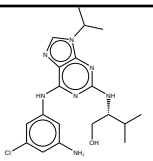
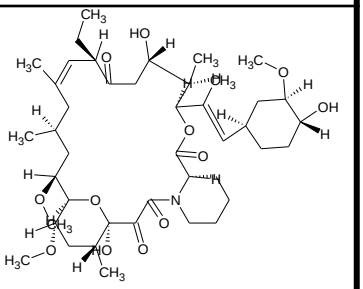
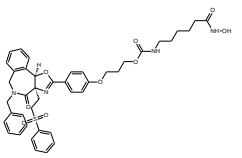
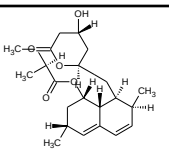
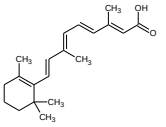
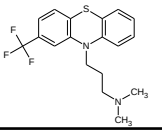
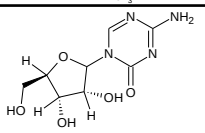
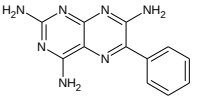
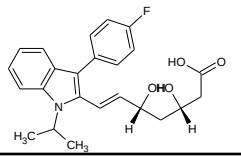
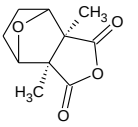
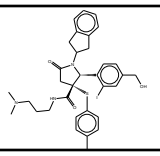
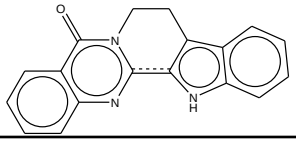
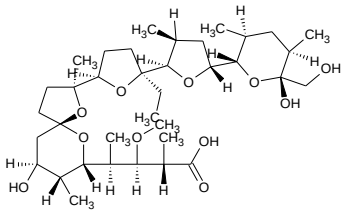
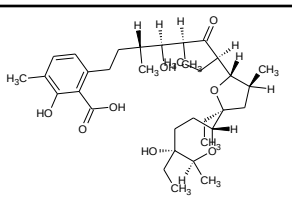
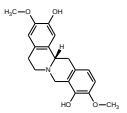
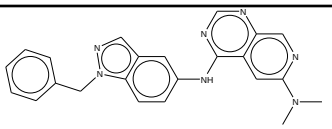
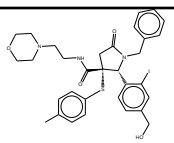
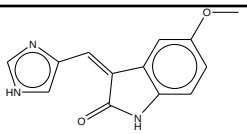
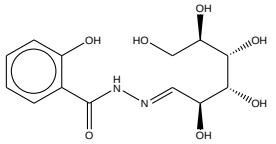
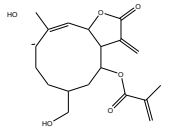
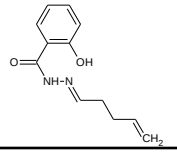
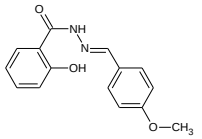
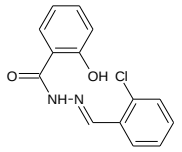
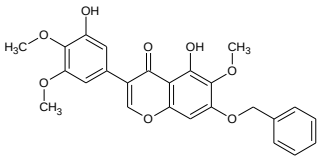
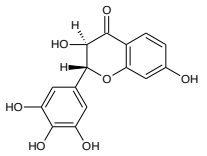
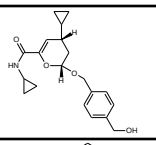
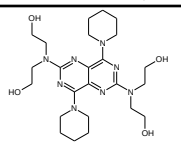
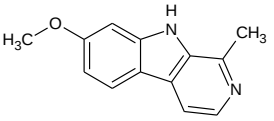
Compound Name	EC50 (μM)	SMILES	Structure
NP-010664(Colchicine)	0.10	COc1cc2CC[C@H](NC(=O)C)c3cc(=O)c(OC)ccc3-c2c(OC)c1OC	
5,6-EPOXYEICOSATRIENOIC ACID	0.25	CCCCC/C=C\C/C=C\C/C=C\CC1OC1CCCC(=O)O	
5(S)-HPETE	0.30	CCCCC/C=C\C/C=C\C/C=C\C=C\[C@H](CCCC(=O)O)OO	
THM 1-90	0.40	OCCN(CCc1c[nH]c2ccccc12)Cc3ccc(/C=C/C(=O)NO)cc3	
AM-580	0.40	CC1(C)CCC(C)(C)c2cc(ccc21)C(=O)Nc3ccc(cc3)C(=O)O	
K252A	1.10	COC(=O)[C@@]1(O)C[C@@H]2O[C@@]1(C)n3c4ccccc4c5c6CNC(=O)c6c7c8ccccc8n2c7c35	
NP-003965	1.30	CC(C)(O)CCC(=O)[C@](C)(O)C1[C@H](O)C[C@@]2(C)C3CC=C4C(C[C@H](O)C(=O)C4(C)C)[C@]3(C)C(=O)C[C@]12C	
JAK3 Inhibitor VI	2.60	CS(=O)(=O)O.C1=CC(=CN=C1)C2=CC3=C(C=C2)NC(=O)C3=CC4=CC=CN4	
(R)-METHANANDAMIDE	2.60	CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)N[C@H](C)CO	
9-CIS RETINOIC ACID	2.68	C/C(=C/C=C/C(=C/C(=O)O)/C)/C=C/C1=C(C)CCCC1(C)C	

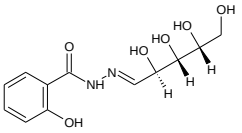
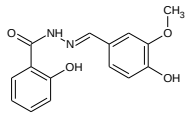
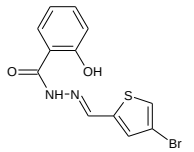
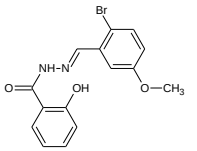
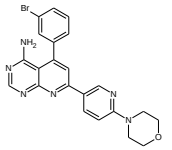
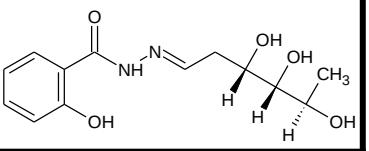
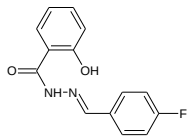
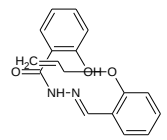
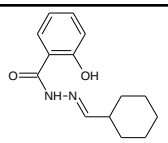
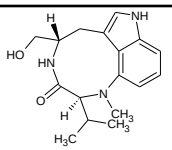
Compound Name	EC50 (μM)	SMILES	Structure
NP-006299	3.00	CN1Cc2c3OCOc3ccc2[C@H]4[C@@H](O)Cc5cc6OCOc6cc5[C@H]41	
Dimethyl fasudil	3.30	C[C@@H]1CNCCCN1S(=O)(=O)c2cccc3cncc(C)c23	
5,8,11-EICOSATRIYNOIC ACID	3.50	CCCCCCCCC#CCC#CCC#CCCCC(=O)O	
356130;WT-III-101-II_XG02	3.61	COc1cc(/C=N/NC(=O)c2ccccn2)ccc1O	
SU6656	3.86	CN(C)S(=O)(=O)c1ccc2NC(=O)/C(=C\c3cc4CCCCc4[nH]3)/c2c1	
NP-010771	4.00	O[C@H]([C@H]1C[C@@H]2CCN1C[C@@H]2C=C)c3ccnc4ccccc34	
SB 225002	4.00	Oc1cc(ccc1NC(=O)Nc2ccccc2Br)[N+](=O)[O-]	
2-Methoxy-Estradiol	4.79	COc1cc2C3CC[C@]4(C)[C@@H](O)CCC4C3CCc2cc1O	
2,5-dihydroxycinnamic acid	5.00	COC(=O)/C=C/c1cc(O)ccc1O	
NP-003964	5.30	CC(C)(O)CCC(=O)[C@](C)(O)C1[C@H](O)C[C@@]2(C)C3CC=C4C(C[C@H](O)[C@@H](O)C4(C)C)[C@]3(C)C(=O)C[C@]12C	

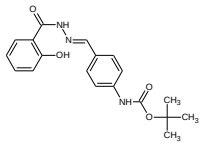
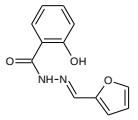
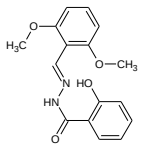
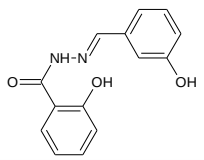
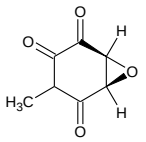
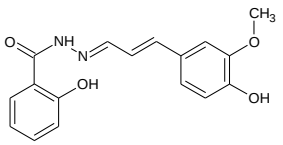
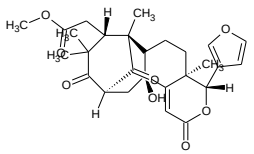
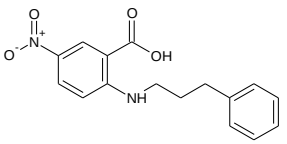
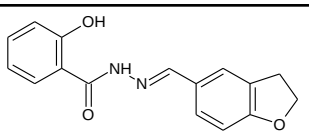
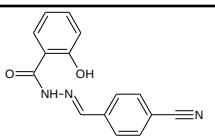
Compound Name	EC50 (μM)	SMILES	Structure
Indanocine	5.40	COc1cc2C/C(=C\c3cc(C)c(O)c(C)c3)/C(=O)c2c(N)c1OC	
DEOXYSAPPANONE B 7,3'-DIMETHYL ETHER ACETATE	5.60	COc1ccc2C(=O)C(Cc3ccc(OC)c(OC(=O)C)c3)COc2c1	
Simvastatin	5.84	CCC(C)(C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@@H]12	
NP-009507	6.00	COc1cc(ccc1O)c2oc3cc(O)c(OC)c(O)c3c(=O)c2OC	
DEOXYSAPPANONE B 7,4'-DIMETHYL ETHER	6.10	COc1ccc2C(=O)C(Cc3ccc(OC)c(O)c3)COc2c1	
Cdk1 Inhibitor	7.20	Clc1[nH]c2ccccc2c1/C=C\3/C(=O)Nc4ccccc34	
379572	7.35	CN(C)CCCNC(=O)[C@H]1[C@@H](N(Cc2cc(cc(c2)C(F)(F)F)C(F)(F)F)C(=O)c3ccccc13)c4ccc(COC(=O)NCCCCCC(=O)NO)cc4	
Prazosin hydrochloride	7.80	COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)c4ccco4	
RLM 2-67	8.26	Nc1ccccc1NC(=O)c2ccc(CNc3nccc(n3)c4cccnc4)cc2	
324803	8.70	Cc1ccc(S[C@@]2(CC(=O)N(Cc3ccccc3Cl)[C@@H]2c4ccc(CO)cc4I)C(=O)NCCN5CCOCC5)cc1	

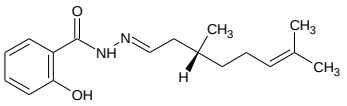
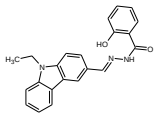
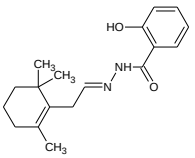
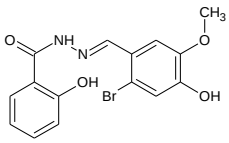
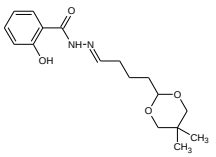
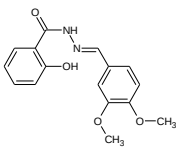
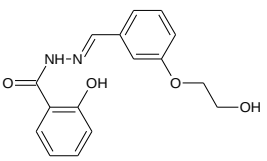
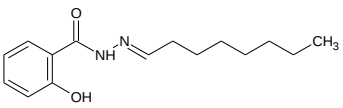
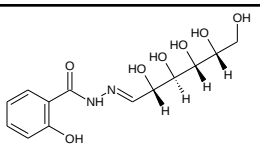
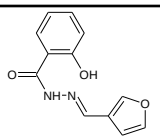
Compound Name	EC50 (μM)	SMILES	Structure
324818	8.80	CN(C)CCCNC(=O)[C@]1(CC(=O)N(Cc2ccccc2C(F)(F)F)[C@@H]1c3ccc(CO)cc3I)Sc4ccc(C)cc4	
Latruculin B	8.82	C[C@H]/1CC[C@@H]2C[C@H](C[C@@](O)(O2)[C@@H]3CSC(=O)N3)OC(=O)\C=C(\C)/CC/C=C1	
Aminopurvalanol A	8.83	CC(C)[C@H](CO)Nc1nc(Nc2cc(N)cc(Cl)c2)c3ncn(C(C)C)c3n1	
ascomycin (FK-520)	8.87	CC[C@@H]1C=C(C)C[C@H](C)C[C@H](OC)[C@H]2O[C@](O)([C@H](C)C[C@@H]2OC)C(=O)C(=O)N3CCCC[C@H]3C(=O)O[C@@H]([C@H](C)[C@@H](O)CC1=O)/C(=C/[C@@H]4CC[C@@H](O)[C@@H](C4)OC)/C	
379505	10.00	ONC(=O)CCCCCNC(=O)OCCCOc1ccc(cc1)C2=N[C@]3(CCS(=O)(=O)c4ccccc4)[C@H](O2)c5ccccc5CN(Cc6ccccc6)C3=O	
Lovastatin	10.66	CC[C@H](C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@@H]12	
Retinoic acid	10.68	C/C(=C\C=C\C(=C\C(=O)O)\C)/C=C/C1=C(C)CCCC1(C)C	
Triflupromazine hydrochloride	10.90	CN(C)CCCN1c2ccccc2Sc3ccc(cc13)C(F)(F)F	
Azacytidine-5	11.15	Nc1ncn(C2O[C@H](CO)[C@@H](O)[C@H]2O)c(=O)n1	
Triamterene	12.30	Nc1nc(N)c2nc(c(N)nc2n1)c3ccccc3	

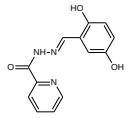
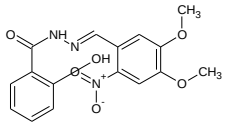
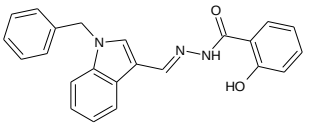
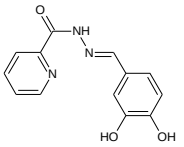
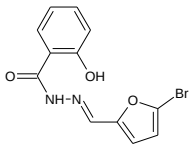
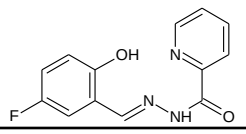
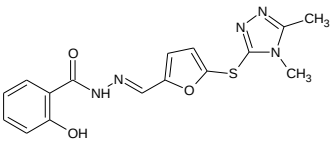
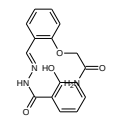
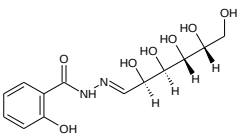
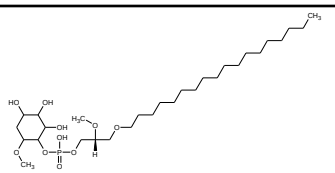
Compound Name	EC50 (μM)	SMILES	Structure
Fluvastatin sodium salt	13.54	CC(C)n1c(/C=C/[C@H](O)C[C@H](O)CC(=O)O)c(c2ccc(F)cc2)c3ccccc13	
CANTHARIDIN	14.83	C[C@]12C3CCC(O3)[C@]2(C)C(=O)OC1=O	
324798	14.98	CN(C)CCCNC(=O)[C@]1(CC(=O)N(C2Cc3ccccc3C2)[C@@H]1c4ccc(CO)cc4I)Sc5ccc(C)cc5	
rutaecarpine	14.99	O=c1n2CCc3c([nH]c4ccccc34)-c2nc5ccccc15	
Monensin sodium salt	15.13	CC[C@]1(CC[C@@H](O1)[C@]2(C)CC[C@]3(C[C@H](O)[C@@H](C)[C@H](O3)[C@@H](C)[C@@H](OC)[C@H](C)C(=O)O)O2)[C@@H]4O[C@H](C[C@@H]4C)[C@H]5O[C@@](O)(CO)[C@H](C)C[C@@H]5C	
Lasalocid sodium salt	15.29	CC[C@H]([C@H]1O[C@@](CC)(C[C@@H]1C)[C@H]2CC[C@](O)(CC)[C@H](C)O2)C(=O)[C@@H](C)[C@@H](O)[C@H](C)CCc3ccc(C)c(O)c3C(=O)O	
Scoulerine	15.52	COc1ccc2C[C@@H]3N(CCc4cc(OC)c(O)cc34)Cc2c1O	
GW8510	15.67	CN(C)c1cc2c(Nc3ccc4n(Cc5ccccc5)ncc4c3)ncnc2cn1	
324833	15.74	Cc1ccc(S[C@@]2(CC(=O)N(Cc3ccccc3)[C@@H]2c4ccc(CO)cc4I)C(=O)NCCN5CCOCC5)cc1	
SU9516	16.39	COc1ccc2NC(=O)/C(=C\c3c[nH]cn3)/c2c1	

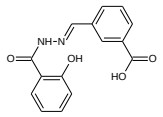
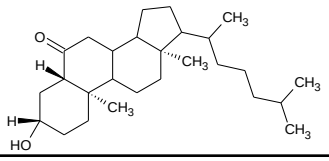
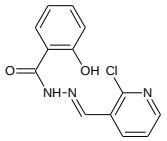
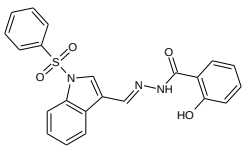
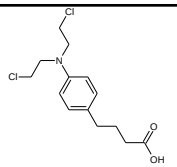
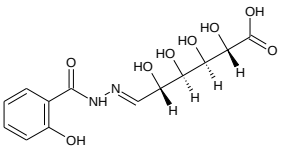
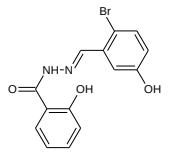
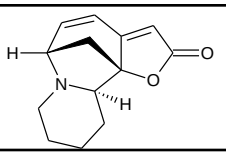
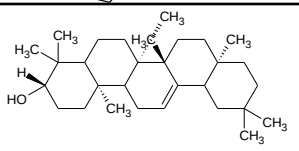
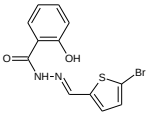
Compound Name	EC50 (μM)	SMILES	Structure
355966;WT-III-101-I_XF03	16.68	OC[C@@H](O)[C@H](O)[C@H](O)[C@@H](O)/C=N/NC(=O)c1ccccc1O	
NP-003918	16.87	CC(=C)C(=O)OC1CC(CO)CCCC(=CC2OC(=O)C(=C)C21)CO	
355939;WT-III-101-I_XB10	17.07	Oc1ccccc1C(=O)N/N=C/CCC=C	
355843;WT-III-101-I_A03	17.12	COc1ccc(/C=N/NC(=O)c2ccccc2O)cc1	
355871;WT-III-101-I_D01	17.29	Oc1ccccc1C(=O)N/N=C/c2ccccc2Cl	
IRIGENIN, 7-BENZYL ETHER	17.34	COc1cc(cc(O)c1OC)c2coc3cc(OCc4ccccc4)c(OC)c(O)c3c2=O	
DIHYDROROBINETIN	17.75	O[C@@H]1[C@H](Oc2cc(O)ccc2C1=O)c3cc(O)c(O)c(O)c3	
372504	17.97	OCc1ccc(CO[C@H]2C[C@H](C=C(O2)C(=O)NC3CC3)C4CC4)cc1	
dipyridamole	18.98	OCCN(CCO)c1nc(N2CCCCC2)c3nc(nc(N4CCCCC4)c3n1)N(CCO)CCO	
harmine	20.88	COc1ccc2c(c1)[nH]c3c(C)nccc23	

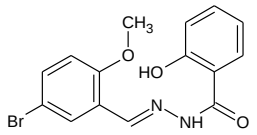
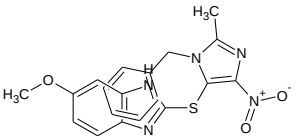
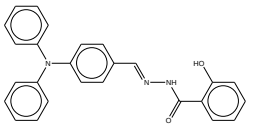
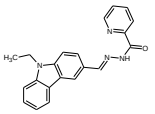
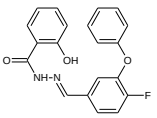
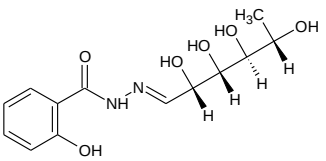
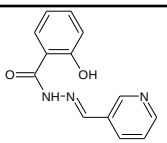
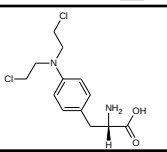
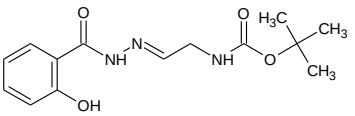
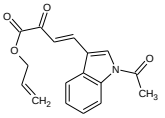
Compound Name	EC50 (μM)	SMILES	Structure
355964;WT-III-101-I_XF01	23.79	OC[C@@H](O)[C@@H](O)[C@H](O)/C=N/NC(=O)c1ccccc1O	
355974;WT-III-101-I_XG02	25.50	COc1cc(/C=N/NC(=O)c2ccccc2O)ccc1O	
355896;WT-III-101-I_F07	25.63	Oc1ccccc1C(=O)N/N=C/c2cc(Br)cs2	
355856;WT-III-101-I_B05	25.76	COc1ccc(Br)c(/C=N/NC(=O)c2ccccc2O)c1	
ABT-702	25.98	Nc1ncnc2nc(cc(c3cccc(Br)c3)c12)c4ccc(nc4)N5CCOCC5	
355965;WT-III-101-I_XF02	26.07	C[C@@H](O)[C@@H](O)[C@@H](O)C/C=N/NC(=O)c1ccccc1O	
355899;WT-III-101-I_F11	26.57	Oc1ccccc1C(=O)N/N=C/c2ccc(F)cc2	
355842;WT-III-101-I_A02	26.89	Oc1ccccc1C(=O)N/N=C/c2ccccc2OCC=C	
355877;WT-III-101-I_D08	26.97	Oc1ccccc1C(=O)N/N=C/C2CCCCC2	
Indolactam V	27.53	CC(C)[C@@H]1N(C)c2cccc3[nH]cc(C[C@@H](CO)NC1=O)c23	

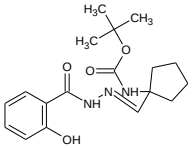
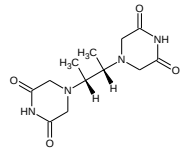
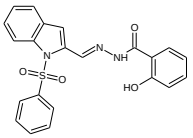
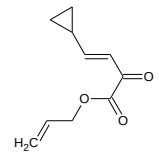
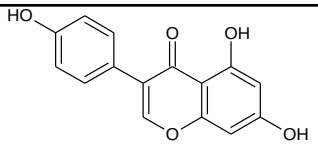
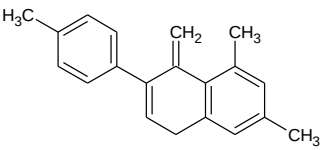
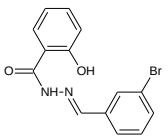
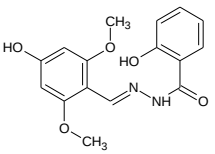
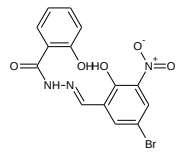
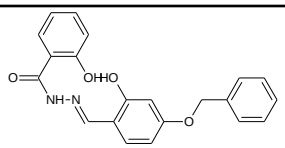
Compound Name	EC50 (μM)	SMILES	Structure
355904;WT-III-101-I_G06	27.55	CC(C)(C)OC(=O)Nc1ccc(/C=N/NC(=O)c2ccccc2O)cc1	
355906;WT-III-101-I_G09	27.57	Oc1ccccc1C(=O)N/N=C/c2ccco2	
355891;WT-III-101-I_F01	27.57	COc1cccc(OC)c1/C=N/NC(=O)c2ccccc2O	
355908;WT-III-101-I_G11	27.65	Oc1cccc(/C=N/NC(=O)c2ccccc2O)c1	
(-)-Terreic Acid	28.63	CC1C(=O)[C@@H]2O[C@@H]2C(=O)C1=O	
355915;WT-III-101-I_H07	28.98	COc1cc(/C=C/C=N/NC(=O)c2ccccc2O)ccc1O	
8beta-HYDROXYCARAPIN	29.33	COC(=O)C[C@H]1C(C)(C)C(=O)[C@@H]2C[C@]3(O)C(CC[C@@]4(C)[C@@H](OC(=O)C=C43)c5ccoc5)[C@@]1(C)C2=O	
NPPB	30.42	OC(=O)c1cc(ccc1NCCCc2ccccc2)[N+](=O)[O-]	
355885;WT-III-101-I_E06	30.63	Oc1ccccc1C(=O)N/N=C/c2ccc3OCCc3c2	
355876;WT-III-101-I_D07	30.96	Oc1ccccc1C(=O)N/N=C/c2ccc(C#N)cc2	

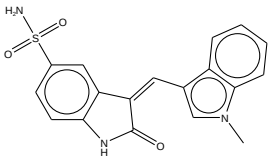
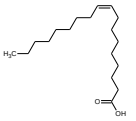
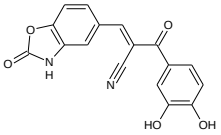
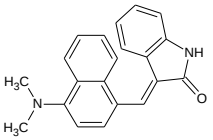
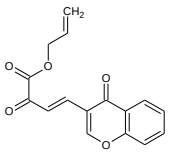
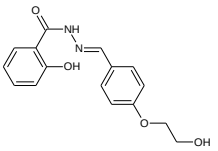
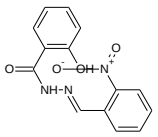
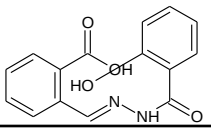
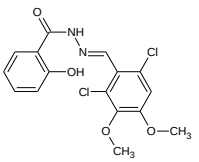
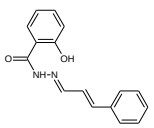
Compound Name	EC50 (μM)	SMILES	Structure
355874;WT-III-101-I_D05	31.08	C[C@H](CCC=C(C)C)C/C=N/NC(=O)c1ccccc1O	
355981;WT-III-101-I_XG11	32.00	CCn1c2ccccc2c3cc(/C=N/NC(=O)c4ccccc4O)ccc13	
355958;WT-III-101-I_XD09	32.22	CC1=C(C/C=N/NC(=O)c2ccccc2O)C(C)(C)CCC1	
355863;WT-III-101-I_C03	32.65	COc1cc(/C=N/NC(=O)c2ccccc2O)c(Br)cc1O	
355894;WT-III-101-I_F05	32.93	CC1(C)COC(CCC/C=N/NC(=O)c2ccccc2O)OC1	
355892;WT-III-101-I_F02	33.15	COc1ccc(/C=N/NC(=O)c2ccccc2O)cc1OC	
355911;WT-III-101-I_H02	34.37	OCCOc1cccc(/C=N/NC(=O)c2ccccc2O)c1	
355949;WT-III-101-I_XC11	34.53	CCCCCCC/C=N/NC(=O)c1ccccc1O	
355967;WT-III-101-I_XF05	34.53	OC[C@@H](O)[C@@H](O)[C@H](O)[C@@H](O)/C=N/NC(=O)c1ccccc1O	
355907;WT-III-101-I_G10	36.12	Oc1ccccc1C(=O)N/N=C/c2ccoc2	

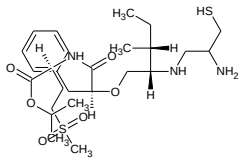
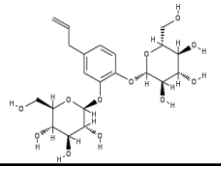
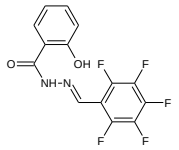
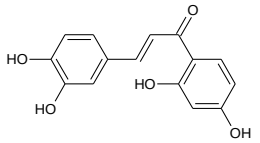
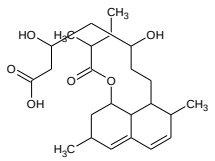
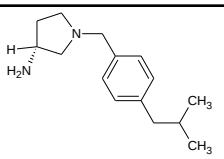
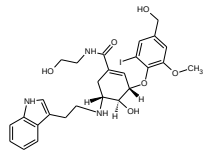
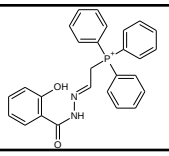
Compound Name	EC50 (μM)	SMILES	Structure
356044;WT-III-101-II_E09	36.24	Oc1ccc(O)c(/C=N/NC(=O)c2ccccn2)c1	
355937;WT-III-101-I_XB07	37.03	COc1cc(/C=N/NC(=O)c2ccccc2O)c(cc1OC)[N+](=O)[O-]	
355985;WT-III-101-I_XH03	37.29	Oc1ccccc1C(=O)N/N=C/c2cn(Cc3ccccc3)c4ccccc24	
356045;WT-III-101-II_E10	37.90	Oc1ccc(/C=N/NC(=O)c2ccccn2)cc1O	
355852;WT-III-101-I_B01	38.68	Oc1ccccc1C(=O)N/N=C/c2ccc(Br)o2	
356058;WT-III-101-II_G03	38.77	Oc1ccc(F)cc1/C=N/NC(=O)c2ccccn2	
355895;WT-III-101-I_F06	38.81	Cc1nnc(Sc2ccc(/C=N/NC(=O)c3ccccc3O)o2)n1C	
355959;WT-III-101-I_XD11	38.94	NC(=O)COc1ccccc1/C=N/NC(=O)c2ccccc2O	
355987;WT-III-101-I_XH05	39.30	OC[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)/C=N/NC(=O)c1ccccc1O	
Akt Inhibitor II	39.94	CCCCCCCCCCCCCCCCCCCCOC[C@H](COP(=O)(O)OC1C(O)C(O)C(O)CC1OC)OC	

Compound Name	EC50 (μM)	SMILES	Structure
355868;WT-III-101-I_C10	40.02	OC(=O)c1cccc(/C=N/NC(=O)c2ccccc2O)c1	
5alpha-CHOLESTAN-3beta-OL-6-ONE	40.13	CC(C)CCCC(C)C1CCC2C3CC(=O)[C@H]4C[C@@H](O)CC[C@]4(C)C3CC[C@]12C	
355872;WT-III-101-I_D03	41.14	Oc1ccccc1C(=O)N/N=C/c2ccccnc2Cl	
355942;WT-III-101-I_XC02	41.30	Oc1ccccc1C(=O)N/N=C/c2cn(c3ccccc23)S(=O)(=O)c4ccccc4	
CHLORAMBUCIL	41.45	OC(=O)CCCc1ccc(cc1)N(CCCl)CCCl	
355975;WT-III-101-I_XG03	41.56	O[C@@H](/C=N/NC(=O)c1ccccc1O)[C@@H](O)[C@@H](O)[C@H](O)C(=O)O	
355854;WT-III-101-I_B03	42.53	Oc1ccc(Br)c(/C=N/NC(=O)c2ccccc2O)c1	
SECURININE	42.80	O=C1O[C@]2(C[C@H]3C=CC2=C1)[C@H]4CCCCN34	
beta-AMYRIN	42.88	CC1(C)CC[C@]2(C)CC[C@]3(C)C(=CCC4[C@@]5(C)CC[C@H](O)C(C)(C)C5CC[C@]43C)C2C1	
355862;WT-III-101-I_C02	44.36	Oc1ccccc1C(=O)N/N=C/c2ccc(Br)s2	

Compound Name	EC50 (μM)	SMILES	Structure
355857;WT-III-101-I_B07	44.46	COc1ccc(Br)cc1/C=N/NC(=O)c2ccccc2O	
5920592	45.28	COc1ccc2nc(Sc3c(nc(C)n3Cc4ccccc4)[N+](=O)[O-])[nH]c2c1	
355962;WT-III-101-I_XE08	48.20	Oc1ccccc1C(=O)N/N=C/c2ccc(cc2)N(c3ccccc3)c4ccccc4	
356137;WT-III-101-II_XG11	48.96	CCn1c2ccccc2c3cc(/C=N/NC(=O)c4ccccn4)ccc13	
355901;WT-III-101-I_G02	49.19	Oc1ccccc1C(=O)N/N=C/c2ccc(F)c(Oc3ccccc3)c2	
355969;WT-III-101-I_XF07	50.28	C[C@H](O)[C@H](O)[C@@H](O)[C@@H](O)/C=N/NC(=O)c1ccccc1O	
355944;WT-III-101-I_XC04	51.67	Oc1ccccc1C(=O)N/N=C/c2ccccnc2	
MELPHALAN	52.01	N[C@@H](Cc1ccc(cc1)N(CCCl)CCCl)C(=O)O	
355897;WT-III-101-I_F09	54.22	CC(C)(C)OC(=O)NC/C=N/NC(=O)c1ccccc1O	
TFB14-I082	54.26	CC(=O)n1cc(/C=C/C(=O)C(=O)OCC=C)c2ccccc12	

Compound Name	EC50 (μM)	SMILES	Structure
355865;WT-III-101-I_C06	54.72	CC(C)(C)OC(=O)NC1(CCCC1)/C=N/NC(=O)c2ccccc2O	
ICRF-193	55.83	C[C@@H]([C@@H](C)N1CC(=O)NC(=O)C1)N2CC(=O)NC(=O)C2	
355995;WT-III-101-I_XE07	60.10	Oc1ccccc1C(=O)N/N=C/c2cc3ccccc3n2S(=O)(=O)c4ccccc4	
DML-I-127-f10-17	61.98	C=CCOC(=O)C(=O)/C=C/C1CC1	
GENISTEIN	62.12	Oc1ccc(cc1)c2coc3cc(O)cc(O)c3c2=O	
genistein	63.15	Cc1ccc(cc1)C2=CCc3cc(C)cc(C)c3C2=C	
355849;WT-III-101-I_A10	63.32	Oc1ccccc1C(=O)N/N=C/c2ccccc(Br)c2	
355893;WT-III-101-I_F03	63.89	COc1cc(O)cc(OC)c1/C=N/NC(=O)c2ccccc2O	
355883;WT-III-101-I_E04	66.29	Oc1ccccc1C(=O)N/N=C/c2cc(Br)cc([N+](=O)[O-])c2O	
355864;WT-III-101-I_C04	69.23	Oc1ccccc1C(=O)N/N=C/c2ccc(OCc3ccccc3)cc2O	

Compound Name	EC50 (μM)	SMILES	Structure
Syk Inhibitor	72.50	Cn1cc(/C=C/2\C(=O)Nc3ccc(cc23)S(=O)(=O)N)c4ccccc14	
Oleic Acid	75.41	CCCCCCCC/C=C\CCCCCCCC(=O)O	
AGL 2263	76.45	Oc1ccc(cc1O)C(=O)/C(=C/c2ccc3oc(=O)[nH]c3c2)/C#N	
VEGF Receptor 3 Kinase Inhibitor, MAZ51	78.41	CN(C)c1ccc(/C=C/2\C(=O)Nc3ccccc23)c4ccccc14	
TFB26-I096	78.77	C=CCOC(=O)C(=O)/C=C/c1coc2ccccc2c1=O	
355912;WT-III-101-I_H03	81.66	OCCOc1ccc(/C=N/NC(=O)c2ccccc2O)cc1	
355936;WT-III-101-I_XB05	81.69	Oc1ccccc1C(=O)N/N=C/c2ccccc2[N+](=O)[O-]	
355869;WT-III-101-I_C11	83.82	OC(=O)c1ccccc1/C=N/NC(=O)c2ccccc2O	
355881;WT-III-101-I_E01	88.09	COc1cc(Cl)c(/C=N/NC(=O)c2ccccc2O)c(Cl)c1OC	
355873;WT-III-101-I_D04	88.85	Oc1ccccc1C(=O)N/N=C/C=C/c2ccccc2	

Compound Name	EC50 (μM)	SMILES	Structure
L-744,832	89.00	CC[C@@H](C)[C@@H](CO[C@@H](Cc1ccccc1)C(=O)N[C@@H](CCS(=O)(=O)C)C(=O)OC(C)C)NCC(N)CS	
NP-006884	90.83	OC[C@H]1O[C@@H](Oc2ccc(CC=C)cc2O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)[C@H](O)[C@@H](O)[C@@H]1O	
355938;WT-III-101-I_XB09	91.91	Oc1ccccc1C(=O)N/N=C/c2c(F)c(F)c(F)c(F)c2F	
Butein	91.99	Oc1ccc(C(=O)/C=C/c2ccc(O)c(O)c2)c(O)c1	
NP-001236	92.31	CCC(C)C(=O)OC1CC(C)C=C2C=CC(C)C(CCC(O)CC(O)CC(=O)O)C12	
TMI-34	93.03	CC(C)Cc1ccc(CN2CC[C@@H](N)C2)cc1	
HUM-SAH20	94.90	COc1cc(CO)cc(I)c1O[C@H]2C=C(C[C@@H](NCCc3c[nH]c4ccccc34)[C@@H]2O)C(=O)NCCO	
355963;WT-III-101-I_XE09	95.02	Oc1ccccc1C(=O)N/N=C/C[P+](c2ccccc2)(c3ccccc3)c4ccccc4	
355900;WT-III-101-I_G01	96.51	Oc1ccc(/C=N/NC(=O)c2ccccc2O)cc1F