

## Electronic Supplementary Information

### **A novel adaptive ensemble classification framework for ADME prediction**

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C91	CacoP	CacoP-	13	O=C1C(CCS(=O)c2ccccc2)C(=O)N(N1c1ccccc1)c1ccccc1
C92	CacoP	CacoP-	13	O=C(NC[C@H]1[NH+](CC)CCC1)c1cc(ccc1OC)S(=O)(=O)N
C93	CacoP	CacoP-	13	cc1c@H]1[C@@H]2[C@@H]1[C@@H](C(=O)[C@@H]1[C@@H](C[C@@H](C(=O)O1)C)O[C@H]1[C@@H]1[C@@H](C[C@@H](O1)C)[NH+](C)C)O(C)OC)C)N(C(=O)O2)CCCC1cc(ne1)c1encec1C
C94	CacoP	CacoP-	13	CC(C)(C)C#C/C=C/C[NH+](C)Cc1c2ccccc2ccc1
C95	CacoP	CacoP-	13	CCC1(c2c(COC1=O)c(=O)n1Cc3c(nc4ccc(c4c3)C[NH+](C)C)O)c1c2)O
C96	CacoP	CacoP-	13	O=C(C1CCC(C[NH3+])CC1)[O-]
C97	CacoP	CacoP-	13	FC(c1cc2c(cc1)Sc1c(cccc1)N2CCC[NH+])1CCN(C)CC1)(F)F
C98	CacoP	CacoP-	13	CC([C@H](N(Cc1ccc(cc1)c1c(cccc1)c1nmm[nH]1)C(=O)CCCC)C(=O)[O-])[O-]C
C99	CacoP	CacoP-	13	O=C(NCC[NH2+][C@@H](O)COc1ccc(cc1)O)N1CCOCC1
C100	CacoP	CacoP-	13	OC[C@H]([C@H]([C@@H]([C@H](CO)O)O)O)O
C101	CacoP	CacoP-	13	O=c1nc(N)ccn1[C@@H]1O[C@H](CO)[C@@H](O)C1(F)F
C102	CacoP	CacoP-	13	CC(C)C[C@H]1C(=O)N2CCC[C@H]2[C@@H]2(N1C(=O)[C@](O2)(C(C)C)NC(=O)[C@H]1C[NH+])([C@@H]2Cc3c([nH]c4cccc(c34)C2=C1)Br)C)O
C103	CacoP	CacoP-	13	O=C([C@H]1CSSC[C@H]([NH3+])C(=O)N[C@H](Cc2ccc(cc2)O)C(=O)N[C@H](Cc2ccccc2)C(=O)N[C@H](CCCC(=O)N)C(=O)N[C@H](CC(=O)N)C(=O)N1[C@H](C(=O)N[C@H](C(=O)N)CCN=C(N)N)CCC1
C104	CacoP	CacoP-	13	O=C1N[C@@H](C(=O)N[C@H](C(=O)N[C@H](Cc2[nH]3c2ccc3)C(=O)N[C@H](CO)C(=O)N[C@H](C(=O)N[C@H](COC(C)C)C(=O)N[C@H](CC(C)C)C(=O)N[C@H](CCCN=C(N)N)C(=O)N2CCC[C@@H]2C(=O)N)C)C2ccc(cc2)O)Cc2en[nH]2)CC1
C105	CacoP	CacoP-	13	O=c1n(NC(=O)N[NH3+])c(=O)c2cc(cc3c2c1cc(c3N)S(=O)(=O)[O-])S(=O)(=O)[O-]
C106	CacoP	CacoP-	13	O=C(NC)[C@H](NC(=O)[C@@H](C)NC(=O)C)Cc1ccccc1
C107	CacoP	CacoP-	13	O=C(NC)[C@H](NC(=O)[C@@H](C(C)C)NC(=O)C)Cc1ccccc1
C108	CacoP	CacoP-	13	O=S(=O)(c1ccc2ccccc2c1)N[C@@H](Cc1cc(ccc1)C(=N)N)CC(=O)N1CCCC[C@@H]1C(=O)OC
C109	CacoP	CacoP-	13	O=S(=O)(c1ccc2ccccc2c1)NC(Cc1cc(ccc1)C(=N)N)CC(=O)N1CCCC(C(=O)[O-])C1
C110	CacoP	CacoP-	13	O=S(=O)(c1ccc2ccccc2c1)NC(Cc1cc(ccc1)C(=N)N)CC(=O)N1CCC(C(=O)[O-])CC1
C111	CacoP	CacoP-	13	O=S(=O)(c1ccc2ccccc2c1)NC(Cc1cc(ccc1)C(=N)N)CC(=O)N1CCC(C(=O)OC)CC1
C112	CacoP	CacoP-	13	O=S(=O)(c1ccc2ccccc2c1)NC(Cc1cc(ccc1)C(=N)NO)CC(=O)N1CCC(C(=O)[O-])CC1
C113	CacoP	CacoP-	13	O=S(=O)(c1ccc2ccccc2c1)NC(Cc1cc(ccc1)C(=N)N)CC(=O)N1CC[NH2+])CC1
C114	CacoP	CacoP-	13	O=C([C@H]1CSSCC(=O)N[C@H](Cc2ccc(cc2)O)C(=O)N[C@H](Cc2ccccc2)C(=O)N[C@H](CCCC(=O)N)C(=O)N[C@H](CC(=O)N)C(=O)N1N1[C@H](C(=O)N[C@H](C(=O)N)CCN=C(N)N)CCC1
C115	CacoP	CacoP-	13	O=S(=O)(c1ccc2ccccc2c1)NC(Cc1cc(ccc1)C(=N)NC)CC(=O)N1CCC(C)CC1
C116	CacoP	CacoP-	13	OC([NH2+])CCNC(=O)N1CCC(O)CC1)COc1ccc(cc1)CCOCCOCC1CC1
C117	CacoP	CacoP-	13	O=S(=O)(Nc1ncccc1)c1ccc(cc1)N/N=C/1\C=C(C(=O)[O-])C(=O)C=C1
C118	CacoP	CacoP-	13	O=C([O-])C[NH2+][C@H](C1CCCC1)C(=O)N1[C@H](C(=O)N(c2ccc(cc2)C(=N)N)C)CC1
C119	CacoP	CacoP-	13	CC1C(O)C(O)C(O)C(O)[C@H]2CC[C@]3(C)[C@H]4CC[C@]5(C)[C@@H](c6coc(=O)cc6)CC[C@]5(O)[C@@H]4CCC3=C2)O1
C120	CacoP	CacoP-	13	Oc1ccc(cc1)C([NH3+])C(=O)N[C@@H]1[C@@H]2SCC(=C(C(=O)[O-])N2C1=O)CSc1n[nH]cn1
C121	CacoP	CacoP-	13	O=C(C(OP(=O)(CCCCc1ccccc1)[O-])CCCC[NH3+])N1C(C(=O)[O-])CCCC1
C122	CacoP	CacoP-	13	CC[N+](Cc1c(cccc1)Br)(C)C
C123	CacoP	CacoP-	13	O=C(C1=CCS[C@H]2N1C(=O)[C@H]2NC(=O)/C(=C)CC(=O)O)/c1csc(n1)N)[O-]
C124	CacoP	CacoP-	13	NC(=N)c1ccc(cc1)OCCCCCOc1ccc(cc1)C(=N)N
C125	CacoP	CacoP-	13	C[C@H]1C[C@H]2[C@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@]1(C(=O)COC1[C@H](O)[C@H](O)[C@H](O)[C@H](CC(=O)[O-])O1)O
C126	CacoP	CacoP-	13	O[C@H]1[C@@H](CO)(O)O[C@@H](CO)[C@@H]1O[C@@H]1O[C@@H]1([C@@H]([C@@H]([C@H]1O)O)CO
C127	CacoP	CacoP-	13	CO/N=C(c1ccco1)/C(=O)NC1C2N(C1=O)C(=C(CS2)COC(=O)N)C(=O)[O-]
C128	CacoP	CacoP-	13	OC(C)C(=O)[O-]
C129	CacoP	CacoP-	13	CN1CC(=O)N=C1N
C130	CacoP	CacoP-	13	C[C@H]1C(=O)N(C)[C@H](C(=O)NC)Cc2cn(cn2)CC(=O)N2[C@H](C(=O)N1)CCC2
C131	CacoP	CacoP-	13	O=C1N[C@H](C(=O)N2[C@@H](CCC2)C(=O)N[C@H](C(=O)N[C@H](Cc2c[nH]c3c2ccccc3)C(=O)N[C@H](C(=O)N[C@H]1[C@@H](CO)CCCC[NH3+])Cc1ccccc1)Cc1ccccc1
C132	CacoP	CacoP-	13	O=C1N[C@H](C(=O)N2[C@@H](CCC2)C(=O)N[C@H](C(=O)N(C)[C@H](Cc2c[nH]c3c2ccccc3)C(=O)N[C@H](C(=O)N[C@H]1[C@@H](CO)CCCC[NH3+])Cc1ccccc1)Cc1ccccc1
C133	CacoP	CacoP-	13	CC(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@H](Cc1ccccc1)C(=O)N[C@@H](Cc1ccccc1)C(=O)N
C134	CacoP	CacoP-	13	NC(=N)c1ccc2c(c1)[nH]c(n2)Cc1nc2c([nH]1)c(ccn2)C
C135	CacoP	CacoP-	13	Fe1cc(ccc1C1CCS(=O)CC1)N1C[C@H](CNC(=O)C)OC1=O
C136	CacoP	CacoP-	13	Fe1cc(ccc1N1CCN(C(=O)CO)CC1)N1C[C@H](CNC(=O)C)OC1=O







C275	CacoP	CacoP+	12	[C@@H]12CC[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@H]1[C@H]2CCCC2=CC(=O)C=C[C@]12C
C276	CacoP	CacoP+	2	C[C@]12CC[C@H]3[C@@H](CCC4=Ce5c(en5)C[C@]34C)[C@@H]1CC[C@@]2(O)C#C
C277	CacoP	CacoP+	11	CCC12CC[NH+](CC(C)(C)O)C(Ce3ccc(cc13)O)C2(C)C
C278	CacoP	CacoP+	10,11,12,6,2	CC(=O)CC(c1cccc1)c1c(O)oc2cccc2c1=O
C279	CacoP	CacoP+	12	OCC(C(=O)OC1C[C@H]2[NH+](C)[C@H](CC2)C1)c1cccc1
C280	CacoP	CacoP+	12	c1c2c(cc(c1OC)OC)[C@@]13CC[NH+]+4CC5=CCOC6CC(=O)N2C1[C@H]6[C@H]5C[C@@H]34
C281	CacoP	CacoP+	13	c1(c(nc(c(n1)Cl)N)N)C(=O)N=C(N)N
C282	CacoP	CacoP+	13	Nc1nc2c(cc(cc2)/C(=C/C(=O)N)/c2cccc(c2)F)n1S(=O)(=O)C(C)C
C283	CacoP	CacoP+	13	Nc1nc2c(cc(cc2)/C(=C/C(=O)N)/c2ccc(ccc2F)F)n1S(=O)(=O)C(C)C
C284	CacoP	CacoP+	13	Nc1nc2c(cc(cc2)/C(=C/C(=O)N)C)/c2ccc(ccc2F)F)n1S(=O)(=O)C(C)C
C285	CacoP	CacoP+	13	Nc1nc2c(cc(cc2)/C(=C/C(=O)N)C)/c2cccc2n1S(=O)(=O)C(C)C
C286	CacoP	CacoP+	13	Nc1nc2c(cc(cc2)/C(=C/C(=O)N)C)/c2cccc(c2)F)n1S(=O)(=O)CCC
C287	CacoP	CacoP+	13	Nc1nc2ccc(cc2n1S(=O)(=O)C(C)C)/C(=C/C(=O)N)/c1ccc(c(c1)F)OC
C288	CacoP	CacoP+	13	Nc1n(c2c(n1)ccc(c2)/C(=C/C(=O)N)/c1c(c(c(c1F)F)F)F)S(=O)(=O)C(C)C
C289	CacoP	CacoP+	13	Nc1nc2ccc(cc2n1S(=O)(=O)C(C)C)/C(=C/C(=O)N)/c1ccc(c(c1)F)F
C290	CacoP	CacoP+	13	Nc1nc2ccc(cc2n1S(=O)(=O)C(C)C)/C(=C/C(=O)N)/c1ccc(cc1F)F
C291	CacoP	CacoP+	13	Nc1n(c2c(n1)ccc(c2)/C(=C/C(=O)N)C)/c1ccc(c1)F)S(=O)(=O)[N-]C(=O)N(C)C
C292	CacoP	CacoP+	13	O=C(NCC1[NH2+]CCCC1)c1ccc(ccc1OCC(F)F)OCC(F)F
C293	CacoP	CacoP+	13	Nc1n(c2c(n1)ccc(c2)/C(=C/C(=O)N)/c1ccc(c1)F)S(=O)(=O)[N-]C(=O)N1CCOCC1
C294	CacoP	CacoP+	13	Nc1nc2c(cc(cc2)/C(=C/C(=O)N)C)/c2cccc(c2F)F)n1C(C)C
C295	CacoP	CacoP+	13	Nc1nc2ccc(cc2n1C1CCCC1)/C(=C/C(=O)N)C)/c1cccc1F
C296	CacoP	CacoP+	13	CC(c1c(c(ccc1)C(C)C)O)C
C297	CacoP	CacoP+	13	c1ccc(ccc1N)S(=O)(=O)N
C298	CacoP	CacoP+	13	Oc1ccc(cc(c1O)O)C(=O)OC
C299	CacoP	CacoP+	13	O=C1C([NH2+]C)(c2cccc2Cl)CCCC1
C300	CacoP	CacoP+	13	O=C(CCCCCCCC)Nc1ccc(cc1)S(=O)(=O)Nc1nncs1
C301	CacoP	CacoP+	13	CC1(C)[C@H]2[C@@H]1CN(C(=O)[C@@H](C(C)(C)C)NC(=O)N[C@H](C(=O)C(C)C)C(C)C)[C@@H]2C(=O)N[C@@H](CCC)C(=O)C(=O)NCC=C
C302	CacoP	CacoP+	13	ClC1(Cl)C2C1CN(C(=O)C(NC(=O)OC(C)(C)C)C(C)C)C2C(=O)NC(Cc1CCCC1)C(=O)C(=O)N
C303	CacoP	CacoP+	13	O=C1N2C(C[C@@H](O)c3ccc(nc4ccc(cc34)OC)c3esc(n3)NC(C)C)C2)C(=O)N[C@@]2([C@@H](/C=C/CCCC[C@@H]1NC(=O)OC1CCCC1)C2)C(=O)[O-]
C304	CacoP	CacoP+	13	C[NH2+]CCC(Oc1ccc(cc1)C)c1cccc1
C305	CacoP	CacoP+	13	O=C(c1cc(nn1c1cccc(c1)C[NH3+])C(F)F)Nc1c(cc(c1)c1cccc1S(=O)(=O)C)F
C306	CacoP	CacoP+	13	COc1ccc(cc(c1OC)OC)C(=O)N1CC[C@@](c2ccc(c2)Cl)Cl)(CC[NH+]2CCC(C(=O)N3CCN(C)CC3)(c3cccc3)CC2)C1
C307	CacoP	CacoP+	13	Oc1c2cccc2ccc1
C308	CacoP	CacoP+	13	Fe1cccc2c1O[C@@H]1[C@H](O2)C[NH2+]C1
C309	CacoP	CacoP+	13	[NH3+][C@@H]([C@@H](O)[C@@H](O)CC(C)C)CC1CCCCC1
C310	CacoP	CacoP+	13	O[C@@H]([C@@H](O)CC(C)C)[C@@H](NC(=O)CCCCc1cccc1)CC1CCCCC1
C311	CacoP	CacoP+	13	O[C@@H]([C@@H](O)CC(C)C)[C@@H](NC(=O)C[C@H](NC(=O)OC(C)(C)C)C(=O)[O-])CC1CCCCC1
C312	CacoP	CacoP+	13	O[C@@H]([C@@H](O)CC(C)C)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](Cc1cccc1)NS(=O)(=O)N1CCN(C(=O)CCC(=O)[O-])CC1)Cc1csc(n1)N)CC1CCCCC1
C313	CacoP	CacoP+	13	O=C(N1CCC(C(C(=O)[O-])C2CNe3c(ccc3)C2)CC1)CCc1nc2c(cc1)CCCN2
C314	CacoP	CacoP+	13	O=c1[nH]c(=O)n(cc1F)[C@H]1O[C@@H](COC(=O)C(C)C)[NH3+][C@H](O)C1
C315	CacoP	CacoP+	13	O=c1[nH]c(=O)n(cc1F)[C@H]1O[C@@H](CO)[C@H](OC(=O)[C@H]([C@@H](C)CC)[NH3+])C1
C316	CacoP	CacoP+	13	Oc1ccc(cc1)C(=O)OCCCC
C317	CacoP	CacoP+	13	Oc1ccc(cc1)C(=O)OCCCCC
C318	CacoP	CacoP+	13	O=C(CC(=O)/C=C/c1ccc(c(c1)OC)O)/C=C/c1ccc(c(c1)OC)O
C319	CacoP	CacoP+	13	cc1=c2[C@@H](O)C(=O)[C@@]3(C)[C@@H](O)[C@@H]C@@H(O)[C@@H](O)[C@@H](O)CO4C[C@H]4[C@@](CO4)(OC(=O)C[C@H]3[C@@H](O)C[C@@H]1OC(=O)[C@@H](O)[C@H](NC(=O)c1cccc1)c1cccc1)O)C2(C)C
C320	CacoP	CacoP+	13	Fe1c(c(c(cc1)OC)c1nc2c(ncc(c2)Cl)s1)F)C(=O)N



C321	CacoP	CacoP+	13	N#Cc1cccc(c1)Cn1ence1
C322	CacoP	CacoP+	13	c1(ccccc1)Cn1ene2c1cccc2
C323	CacoP	CacoP+	13	O=C([O-])c1cccc(cc1)Cn1ene2c1cccc2
C324	CacoP	CacoP+	13	NS(=O)(=O)c1cccc(cc1)Cn1ene2c1cccc2
C325	CacoP	CacoP+	13	N#Cc1cccc(c1)Cn1nccc1
C326	CacoP	CacoP+	13	O=C([O-])c1cccc(cc1)Cn1nccc1
C327	CacoP	CacoP+	13	O=C([O-])Cc1cccc(cc1)Cn1nccc1
C328	CacoP	CacoP+	13	[O-]C(=O)c1cccc(c1)Cc1nccc1
C329	CacoP	CacoP+	13	NC(=O)c1cccc(c1)Cn1ene2c1cccc2
C330	CacoP	CacoP+	13	NC(=O)c1cccc(c1)Cn1nccc1
C331	CacoP	CacoP+	13	[NH3+]Cc1cccc(c1)Cn1nccc1
C332	CacoP	CacoP+	13	CC(=O)N[C@H](Cc1cccc1)C(=O)N(C)[C@H](Cc1cccc1)C(=O)N[C@H](Cc1cccc1)C(=O)N
C333	CacoP	CacoP+	13	CC(=O)N[C@H](Cc1cccc1)C(=O)N[C@H](Cc1cccc1)C(=O)N[C@H](Cc1cccc1)C(=O)NC
C334	CacoP	CacoP+	13	FC(c1c(nc(cc1)N1CC[NH2+]CC1)Cl)(F)F
C335	CacoP	CacoP+	13	O=C1CC(C)(C)CC(=O)N1CCCC[NH+]1CCN(c2ncccn2)CC1
C336	CacoP	CacoP+	13	O=C1C(O)C(C)(C)CC(=O)N1CCCC[NH+]1CCN(c2ncccn2)CC1
C337	CacoP	CacoP+	13	FC(c1cc(ncc1)N1CC[NH+])(CCCCN2CCCC2=O)CC1)(F)F
C338	CacoP	CacoP+	13	Clc1cccc(cc1)C1c2c(cccc2)C2=NCCN2C1
C339	CacoP	CacoP+	13	O=C1CC(C)C(=NN1)c1cc2cc(c(cc2s1)OC)OC
C340	CacoP	CacoP+	13	[NH3+]C(CC=C)c1cccc1e1noc2c1cccc2
C341	CacoP	CacoP+	13	O=C([C@H](OCc1cccc1)[C@H](O)[C@@H](O)[C@@H](OCc1cccc1)C(=O)N[C@@H](C(C)C)C(=O)NCC(F)(F)F)N[C@@H]1[C@H](O)Cc2c1cccc2
C342	CacoP	CacoP+	13	O=C(c1cc(nc(c1)N(C)[C@H]1[C@@H](C)C1)C)N(C)S(=O)(=O)C)N[C@@H](Cc1cccc1)[C@@H](O)C[C@@H](OC)C(=O)N[C@@H](C(C)C)C(=O)NCc1cccc1
C343	CacoP	CacoP+	13	O=C([O-])C[C@H](O)C[C@H](O)/C=C/c1c(c(c(nc1C(C)C)C(C)C)COC)c1cccc(c1)F
C344	CacoP	CacoP+	13	O=C1NCC2(CCC[NH2+]C2)c2c1cc([nH]2)c1eene(n1)c1cc2e(cc1)OCO2
C345	CacoP	CacoP+	13	c1(ccccc1)Cn1c(nnn1)C([NH+]1CCN(C2CCC2)CCC1)c1ccc2occc2c1
C346	CacoP	CacoP+	13	O=C1CC([NH+]2CCC[NH+])(CCCN3c4c(ccc(c4)C(=O)[O-])OCc4c3cccc4)CC2)N(C)C(=O)N1C
C347	CacoP	CacoP+	13	O=C1C[C@@H]([N@H+]2CC[N@@H+])(CCCN3c4c(ccc(c4)CC(=O)[O-])OCc4c3cccc4)CC2)N(C)C(=O)N1C
C348	CacoP	CacoP+	13	O=C1CC([NH+]2CCC[NH+])(CCCN3c4c(ccc(c4)C(C)(C)C(=O)[O-])CCc4c3cccc4)CC2)N(C)C(=O)N1C
C349	CacoP	CacoP+	13	Clc1c(cc(c2c1O[C@@]1(C(=CC(=O)C[C@H]1C)OC)C2=O)OC)OC O=C1CC([NH+]2CCC[NH+])(CCCN3c4c(ccc(c4)C(=O)[O-])OCc4c3cccc4)CC2)N(C)C(=O)N1C
C350	CacoP	CacoP+	13	O=C1C[C@@H]([N@H+]2CC[N@@H+])(CC/C=C/3\c4c(ccc(c4)CC(=O)[O-])OCc4c3cccc4)CC2)N(C)C(=O)N1C
C351	CacoP	CacoP+	13	O=C1C[C@@H]([N@H+]2CC[N@@H+])(CC/C=C/3\c4c(ccc(c4)C(=O)[O-])OCc4c3cccc4)CC2)N(C)C(=O)N1C
C352	CacoP	CacoP+	13	O=C1C[C@@H]([N@H+]2CC[N@@H+])(CC/C=C/3\c4c(ccc(c4)CC(=O)[O-])OCc4c3cccc4)CC2)N(C)C(=O)N1C
C353	CacoP	CacoP+	13	O=C1CC([NH+]2CCC[NH+])(CC/C=C/3\c4c(ccc(c4)CC(=O)[O-])OCc4c3cccc4)CC2)N(C)C(=O)N1C
C354	CacoP	CacoP+	13	O=C1C(c2cccc2)(c2cccc2)C(=O)N(COC)C(=O)N1COC
C355	CacoP	CacoP+	13	[NH3+][C@@H](CCCCC)C(=O)N[C@@H](Cc1ccc(cc1)O)C(=O)NCC(=O)NCC(=O)N[C@@H](Cc1cccc1)C(=O)N[C@@H](CC(C)C)C(=O)N
C356	CacoP	CacoP+	13	CCCCCCCCC(=O)OC
C357	CacoP	CacoP+	13	CCCCCCCCC(=O)OCCC
C358	CacoP	CacoP+	13	CCCCCCCCC(=O)Oc1c(cccc1)F
C359	CacoP	CacoP+	13	O=C(c1ccc(cc1)F)CCC[NH+]1CCC(O)(c2ccc(cc2)Cl)CC1
C360	CacoP	CacoP+	13	CCCCCCCCC(=O)Oc1cccc1
C361	CacoP	CacoP+	13	CCCCCCCCC(=O)Nc1nccc1
C362	CacoP	CacoP+	13	CCCCCCCCC(=O)Nc1enccc1
C363	CacoP	CacoP+	13	CCCCCCCCC(=O)OCC(C)C
C364	CacoP	CacoP+	13	CCCCCCCCC(=O)Nc1c(c(ccc1)C)C
C365	CacoP	CacoP+	13	[NH3+]Nc1nccc2cccc12
C366	CacoP	CacoP+	13	

C367	CacoP	CacoP+	13	CCCCCCCCC(=O)NCCO
C368	CacoP	CacoP+	13	CCCCCCCCC(=O)NNe1cccc1
C369	CacoP	CacoP+	13	CCCCCCCCC(=O)NCe1cccc1
C370	CacoP	CacoP+	13	CCCCCCCCC(=O)N1CC[NH2+]CC1
C371	CacoP	CacoP+	13	Oe1cc2c(c(c1)O)C(=O)OCC(CCC(CCCCC2)O)C
C372	CacoP	CacoP+	13	O=c1c2c(cc(cc2O)O)oc(c1)c1cc(c(c1)OC)OC)O
C373	CacoP	CacoP+	13	O=c1c2c(cc(c(c2O)OC)OC)oc(c1OC)c1cc(c(cc1)O)O
C374	CacoP	CacoP+	13	C[C@]12CCCC(=O)C=C1CC[C@@H]1[C@@H]2[C@H](C[C@]2([C@H]1CC[C@@]2(C(=O)CO)O)C)O
C375	CacoP	CacoP+	13	CCC[C@@H](C(=O)C(=O)NC1CC1)NC(=O)[C@H]1[C@H]2CCC[C@H]2CN1C(=O)[C@@H](C(C)C)NC(=O)[C@@H](C1CCCC1)NC(=O)c1cccc1
C376	CacoP	CacoP+	13	O=c1n2c(nc3c1cccc3)C(=O)c1c2cccc1
C377	CacoP	CacoP+	13	O[C@](C[NH+](Cc1ccc(cc1)Br)NC(=O)[C@@H](C(C)C)CC(=O)OC)(Cc1cccc1)C(=O)NC1c2cccc2C[C@H]1O
C378	CacoP	CacoP+	13	O[C@@](C[N@@H+](Cc1ccc(cc1)/C=C\c1cccc1)NC(=O)[C@@H](C(C)C)CC(=O)OC)(Cc1cccc1)C(=O)N[C@H]1c2cccc2C[C@@H]1O
C379	CacoP	CacoP+	13	O[C@](C[NH+](Cc1ccc(cc1)Br)NC(=O)C(C)C)CC(=O)OC)(Cc1cccc1)C(=O)N[C@H](C(C)C)C(=O)NCCOC
C380	CacoP	CacoP+	13	O[C@](C[NH+](Cc1ccc(cc1)Br)NC(=O)[C@@H](C(C)C)CC(=O)OC)(Cc1cccc1)C(=O)N[C@H](C(C)C)C(=O)NC
C381	CacoP	CacoP+	13	O[C@](C[NH+](Cc1ccc(cc1)c1cccc1)NC(=O)[C@@H](C(C)C)CC(=O)OC)(Cc1cccc1)C(=O)N[C@H](C(C)C)C(=O)NC
C382	CacoP	CacoP+	13	O=C1[C@@H]2C[C@@H](Oc3nc(nc4c3cccc4)c3cccc3)C[C@H]2C(=O)N(CCCC/C=C\C[C@H]2[C@@](N1)(C(=O)[N-]S(=O)(=O)C1CC1)C2)C
C383	CacoP	CacoP+	13	O=C1[C@@H]2C[C@@H](Oc3nc(nc4c3ccc(e4)OC)c3nc(es3)C(C)C)[C@H]2C(=O)N(CCCC/C=C\C[C@H]2[C@@](N1)(C(=O)[N-]S(=O)(=O)C1CC1)C2)C
C384	CacoP	CacoP+	13	CC(C)Cc1ccc(cc1)C(C)C(=O)NO
C385	CacoP	CacoP+	13	O=C1[C@@H]2C[C@@H](Oc3nc(nc4c3ccc(e4)OC)c3ccc(cc3)F)C[C@H]2C(=O)N(CCCC/C=C\C[C@H]2[C@@](N1)(C(=O)[N-]S(=O)(=O)C1CC1)C2)C
C386	CacoP	CacoP+	13	O=C1N[C@@]2C[C@H]2/C=C/CCCN(C)C(=O)[C@H]2[C@H]1C[C@H](C2)Oe1nc(nc2c1ccc(e2C)OC)c1cccc1)C(=O)[N-]S(=O)(=O)C1CC1
C387	CacoP	CacoP+	13	O=C1[C@@H]2C[C@@H](Oc3nc(nc4c3ccc(e4)OC)c3ccc(cc3)OC)C[C@H]2C(=O)N(CCCC/C=C\C[C@H]2[C@@](N1)(C(=O)[N-]S(=O)(=O)C1CC1)C2)C
C388	CacoP	CacoP+	13	O=C1N[C@@]2C[C@H]2/C=C/CCCCNC(=O)[C@H]2[C@H]1C[C@H](C2)Oe1nc(nc2c1ccc(e2C)OC)c1cccc1)C(=O)[N-]S(=O)(=O)C1CC1
C389	CacoP	CacoP+	13	Ce1c(cc(cc1)NC(=O)c1ccc(cc1)C[NH+]1CCN(C)CC1)Nc1cccc(n1)c1cccc1
C390	CacoP	CacoP+	13	N#Cc1c(nc(c1)F)Cl)Cl
C391	CacoP	CacoP+	13	O=C([O-])Cc1cccc(c1N)C(=O)c1cccc1
C392	CacoP	CacoP+	13	C[C@H]1C[C@@H](C(=O)[C@@H](C1)[C@@H](CC1CC(=O)NC(=O)C1)O)C
C393	CacoP	CacoP+	13	O=C(OCC)C(SP(=S)(OC)OC)CC(=O)OCC
C394	CacoP	CacoP+	13	C[NH+](C)CCCN1c2cccc2CCe2c1cccc2
C395	CacoP	CacoP+	13	Oe1c(c(c(c1Cl)Cl)Cl)Cl)Cl
C396	CacoP	CacoP+	13	O=c1[nH]c(nc2c1c(c(cc2)C)Sc1cccc1)N
C397	CacoP	CacoP+	13	CN(CCCNC(=O)C1CCCO1)c1nc2cc(c(cc2c(n1)N)OC)OC
C398	CacoP	CacoP+	13	O=C(c1c(oc2cccc12)CCCC)c1cc(c(c1)I)OCC[NH+](CC)CC)I
C399	CacoP	CacoP+	13	O=C(NCc1ccc(cc1)OCC[NH+](C)C)c1cc(c(c1)OC)OC)OC
C400	CacoP	CacoP+	13	CCCCC1=NC2(CCCC2)C(=O)N1Cc1ccc(cc1)c1cccc1c1n[n-]nn1
C401	CacoP	CacoP+	13	O=c1n(CC[NH+]2CCC(C(=O)c3ccc(cc3)F)CC2)c(=O)c2c(cccc2)[nH]1
C402	CacoP	CacoP+	13	CC(=O)N1CCN(c2ccc(cc2)OC)[C@@H]2CO[C@@](Cn3ccnc3)(c3c(cc(cc3)Cl)Cl)O2)CC1
C403	CacoP	CacoP+	13	CC(c1cccc(c1)C(=O)c1cccc1)C(=O)[O-]
C404	CacoP	CacoP+	13	O=C(C1c2ccc(nc2CC1)C(=O)c1cccc1)[O-]
C405	CacoP	CacoP+	13	C[NH+]1CC/C=C\2/e3c(sec3)C(=O)Cc3cccc23)/CC1
C406	CacoP	CacoP+	13	OC(C[NH2+]C(C)CCc1cccc1)c1ccc(c(c1)C(=O)N)O
C407	CacoP	CacoP+	13	O=c1nc(N)ccn1[C@@H]1CS[C@H](CO)O1
C408	CacoP	CacoP+	13	Ce1c(ccnc1CS(=O)c1nc2cccc2[nH]1)OCC(F)(F)F c1c(cc(c(c1)O)c1cc(c(c1)I)O)I)CC(C(=O)[O-])
C409	CacoP	CacoP+	13	][NH3+] CCN(CC)C(=O)N[C@@H]1C[NH+](C[C@@H]2Cc3c[nH]c4cccc(c34)C2=C1)C
C410	CacoP	CacoP+	13	C[C@H]([NH3+])Cc1cccc1
C411	CacoP	CacoP+	13	CCC(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC1CC(C(=O)O1)O)C
C412	CacoP	CacoP+	13	



C459	CacoP	CacoP+	13	O=C1c2e(ccs2)S(=O)(=O)N(/C/1=C(\O)/Nc1ncccc1)C
C460	CacoP	CacoP+	13	O=C(Nc1ccc(c(c1)C(F)(F)F)C#N)C(C)(O)CS(=O)(=O)c1ccc(cc1)F
C461	CacoP	CacoP+	13	CC(C)(C)c1ccc(cc1)C(CCC[NH+])1CCC(CC1)C(c1cccc1)(c1cccc1)O)O
C462	CacoP	CacoP+	13	O=C1CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@@H]3CCCC=C1
C463	CacoP	CacoP+	13	OC1=C(C(=O)N)C(=O)[C@@]2(O)C(=C3C(=O)c4c(cccc4[C@](O)(C)C3CC2[C@@H]1[NH+](C)C)O)O
C464	CacoP	CacoP+	13	O=C1N(C2CCC(=O)NC2=O)C(=O)c2c1cccc2
C465	CacoP	CacoP+	13	CSc1ccc2c(c1)c(=O)n(en2)/C=C/C(=O)[O-]
C466	CacoP	CacoP+	13	CC(C)(C)[NH2+]C[C@H](O)COc1nsnc1N1CCOCC1
C467	CacoP	CacoP+	13	OC(COc1ccc(cc1)COCCOC(C)C)[NH2+]C(C)C
C468	CacoP	CacoP+	13	O=C([O-])Cc1ccc(n1C)C(=O)c1ccc(cc1)C
C469	CacoP	CacoP+	13	OC1(c2cc(ccc2)OC)C(C[NH+](C)C)CCCC1
C470	CacoP	CacoP+	13	O=c1n(CCC[NH+]2CCN(c3cccc(c3)Cl)CC2)nc2cccn12
C471	CacoP	CacoP+	13	Cc1nnc2n1c1ccc(cc1C(=NC2)c1cccc1Cl)Cl
C472	CacoP	CacoP+	13	COc1cc(cc(c1OC)OC)Cc1nnc(nc1N)N
C473	CacoP	CacoP+	13	C1[C@@H]2[C@H](C2[NH3+])CN1c1c(cc2c(n1)n(cc2=O)C(=O)[O-])c1c(cc(cc1)F)F
C474	CacoP	CacoP+	13	CC(c1ccc2c(c1)CC(=O)c1e(cccc1)S2)C(=O)[O-]
C475	CacoP	CacoP+	13	Cc1cn(c(=O)[nH]c1=O)C1CC(C(O1)CO)N=[N+]=[N-]
C476	CacoP	CacoP+	13	O=C1Cc2cc(c(cc2N1)Cl)CC[NH+]1CCN(c2nsc3cccc23)CC1
C477	CacoP	CacoP+	13	Oc1cccc1C(=O)[O-]
C478	CacoP	CacoP+	13	O=c1cc(c2cccc2)oc2c1cccc2
C479	CacoP	CacoP+	13	[NH3+]CCc1ccc(c(c1)O)O
C480	CacoP	CacoP+	13	CC1(C)[C@@]2(CC)CC[N@@H+](CC3(CC3)O)[C@@H]1Cc1ccc(cc21)O
C481	CacoP	CacoP+	13	O=C(NC)[C@H](NC(=O)C(Cc1cccc1)NC(=O)C)Cc1cccc1
C482	CacoP	CacoP+	13	O=C([C@@H](C(C)C)NC(=O)C)NCCc1cccc1
C483	CacoP	CacoP+	13	O=C([C@H](Cc1cccc1)NC(=O)C)NCCc1cccc1
C484	CacoP	CacoP+	13	O=C(C(CC1CCCC1)NC(=O)C)NCCc1cccc1
C485	CacoP	CacoP+	13	CC([NH2+]C(C)C)C(=O)c1cc(ccc1)Cl
C486	CacoP	CacoP+	13	O=S(=O)(c1ccc2cccc2c1)NC(Cc1cc(ccc1)C[NH3+])CC(=O)N1CCC(C)CC1
C487	CacoP	CacoP+	13	O=C1CC[C@]2(C)[C@H]3[C@@H](O)C[C@]4(C)[C@@H](C(=O)CO)CC[C@H]4[C@@H]3CCCC=C1
C488	CacoP	CacoP+	13	O=C(CCC)Nc1ccc(c(c1)C(=O)C)OCC(OC(=O)C1CC1)C[NH2+]C(C)C
C489	CacoP	CacoP+	13	C=CCc1cccc1OCC(OC(=O)C1CC1)C[NH2+]C(C)C
C490	CacoP	CacoP+	13	CC(C)[NH2+]CC(OC(=O)C1CC1)COc1ccc(cc1)CCOCC1CC1
C491	CacoP	CacoP+	13	O=C([O-])C1=CC(C(C(O1)C(C(O)CO)OC(=O)CNC(=O)C(C)C)C[NH3+])NC(=O)C)N=C(N)N
C492	CacoP	CacoP+	13	CC(C)(C)[NH2+]C[C@H](OC(=O)C1CC1)COc1nsnc1N1CCOCC1
C493	CacoP	CacoP+	13	O=c1c(en(C2CC2)c2c1cc(c(c2)N1CC[NH2+]C(C)C1)F)C(=O)[O-]
C494	CacoP	CacoP+	13	O=c1c(en(C2CC2)c2c1cc(c(c2)N1CC[NH+](CCCC)C(C)C1)F)C(=O)[O-]
C495	CacoP	CacoP+	13	[C@@H]12CC[C@]3(C)O[C@@H]4[C@]1(OO3)[C@H]([C@@H](C)C(=O)O4)CC[C@H]2C
C496	CacoP	CacoP+	13	O=C(Nc1cccc(c1)OCCC)OCC[NH+]1CCCC1
C497	CacoP	CacoP+	13	O=C(Nc1cccc(c1)OCCCCC)OCC[NH+]1CCCC1
C498	CacoP	CacoP+	13	CCCC(C)(COC(=O)N)COC(=O)NC(C)C
C499	CacoP	CacoP+	13	N/C(=N\OC)/c1ccc(cc1)c1ccc(o1)c1ccc(cc1)/C(=N\OC)/N
C500	CacoP	CacoP+	13	N#C[C@@](CCC[NH2+]CCc1cc(c(cc1)OC)OC)(c1cc(c(cc1)OC)OC)C(C)C
C501	CacoP	CacoP+	13	O=S(=O)(c1cc(c(cc1)OCCC)c1nc(=O)c2n(nc2[nH]1)CCC)NCCC1CCC[NH+]1C
C502	CacoP	CacoP+	13	C[C@H]1Cc2c(c(c3c(c2)OCO3)OC)c2c(cc(c(c2OC)OC)OC)C[C@]1(C)O
C503	CacoP	CacoP+	13	Fc1ccc2c(c1)CC[C@](OC(=O)COC)(CC[NH+](C)CCCc1nc3cccc3[nH]1)[C@H]2C(C)C
C504	CacoP	CacoP+	13	CC(n1c2cccc2n2cnc(c2c1=O)c1noc(n1)C1CC1)C

C505	CacoP	CacoP+	13	[NH3+][C@@H](C1cccc1)C(=O)N1[C@H](C(=O)[O-])CCC1
C506	CacoP	CacoP+	13	O=c1[nH]c(=O)n(cc1/C=C/Br)[C@@H]1[C@H](O)[C@@H](O)[C@H](CO)O1
C507	CacoP	CacoP+	13	C[NH+]1CCC(c2c[nH]c3c2cc(cc3)NC(=O)c2ccc(cc2)F)CC1
C508	CacoP	CacoP+	13	CCCOe1cc2c(cc1)[C@H](c1ccc3c(c1)OCO3)[C@@H](C(=O)[O-])[C@@H]2c1c(cc(cc1)OC)OCCO
C509	CacoP	CacoP+	13	[NH3+][C@@H](C)C(=O)[O-]
C510	CacoP	CacoP+	13	NC(=Nc1nc(cs1)CSCCN/C(=N/C)/NC#N)N
C511	CacoP	CacoP+	13	COe1ccc2c(ccc(c2)C(C)C(=O)[O-])c1
C512	CacoP	CacoP+	13	O=C([C@@H](C1cccc1)NC(=O)C1(CCCC1)NC(=O)c1cc2ccc(cc2s1)C)NCC1CC[NH+](CC1)CC1CCOCC1
C513	CacoP	CacoP+	13	OC(C[NH2+])C(C)C)COe1ccc(cc1)NC=O
C514	CacoP	CacoP+	13	[NH3+]c1cc(c[nH]c1=O)c1ccncc1
C515	CacoP	CacoP+	13	CC1=C(N2[C@@H]([C@@H](C2=O)NC(=O)C(C2=CCC=CC2)[NH3+])SC1)C(=O)[O-]
C516	CacoP	CacoP+	13	CC(=O)N[C@@H](C1cccc1)C(=O)N(C)[C@H](C1cccc1)C(=O)N(C)[C@@H](C1cccc1)C(=O)N
C517	CacoP	CacoP+	13	CC(=O)N(C)[C@@H](C1cccc1)C(=O)N(C)[C@@H](C1cccc1)C(=O)N(C)[C@@H](C1cccc1)C(=O)N
C518	CacoP	CacoP+	13	O=C([O-])COCC[NH+]1CC[NH+](C(c2ccc(cc2)Cl)c2ccc(c2)CC1
C519	CacoP	CacoP+	13	Fe1cc(ccc1N1CCOCC1)N1C[C@H](CNC(=O)C)OC1=O
C520	CacoP	CacoP+	13	Fe1cc(ccc1N1CCN(C(=O)CO)CC1)N1C[C@H](CNC(=S)C)OC1=O
C521	CacoP	CacoP+	13	Fe1cc(ccc1N1CCS(=O)CCC1)N1C[C@H](CNC(=S)C)OC1=O
C522	CacoP	CacoP+	13	Fe1cc(ccc1N1CCN(C(=O)CC1)N1C[C@H](CNC(=S)CC)OC1=O
C523	CacoP	CacoP+	13	Fe1c(ccc(c1)N1C[C@H](CNC(=O)CC)OC1=O)c1nnes1
C524	CacoP	CacoP+	13	Fe1c(ccc(c1)N1C[C@H](CNC(=O)C)OC1=O)c1ene(cc1)C#N
C525	CacoP	CacoP+	13	Fe1c(ccc(c1)N1C[C@H](CNC(=S)C)OC1=O)c1nne(s1)C[NH3+]
C526	CacoP	CacoP+	13	Fe1c(ccc(c1)N1C[C@H](CNC(=O)CC)OC1=O)n1ncc(c1)C#N
C527	CacoP	CacoP+	13	Fe1c(ccc(c1)N1C[C@H](CNC(=S)C)OC1=O)N1CCS(=O)(=O)CCC1
C528	CacoP	CacoP+	13	Fe1c(ccc(c1)N1C[C@H](CNC(=O)C)OC1=O)c1nne(s1)CC/C(=N\O)/C
C529	CacoP	CacoP+	13	Fe1c(ccc(c1)N1C[C@H](CNC(=S)C)OC1=O)c1nne(s1)CNS(=O)(=O)C
C530	CacoP	CacoP+	13	Ne1nc2ccc(cc2n1C(C)C)C(C(=O)NC)c1cccc(c1)F
C531	CacoP	CacoP+	13	O=C([C@@H](NC(=O)c1ccc(cc1)C(=O)N1CCOCC1)C(C)C)N1[C@H](C(=O)NC(C(C)C)C(=O)C(F)F)C(F)F)CCC1
C532	CacoP	CacoP+	13	Ne1nc2ccc(cc2n1S(=O)(=O)NC(C)C)C(C(=O)N)c1cccc(c1)F
C533	CacoP	CacoP+	13	C[NH+](C)CCC(c1ccc(cc1)Cl)c1ncccc1
C534	CacoP	CacoP+	13	Cc1c(sc[n+])1Cc1enc(nc1N)C)CCO
C535	CacoP	CacoP+	13	CCCSelcc2c(cc1)nc([nH]2)NC(=O)OC
C536	CacoP	CacoP+	13	COe1cc(c(c2c1OCO2)c1c(cc(c2c1OCO2)OC)C(=O)OC)CO
C537	CacoP	CacoP+	13	O=c1[nH]c(=O)n(cc1F)[C@H]1O[C@@H](COC(=O)C(Cc2ccc2)[NH3+])[C@H](O)C1
C538	CacoP	CacoP+	13	O=c1[nH]c(=O)n(cc1F)[C@H]1O[C@@H](COC(=O)C[NH3+])[C@H](O)C1
C539	CacoP	CacoP+	13	O=c1[nH]c(=O)n(cc1F)[C@H]1O[C@@H](COC(=O)CNC(=O)C(CC(C)C)[NH3+])[C@H](O)C1
C540	CacoP	CacoP+	13	C[NH+](C)CC/C=C/1\c2c(ccc(c2)Cl)Sc2c1cccc2
C541	CacoP	CacoP+	13	O=c1[nH]c(=O)n(cc1F)[C@H]1O[C@@H](COC(=O)C(CC(C)C)NC(=O)C[NH3+])[C@H](O)C1
C542	CacoP	CacoP+	13	O=c1[nH]c(=O)n(cc1F)[C@@H]1O[C@@H](COC(=O)[C@@H](Cc2ccc(cc2)O)NC(=O)[C@@H](Cc2ccc2)[NH3+])[C@@H](O)C1
C543	CacoP	CacoP+	13	Oe1cc(ccc1O)C=O
C544	CacoP	CacoP+	13	CN(C)c1ccc(cc1)C(=O)NCCCCNC(=O)CS
C545	CacoP	CacoP+	13	NC(=O)[C@@H](NC(=O)C(Cc1c[nH]c2c1cccc2)NC(=O)[C@@H]1N(C(=O)[C@H](Cc2ccc(cc2)O)NC(=O)C([NH3+])CCCC)CCC1)Cc1cccc1
C546	CacoP	CacoP+	13	Ce1c(c(ccc1)C)OCC(=O)N[C@@H](Cc1cccc1)[C@@H](OC(=O)[C@H](C(C)C)NC(=O)C[NH3+])C[C@@H](Cc1cccc1)NC(=O)[C@@H](C(C)C)N1CCNC1=O
C547	CacoP	CacoP+	13	O=C(c1en(C2CC2)c2c(cc(c2)N2CC[NH2+])CC2)F)c1=O)[O-]
C548	CacoP	CacoP+	13	O=c1ccc2c(cc(cc2)O)o1
C549	CacoP	CacoP+	13	C/C=C(C(=O)O)[C@@H]([C@H](O)C(C)O)C)c1c(cc2c(c1)ccc(=O)o2)OC)/C
C550	CacoP	CacoP+	13	CC(=O)CCCC/C=C\CC#CC#C

C551	CacoP	CacoP+	13	COC1C[NH+](CCC1NC(=O)c1ccc(cc1OC)N)C1CCCOc1ccc(cc1)F
C552	CacoP	CacoP+	13	O=S(=O)(Nc1ccc2c1CCN(c1nc(c3c(c(cc3n1)OC)OC)c1ccc1)N)C2)C
C553	CacoP	CacoP+	13	O=C(NO)/C=C/c1cc2c(cc1)n(c(n2)CCc1ccc1)CC[NH+]1CCCC1
C554	CacoP	CacoP+	13	O=S(=O)(N(Cc1ccc(c1)n1ccc1)C1CN(Cc2cnc2C)c2ccc(cc2C1)C#N)c1ccc1
C555	CacoP	CacoP+	13	O=S(=O)(N(Cc1c(oc1C)C)C1CN(Cc2cnc2C)c2ccc(cc2C1)C#N)c1ccc1
C556	CacoP	CacoP+	13	O=S(=O)(N(CC1CCN(C(=O)OC(C)C)CC1)C1CN(Cc2cnc2C)c2ccc(cc2C1)C#N)c1ccc1
C557	CacoP	CacoP+	13	Clc1ccc(c1NC1=NCCN1)C1
C558	CacoP	CacoP+	13	O=C(N[C@H](C(=O)NCCC[NH+]1CCOCC1)Cc1ccc1)C1(NC(=O)c2cc3ccc3s2)CCCC1
C559	CacoP	CacoP+	13	O=C(NCCC[NH+]1CCOCC1)[C@@H](Cc1ccc1)NC(=O)C1(CCCC1)NC(=O)c1ccc(cc1)c1ccc1
C560	CacoP	CacoP+	13	O=C(NCCC[C@H]1CC[N@@H+](CC2CCOCC2)CC1)[C@@H](Cc1ccc1)NC(=O)C1(CCCC1)NC(=O)c1cc2ccc2s1
C561	CacoP	CacoP+	13	Nc1ccc1
C562	CacoP	CacoP+	13	O=C(N)c1ccc1
C563	CacoP	CacoP+	13	Clc1ccc1
C564	CacoP	CacoP+	13	O=Cc1ccc1
C565	CacoP	CacoP+	13	Nc1ccc1
C566	CacoP	CacoP+	13	c1(ccnc1)Cc1ccc1
C567	CacoP	CacoP+	13	CCc1ccc1
C568	CacoP	CacoP+	13	c1(ccnc1)c1ccc1
C569	CacoP	CacoP+	13	C[NH+]1C2CC[C@@H]1C[C@H](OC(c1ccc1)Cl)c1ccc1)C2
C570	CacoP	CacoP+	13	CCCCCCCCCCCCCOP(=O)([O-])OCC[N+](C)(C)C
C571	CacoP	CacoP+	13	O=c1cc(c2ccc2)oc2c1ccc(c2)OC
C572	CacoP	CacoP+	13	O=c1cc(c2ccc(cc2)OC)oc2c1c(cc(c2)OC)OC
C573	CacoP	CacoP+	13	O=c1cc(c2ccc(cc2)O)oc2c1ccc(c2)O
C574	CacoP	CacoP+	13	O=c1cc(c2ccc2)oc2c1c(cc(c2)O)O
C575	CacoP	CacoP+	13	C1C(C(=O)NO1)[NH3+]
C576	CacoP	CacoP+	13	Oc1ccc1C(=O)OC(=O)C
C577	CacoP	CacoP+	13	NC(=N)c1ccc(cc1)COc1ccc2c(c1)C(=O)N(CC(=O)N2C)CCC(=O)[O-]
C578	CacoP	CacoP+	13	CC1C(C(CC(O1)OC1CCC2(C3CCC4(C(CCC4(C3CCC2(C1)O)O)C1=CC(=O)OC1)C)C=O)OC)O
C579	CacoP	CacoP+	13	CC[C@@]1(O)c2c(c(=O)n3c(c2)Cc2nc4ccc4cc32)COC1=O
C580	CacoP	CacoP+	13	Nc1nc2ccc(cc2n1S(=O)(=O)NC(C)C)C(C(=O)N)c1ccc2c1ccc2
C581	CacoP	CacoP+	13	C#CC#CCC/C=C\C=C(=O)NCC(C)C
C582	CacoP	CacoP+	13	C/C=C/C#CCC/C=C\C=C(=O)NCC(C)C
C583	CacoP	CacoP+	13	CCC/C=C\CC/C=C/C=C(=O)NCC(C)C
C584	CacoP	CacoP+	13	CC#CC#CCCC/C=C/C(=O)NCC(C)CC
C585	CacoP	CacoP+	13	C#CC#CC/C=C\CCCC/C=C/C(=O)NCC(C)C
C586	CacoP	CacoP+	13	CC1=NCCc2c1[nH]c1c2ccc(c1)O
C587	CacoP	CacoP+	13	Cc1ccc2c1[nH]c1c2ccc(c1)OC
C588	CacoP	CacoP+	13	Nc1nc2c(ncn2COCCOC(=O)C(C)C)NC(=O)C[NH3+])c(=O)[nH]1
C589	CacoP	CacoP+	13	O=c1c(coc2c1c(cc2)O)O)c1ccc(cc1)O
C590	CacoP	CacoP+	13	O=C([C@H]1N(C(=O)[C@H](C)CSN=O)CCC1)[O-]
C591	CacoP	CacoP+	13	O=C([N-]S(=O)(=O)c1ccc(cc1OC)C)C(c1cc2c(cc1)OCO2)c1cn(c2c1ccc(c2)Cl)C
C592	CacoP	CacoP+	13	O=C([N-]S(=O)(=O)c1ccc(cc1OC)C)C(c1cc2c(cc1)OCO2)c1cn(c2c1ccc(c2)COC)C
C593	CacoP	CacoP+	13	C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@]1(C(=O)CO)O
C594	CacoP	CacoP+	13	O=C(NC(=O)c1cc2c(s1)CC[NH2+]C2)c1ccc(c(c1)OCC(=O)OCCCC)OCC(=O)OCCCC
C595	CacoP	CacoP+	13	Cc1c(c(cc1O)C)C[C@H]([NH3+])C(=O)N[C@@H](CCCNC(=N)N)C(=O)NC(Cc1ccc1)C(=O)NC(CCCCN)C(=O)N
C596	CacoP	CacoP+	13	O=C(NCCC[NH+]1CCOCC1)[C@@H](Cc1ccc1)NC(=O)C1(CCCC1)NC(=O)c1cc2ccc2n1C









C735	CacoP	CacoP-	13	Ne1nc2c(ncn2C2[C@@H](CO)C[C@@H]2CO)c(=O)[nH]1
C736	CacoP	CacoP-	13	[C@H]1(NC(=O)OCOC(=O)[C@H](C)NC(=O)[C@@H](NC(=O)CNC(=O)CNC(=O)[C@@H](NC1=O)C)CC(=O)[O-])Cc1c[nH]c2c1cccc2
C737	CacoP	CacoP-	13	CC(Cc1cccc(c1)O)[NH2+][C@H](C1cc(cc1)O)O
C738	CacoP	CacoP-	13	c1(ccccc1)Cn1c(nnn1)C([NH+])CCN(C2CCC2)CCC1)c1ccc(cc1)Cn1cncn1
C739	CacoP	CacoP-	12,2	CC([NH3+])(Cc1cc(c(cc1)O)O)C(=O)[O-]
C740	CacoP	CacoP-	13	O=C(N[C@@H](C(=O)[O-])CCC(=O)O)c1ccc(cc1)NCc1cnc2c(n1)c(=O)nc(N)[nH]2
C741	CacoP	CacoP-	13	O=C([C@H](NC(=O)[C@H]1CCC(=O)N1)Cc1c[nH]cn1)N1[C@H](CCC1)C(=O)N
C742	CacoP	CacoP-	13	C[C@H](NC(=O)[C@@H](Cc1cccc1)[NH3+])C(=O)N[C@H](CO)C(=O)[O-]
C743	CacoP	CacoP-	13	NC(=N)c1ccc(cc1)C#Cc1ccc2c(c1)C(=O)N(CC(=O)N2C)CCC(=O)[O-]
C744	CacoP	CacoP-	12	CC/C=C(C(=O)N[C@H]1[C@H]2SCC(=C(N2C1=O)C(=O)[O-])COC(=O)N)/c1csc(n1)N
C745	CacoP	CacoP-	13	Cc1e2c(c(c1)CCO[C@H]1O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]1O)O)[C@H]1O[C@@H](CO)[C@@H](O)[C@@H](O)[C@@H]1O)CC(C)C2=O
C746	CacoP	CacoP-	13	O=S(=O)(c1cccc1)N[C@@H](Cc1cc(c(cc1)[C@@H]1CC(=O)[N-]S1(=O)=O)C)c1nc2cccc2[nH]1
C747	CacoP	CacoP-	13	O=C([O-])c1cccc(c1)Cn1cnc1
C748	CacoP	CacoP-	13	O=C([N-]S(=O)(=O)c1ccc(cc1)OC)C(C1cc2c(cc1)OCO2)c1cn(c2c1ccc(c2)C(=O)C)C
C749	CacoP	CacoP-	13	C[C@]12CC[C@H](O)C(C)(C)[C@@H]1CC[C@]1(C)[C@@H]2CC=C2[C@@]1(C)CC[C@]1(C(=O)[O-])[C@H]2CC(C)(C)CC1
C750	CacoP	CacoP-	13	Fe1c(ccc(c1)N1C[C@H](CNC(=S)N)OC1=O)N1CCN(C(=O)CO)CC1
C751	CacoP	CacoP-	13	O=C([O-])[C@H](OC(=O)/C=C/c1ccc(c(c1)O)O)[C@@H](O)C(=O)O
C752	CacoP	CacoP-	13	[NH3+][C(Cc1ccc(cc1)O)C(=O)NC(CCCNC(=N)N)C(=O)NC(Cc1cccc1)C(=O)NC(Cc1cccc1)C(=O)N
C753	CacoP	CacoP-	13	Oc1cc(ccc1O)CC(C(=O)[O-])OC(=O)/C=C/c1ccc(c(c1)CC(=O)O)O
C754	CacoP	CacoP-	13	O=c1nc(N)[nH]c2c1nnc2COCCO
C755	CacoP	CacoP-	13	NC(=N)c1ccc2c(c1)[nH]c(n2)Cc1nc2c([nH]1)cccc2
C756	CacoP	CacoP-	13	O=S(=O)(Nc1cccc1)c1ccc(cc1)/N=N/c1cc(c(cc1)O)CC(=O)[O-]
C757	CacoP	CacoP-	13	O=C(NCCC(=O)N1CC[NH+](C2CCOCC2)CC1)[C@@H](Cc1cccc1)NC(=O)C1(CCCC1)NC(=O)c1cc2cccc2s1
C758	CacoP	CacoP-	13	NC(=O)[C@@H](NC(=O)C(Cc1c[nH]c2c1cccc2)NC(=O)[C@@H]1N(C(=O)[C@H](Cc2c(cc(cc2)O)C)[NH3+])CCC1)Cc1cccc1 O=C([N-
C759	CacoP	CacoP-	13	]S(=O)(=O)c1ccc(cc1)OC)[C@H](c1cc2c(cc1)OCO2)c1cn(c2c1ccc(c2)COC)CCOC
C760	CacoP	CacoP-	13	O=C1CC([NH+])2CCC[NH+](CCCNC3c4c(ccc4)C(C)C(=O)[O-])OCc4c3cccc4)CC2)N(C)C(=O)N1C
C761	CacoP	CacoP-	13	O=C(c1cc(nn1c1cccc(c1)C[NH3+])C)Nc1c(cc(cc1)c1cccc1S(=O)(=O)N)F
C762	CacoP	CacoP-	13	O=C(N[C@H]1O[C@@H](C@@H)(O)[C@@H](O)[C@@H]1O)C(=O)N[C@@H](NC(=O)[C@@H](Cc1c[nH]c2c1cccc2)NC(=O)[C@H]1N(C(=O)[C@@H](Cc2ccc(cc2)O)[NH3+])CCC1)Cc1cccc1
C763	CacoP	CacoP-	13	O=C(NCC1CC[NH+](CC2CCOCC2)CC1)[C@@H](Cc1cccc1)NC(=O)C1(CCCC1)NC(=O)c1cc2ccc(cc2s1)F
C764	CacoP	CacoP-	13	Fe1c(ccc(c1)N1C[C@H](CNC(=S)N)OC1=O)C1CCS(=O)(=O)CC1
C765	CacoP	CacoP-	13	Oc1ccc(cc1)CC(C(=O)NC(C(=O)NC(C(=O)NC(C(=O)N)Cc1cccc1)Cc1cccc1)C)[NH3+]
C766	CacoP	CacoP-	13	O=S(=O)(c1ccc2cccc2c1)NC(Cc1ccc(cc1)C(=N)N)CC(=O)N1CCCC(C(=O)OC)C1
C767	CacoP	CacoP-	13	O=C(NC)[C@H](NC(=O)CNC(=O)C)Cc1cccc1
C768	CacoP	CacoP-	13	Clc1ccc(c(c1)OC)C[C@@H](C)C(=O)N1CCN(c2c(cc(cc2)Cl)[C@@H](NC(=O)C2C[NH2+]C2)C(C)C)CC1
C769	CacoP	CacoP-	13	O=C(N[C@@H](Cc1cc(c(cc1)O)C(C)(C)C)C(=O)N)C(C(C)C)N(C)C(=O)[C@@H]([NH3+])Cc1cccc1
C770	CacoP	CacoP-	13	O=S(=O)(c1ccc2cccc2c1)NC(Cc1ccc(cc1)C(=N)N)CC(=O)N1CCN(C(=O)C)CC1
C771	CacoP	CacoP-	10	CC1(C)SC2C(NC(=O)C([NH3+])c3ccc(cc3)O)C(=O)N2C1C(=O)[O-]
C772	CacoP	CacoP-	13	O=C(NC)[C@H](NC(=O)[C@@H](CC(C)C)NC(=O)C)Cc1cccc1
C773	CacoP	CacoP-	13	O=c1c(coc2c1ccc(c2)O)[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@@H]1O)c1ccc(cc1)O
C774	CacoP	CacoP-	13	O=C1NCC2(CC[NH+](CC)CC2)c2c1cc([nH]2)c1cnc(n1)c1cc2cccc2o1
C775	CacoP	CacoP-	13	CC1(C)C2C1N(C(=O)C(NC(=O)NC(C)C(C)C)C2C(=O)NC(CC1CC1)C(=O)C(=O)N
C776	CacoP	CacoP-	13	O[C@H]1[C@H](c2cc(c(c(c2)O)O)O)O)c2c(c(cc(c2)O)O)C1
C777	CacoP	CacoP-	13	O=C1OC2(c3c(cc(cc3)O)O)c3c2ccc(c3)O)c2c1cc(cc2)NC(=S)NCCCC[C@@H]([NH3+])C(=O)OC
C778	CacoP	CacoP-	13	NC(=N)c1ccc(cc1)COc1ccc2c(c1)C(=O)N(CC(=O)N2C)CCC(=O)OCC
C779	CacoP	CacoP-	13	O=C(N[C@@H](C)C(=O)NCC(=O)NCC(=O)N[C@@H](CC(=O)N)C(=O)N[C@@H](C)C(=O)N)C(Cc1c[nH]c2cccc12)NC(=O)C
C780	CacoP	CacoP-	13	O=C(C1CCC(F)(F)CC1)N[C@@H](CC[NH+])1C2CCC1CC(n1c(nnc1C)C(C)C)C2)c1cccc1



C827	CacoP	CacoP+	13	Cc1c(c(no1)c1cccc1)C(=O)N[C@H]1[C@H]2SC(C)(C)[C@@H](N2C1=O)C(=O)[O-]
C828	CacoP	CacoP+	13	O=C1NC(C2CCCC2)C(=O)N2CC(OC(CCOc3cc(ecc3)C1)(C)C)CC2C(=O)NC(CCC)C(=O)C(=O)NCC=C
C829	CacoP	CacoP+	13	Cc1c(c(ccc1)Cl)NC(=O)c1nc(s1)Nc1nc(nc(c1)N1CC[NH+](CC1)CCO)C
C830	CacoP	CacoP+	13	O=C(N[C@@H](C(=O)N[C@H]1(CCC[C@H](C(=O)[O-])C1)NC(=O)[C@H]1CCCC[C@@H]1[NH3+])Cc1cccc1)C1(CCCCC1)NC(=O)c1cc2cccc2s1
C831	CacoP	CacoP+	13	O=c1cc(CCC)[nH]c(=S)[nH]1
C832	CacoP	CacoP+	12	COC(=O)C1=C(C)NC(=C(C1c1cc(ccc1)[N+](=O)[O-])C(=O)OCC[NH+](C)Cc1cccc1)C
C833	CacoP	CacoP+	13	FC(F)(F)c1nn(c(c1)c1ccc(cc1)C)c1ccc(cc1)S(=O)(=O)N
C834	CacoP	CacoP+	13	O=c1oe2c(c3c(cco3)cc2cc1)OCC(C(=C)C)OC(C)(C)C(O)COc1c2c(cc3c1occ3)ccc(=O)o2
C835	CacoP	CacoP+	13	O=C(c1nn(c(c1)C)c1ccc(cc1)Cl)c1ccc(cc1Cl)Cl)N[NH+]1CCCCC1
C836	CacoP	CacoP+	13	O=c1c(c(nc2n1CCCC2)C)CC[NH+]1CCC(CC1)c1noc2c1ccc(e2)F
C837	CacoP	CacoP+	13	CN(C(=O)C[NH3+])CC(=O)[O-]
C838	CacoP	CacoP+	13	O=c1c(c(CC)oc(c1Cc1c(c(c(c1O)C(=O)C)O)CC=C(C)C)O)O)C
C839	CacoP	CacoP+	13	Cc1c2c(c(c(c1CCO)C)O)CC(C)(C)C2=O
C840	CacoP	CacoP+	13	COc1cc2nnc(c2cc1OCCC[NH+]1CCOCC1)Nc1ccc(c(c1)Cl)F
C841	CacoP	CacoP+	10,11,12,4,6,2	O=C1NC(=O)C(N1)(c1cccc1)c1cccc1
C842	CacoP	CacoP+	13	[O-]C(=O)CC1(CNC(=O)OC(C)OC(=O)C(C)C)CCCCC1
C843	CacoP	CacoP+	13	O=C([O-])CC1(C[NH3+])CCCCC1
C844	CacoP	CacoP+	13	O=S(=O)(c1ccc(cc1)CCCCCCCCCCCC)Nc1nncs1
C845	CacoP	CacoP+	13	O=S(=O)(c1ccc2ccccc2c1)NC(Cc1cc(ccc1)C(=N)NO)CC(=O)N1CCC(C)CC1
C846	CacoP	CacoP+	13	C1Cc2c(ccc(c2)Cl)C(=C2CC[NH2+])CC2)c2c1ccn2
C847	CacoP	CacoP+	13	O=C(c1ncc(nc1)C)NCCc1ccc(cc1)S(=O)(=O)[N-]C(=O)NC1CCCCC1
C848	CacoP	CacoP+	13	Clc1cccc1C[NH+]1CCc2c(ccs2)C1CCC1(CC(=O)[O-])
C849	CacoP	CacoP+	13	]OCC=C2c3c(c(ccc3)CC)NC12
C850	CacoP	CacoP+	13	CCCC1O[C@@H]2[C@H]3[C@@H]4CCC5=CC(=O)C=C[C@@]5([C@H]4[C@H](C[C@@]3([C@@]2(O1)C(=O)CO)C)O)C
C851	CacoP	CacoP+	13	O=C(N(C)C)C(c1cccc1)(c1cccc1)CC[NH+]1CCC(O)(c2ccc(cc2)Cl)CC1
C852	CacoP	CacoP+	13	O=C(OC1C(=O)N(C)c2ccc(cc2C(=N1)c1cccc1)Cl)N(C)C
C853	CacoP	CacoP+	13	Oc1c(c(nc1)CO)CO
C854	CacoP	CacoP+	13	C[NH+]1C[C@H]2[C@@H](c3c(ccc(c3)Cl)Oe3ccccc23)C1
C855	CacoP	CacoP+	13	Cc1ncc(cc1)c1ncc(cc1c1ccc(cc1)S(=O)(=O)C)Cl
C856	CacoP	CacoP+	10	Cn1c2c([nH]en2)c(=O)n(C)c1=O
C857	CacoP	CacoP+	13	O=c1cc2oe3c(ccc(c3)O)c(c2cc1)c1cccc1C(=O)[O-]
C858	CacoP	CacoP+	13	O=C(OC)Nc1nc2ccccc2[nH]1
C859	CacoP	CacoP+	13	Cc1ccncc1
C860	CacoP	CacoP+	13	O=C(NCC1CC[NH+](CC2CCOCC2)CC1)[C@@H](Cc1cccc1)NC(=O)C1(CCCC1)NC(=O)c1cc2ccc(cc2s1)C(F)(F)F
C861	CacoP	CacoP+	13	O=C(CCCCCNC(=O)CS)Nc1c2ncccc2cc1
C862	CacoP	CacoP+	13	O=C([C@@H](NC(=O)N1CCOCC1)C(C)C)N1[C@H](C(=O)NC(C)C)C(=O)C(F)(F)C(F)(F)C)CCC1
C863	CacoP	CacoP+	13	CC(CN1c2c(cccc2)Sc2c1cccc2)[NH+](C)C
C864	CacoP	CacoP+	13	O=C1N(c2ccccc2)c2c(cccc2)C1(Cc1ccncc1)Cc1ccncc1
C865	CacoP	CacoP+	12	[O-]C(=O)CCC(=O)O[C@H]1O[C@@H]2OC3(OO[C@@]42[C@@H](CC[C@@H](C)[C@@H]4CC3)[C@H]1)C
C866	CacoP	CacoP+	13	Fe1c(ccc(c1)N1C[C@H](CNC(=S)N)OC1=O)N1CCOCC1
C867	CacoP	CacoP+	13	Cc1nc(c(c1OC)C)CS(=O)c1nc2c([nH]1)cc(cc2)OC
C868	CacoP	CacoP+	13	Fe1cc(ccc1C1CCS(=O)CC1)N1C[C@H](CNC(=O)CC)OC1=O
C869	CacoP	CacoP+	13	Oc1cc(ccc1[C@@H]1COe2c3c(ccc2C1)OC(C=C3)(C)C)O
C870	CacoP	CacoP+	13	COc1c(cc2c(c1)[C@@]13CC[N+](4([O-])[C@@H]1C[C@H]1[C@H]5[C@H]3N2C(=O)C[C@H]5OCC=C1C4)OC
C871	CacoP	CacoP+	13	O=C(N)c1cccc(c1)Cc1nc(c([nH]1)c1nc(ccc1)C)c1cc2nccnc2cc1
C872	CacoP	CacoP+	13	Cn1c(nc2ncc(cc12)c1cccc1)N

C873	CacoP	CacoP+	13	<chem>Cc1c(c(ccc1)C)OCC(=O)N[C@@H](Cc1ccccc1)[C@H](C[C@H](Cc1ccccc1)NC(=O)[C@H](C(C)C)N1CCCNC1=O)O</chem>
C874	CacoP	CacoP+	13	<chem>O=C([O-])c1ccc(cc1)c1cc2ccnc2c(n1)c1cc2nonc2cc1</chem>
C875	CacoP	CacoP+	13	<chem>O=C([C@H](NC(=O)[C@H]1CCC(=O)N1)Cc1c[nH]cn1)N1[C@H](CCC1)C(=O)NC1[C@@H]([C@H]([C@@H]([C@@H](C(=O)N)O1)O)O)O</chem>
C876	CacoP	CacoP+	13	<chem>CS(=O)(=O)Nc1ccc(cc1)C(O)C[NH2+]C(C)C</chem>
C877	CacoP	CacoP+	13	<chem>O=C1Nc2ccc(cc2C(=NC1)c1ncccc1)Br</chem>
C878	CacoP	CacoP+	12	<chem>CC/C(=C(\c1ccccc1)/c1ccc(cc1)OCC[NH+](C)C)/c1ccccc1</chem>
C879	CacoP	CacoP+	13	<chem>O=C(Nc1ccc2c(c1)NCC2(C)C)c1ccccc1Nc1ccccc1</chem>
C880	CacoP	CacoP+	13	<chem>O=S(=O)(c1ccc(cc1)N)Nc1c(c(no1)C)C</chem>
C881	CacoP	CacoP+	12,8,2	<chem>OC[C@@H](NC(=O)C(C)C)[C@H](O)c1ccc(cc1)[N+](=O)[O-]</chem>
C882	CacoP	CacoP+	13	<chem>Cc1c(c(ccc1)C)OCC(=O)N[C@@H](Cc1ccccc1)[C@@H](OC(=O)[C@H](C(C)C)NC(=O)[C@H](C(C)C)[NH3+])C[C@@H](Cc1ccccc1)NC(=O)[C@H](C(C)C)N1CCCNC1=O</chem>
C883	CacoP	CacoP+	13	<chem>O=C([O-])C1=CC(C(C(O)C)C(O)CO)OC(=O)C(COC)NC(=O)C(C(C)C)C[NH3+])NC(=O)C)N=C(N)N</chem>
C884	CacoP	CacoP+	13	<chem>OCc1ccccc1</chem>
C885	CacoP	CacoP+	11,4,8,2	<chem>CC(=O)Oc1c(cccc1)C(=O)[O-]</chem>
C886	CacoP	CacoP+	13	<chem>O[C@](C[NH+](Cc1ccc(cc1)Br)NC(=O)[C@@H](C(C)C)C)CC(=O)OC)(Cc1ccccc1)C(=O)NC1CCOC1</chem>
C887	CacoP	CacoP+	10,11	<chem>CC(C)(C)[NH2+]CC(O)COc1ccc2c1CC(O)C(O)C2</chem>
C888	CacoP	CacoP+	13	<chem>Cc1cc(no1)N/C(=C/1\C(=O)c2ccccc2S(=O)(=O)N1C)/O</chem>
C889	CacoP	CacoP+	13	<chem>O=C(N1CCCC1)CCC[NH+]1CCC(=C(c2ccc(cc2)F)CC1</chem>
C890	CacoP	CacoP+	10	<chem>CCOC(=O)C(CCCc1ccccc1)[NH2+]C(C)C(=O)N1CCCC1C(=O)[O-]</chem>
C891	CacoP	CacoP+	13	<chem>c1(ccncc1)c1ccccc1</chem>
C892	CacoP	CacoP+	13	<chem>CC(C)CN(C[C@@H]([C@@H](Cc1ccccc1)NC(=O)O[C@H]1CO[C@H]2[C@@H]1CCO2)O)S(=O)(=O)c1ccc(cc1)N</chem>
C893	CacoP	CacoP+	10	<chem>CSc1ccc2c(c1)c(=C)n(cn2)/C=C/C(=O)[O-]</chem>
C894	CacoP	CacoP+	13	<chem>O[C@](C[NH+](Cc1ccc(cc1)Br)NC(=O)[C@@H](C(C)C)C)CC(=O)OC)(Cc1ccccc1)C(=O)Nc1ccc(cc1)C)O</chem>
C895	CacoP	CacoP+	12	<chem>C[C@@H]1O[C@H](OC[C@H]1[NH3+])c1ccc(cc1)[N+](=O)[O-]</chem>
C896	CacoP	CacoP+	13	<chem>C[NH+](C)CCN(Cc1ccc(cc1)OC)c1ncccc1</chem>
C897	CacoP	CacoP+	12	<chem>CC[C@]1(O)C(=O)OCc2c1cc1n(Cc3c1nc1ccccc1c3)[N+](=O)[O-]c2=O</chem>
C898	CacoP	CacoP+	13	<chem>O=C(CCCCCC(=O)NO)Nc1ccccc1</chem>
C899	CacoP	CacoP+	12	<chem>C[NH2+]CCC(Oc1ccc(cc1)C(F)(F)F)c1ccccc1</chem>
C900	CacoP	CacoP+	13	<chem>O=C([O-])Cc1ccc2c1oc1c(ccc1C)C)c2=O</chem>
C901	CacoP	CacoP+	13	<chem>O=C([O-])c1ccccc1Nc1ccccc1C)C</chem>
C902	CacoP	CacoP+	13	<chem>Cn1ccc1CN(CCN(Cc1ccccc1)S(=O)(=O)c1ccccc1)c1ccc(cc1)C#N</chem>
C903	CacoP	CacoP+	13	<chem>Oc1ccccc1NC(=O)C</chem>
C904	CacoP	CacoP+	13	<chem>O=C([N-]S(=O)(=O)c1ccc(cc1OC)C)C(c1cc2c(cc1)OCO2)c1cn(c2c1ccc(c2)C(=O)OCC)C</chem>
C905	CacoP	CacoP+	13	<chem>O=C(NCCC(=O)N1CC[NH+](CC2CCOCC2)CC1)[C@@H](Cc1ccccc1)NC(=O)C1(CCCC1)NC(=O)c1cc2ccccc2s1</chem>
C906	CacoP	CacoP+	13	<chem>O=C([O-])/C=C/c1ccccc1</chem>
C907	CacoP	CacoP+	13	<chem>O=C(c1nccc1[NH2+]Cc1ccccc1)Nc1ccc(cc1)C(C)C)C</chem>
C908	CacoP	CacoP+	13	<chem>Nc1nc2ccc(cc2n1S(=O)(=O)NC(C)C)C(C(=O)N)c1c(ccc(c1)F)F</chem>
C909	CacoP	CacoP+	13	<chem>CC(=O)CCCCC(O)/C=C/C#C/C=C/C</chem>
C910	CacoP	CacoP+	13	<chem>COc1cc(cc1OC)OC)C(=O)N1CC[C@@](c2ccc(c(c2)Cl)Cl)(CC[NH+]2CCC(C(=O)N)(c3ccccc3)CC2)C1</chem>
C911	CacoP	CacoP+	13	<chem>Oc1ccccc1</chem>
C912	CacoP	CacoP+	13	<chem>O[C@@H]1[C@H](O)C[C@]2(C(=O)C=C3C([C@@H](O)C[C@@]4(C)[C@@]3(O)CC[C@@H]4[C@@](C)(O)[C@H](O)CCC(C)C)[C@]2(C)C1)O</chem>
C913	CacoP	CacoP+	13	<chem>Fc1cc(cc(c1c1ccccc1)F)N1CC(CNC(=O)C)OC1=O</chem>
C914	CacoP	CacoP+	13	<chem>CC(=O)N[C@@H](Cc1ccccc1)C(=O)N</chem>
C915	CacoP	CacoP+	13	<chem>CCOc1ccccc1OCC1C[NH2+]CCO1</chem>
C916	CacoP	CacoP+	13	<chem>O=C1N(Cc2ccc3[nH]nc(c3c2)N)[C@@H](Cc2ccccc2)[C@@H](O)[C@@H](O)[C@@H](Cc2ccccc2)N1CCCC</chem>
C917	CacoP	CacoP+	13	<chem>O=C1Nc2c(cc(c2)Cl)C(=NC1O)c1c(cccc1)Cl</chem>
C918	CacoP	CacoP+	13	<chem>Cc1nccc2c1[nH]c1c2ccccc1</chem>

C919	CacoP	CacoP+	13	Oc1cc2c(c(c1)O)C(=O)OCC(CCC(=O)CCC/C=C\2)C
C920	CacoP	CacoP+	13	O=C([O-])Cc1cc(c(n1C)C(=O)c1ccc(cc1)Cl)C
C921	CacoP	CacoP+	13	CCC(C)(C(=O)O)[C@@H]1C[C@@H](C=C2C=C[C@H]([C@H]([C@H]12)CC[C@@H]1C[C@@H](CC(=O)O1)O)C)C
C922	CacoP	CacoP+	13	Clc1ccc(c(c1)F)C[C@@H](C)C(=O)N1CCN(c2c(cc(cc2)C)[C@@H]([NH2+])CCNC)C(C)C)CC1
C923	CacoP	CacoP+	13	O=c1c2c(cccc2)nc2n1CCc1c2[nH]e2c1cccc2
C924	CacoP	CacoP+	12	CCc1c2cc(ccc2nc2c1Cn1c2cc2c(COC(=O)[C@]2(O)CC)c1=O)O
C925	CacoP	CacoP+	13	O=C(c1cc(nn1c1cccc(c1)C[NH3+])C(F)(F)F)Nc1ccc(cc1)c1cccc1S(=O)(=O)C
C926	CacoP	CacoP+	13	COe1c(e2c(c(cc(n2)n2ccc(n2)C(C)C)O[C@H]2[C@H]3C(=O)N(CCCC/C=C\C@H]4[C@@](NC(=O)[C@@H]3C2)(C(=O)[N-]S(=O)(=O)C2CC2)C4)C)cc1)C
C927	CacoP	CacoP+	13	Clc1ccc(cc1)C[C@@H](C)C(=O)N1CCN(c2c(cccc2F)[C@@H](NC(=O)CC[NH+](C)C)C(C)C)CC1
C928	CacoP	CacoP+	13	CC1=C(CCC(=O)O)/C=C/c2c(c(c([nH]2)/C=C/2/C(=C(C)C(=O)N2)C=C)C)CCC(=O)[O-]/N=C1/C=C/1\C(=C(C=C)C(=O)N1)C
C929	CacoP	CacoP+	13	O=Cc1c(nc(n1Cc1ccc(cc1)c1cccc1c1nn[n-]1)CCC)CC
C930	CacoP	CacoP+	13	O[C@@H]([C@@H](O)CC(C)C)[C@@H](NC(=O)C[NH3+])CC1CCCC1
C931	CacoP	CacoP+	13	O=S(=O)(N(CC1CCN(C(=O)OCC(C)C)CC1)C1CN(Cc2cncn2C)c2ccc(cc2C1)C#N)c1ncccc1
C932	CacoP	CacoP+	13	O=C1CC([NH+])2CC[NH+](CCCN3c4cccc4Sc4c3cc(cc4)CC(=O)[O-])CC2)N(C)C(=O)N1C
C933	CacoP	CacoP+	10,6,2	COc1ccc(cc1OC)CC[NH+](C)CCCC(C#N)(C(C)C)c1ccc(c(c1)OC)OC
C934	CacoP	CacoP+	13	Ne1n(c2c(n1)ccc(c2)/C=C/C(=O)NC)/c1cccc(c1)F)S(=O)(=O)[N-]C(=O)N1CCCC1
C935	CacoP	CacoP+	13	c1cc(c(c1)Cl)/C=N/N=C(N)N)Cl
C936	CacoP	CacoP+	13	CC/C=C(\C(=O)N)[C@@H]1[C@H]2N(C(=C(COC(=O)N)CS2)C(=O)OCOC(=O)C(C)(C)C)C1=O)/c1csc(n1)N
C937	CacoP	CacoP+	12,5	[nH]1c2c(n(nc2CC)C)c(=O)nc1c1c(ccc(c1)S(=O)(=O)N1CC[NH+](C)CC1)OCC
C938	CacoP	CacoP+	13	O=C1C(c2cccc2)(c2cccc2)C(=O)N(COC)C(=O)N1
C939	CacoP	CacoP+	13	O=C(c1cenn1CCc1cnccl)Nc1ccc(cc1)Cl
C940	CacoP	CacoP+	13	O=C1CC(c2ccc(cc2)O)Oe2c1c(cc(c2CC=C(C)C)O)O
C941	CacoP	CacoP+	13	Cc1nnc2n1c1c(cc(cc1)Cl)C(=NC2)c1cccc1
C942	CacoP	CacoP+	13	C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@]2(C#C)O)CCc1c3ccc(c1)O
C943	CacoP	CacoP+	12	CC[C@]1(O)[C@H]2CN(C1)CCc1c([nH]3cccc13)[C@@](C2)(C(=O)OC)c1c(cc2c(c1)[C@]13[C@@H](N2C)[C@@]2[C@@]4(C=CC[NH+](CC1)[C@H]34)CC)OC(=O)N(CCC1)C2=O)OC
C944	CacoP	CacoP+	13	O=C(CNC(=O)C)NCCc1cccc1
C945	CacoP	CacoP+	10,11,12,8	Clc1cccc(c1N=C1NCCN1)Cl
C946	CacoP	CacoP+	12	COe1c(cc2c(c1)oc(=O)cc2)[C@@H](O)[C@H](OC(=O)/C=C/C)C(C)C)O
C947	CacoP	CacoP+	13	O[C@@H]1[C@H](COC(=O)[C@H](C(C)C)[NH3+])O[C@H]([C@H]1O)n1c(=O)nc(O)cc1
C948	CacoP	CacoP+	10,11	COc1cc(c(c2c1C(=O)C1(O2)C(C)CC(=O)C=C1OC)Cl)OC
C949	CacoP	CacoP+	13	O=C(NC)[C@@H](NC(=O)[C@@H](CC1CCCC1)NC(=O)C)Cc1cccc1
C950	CacoP	CacoP+	13	c1c(c(=O)[nH]c(=O)n1[C@H]1[C@H]([C@@H]([C@H](O1)CO)O)O)/C=C/Br
C951	CacoP	CacoP+	13	CC(c1cccc(c1)O)c1cccc1C(=O)[O-]
C952	CacoP	CacoP+	13	CCCCCCCCC(=O)[O-]
C953	CacoP	CacoP+	10,11,12,4,2	Cc1cn([C@H]2C[C@H](N=[N+]=[N-])[C@@H](CO)O2)c(=O)[nH]c1=O
C954	CacoP	CacoP+	12	cc[C@H]1OC(=O)[C@H](C)C(O)[C@H]2C[C@@](C)OC[C@H](O)[C@H](O2)[C@H](C)C(O)[C@@H]2O[C@H](C)[C@@H]([C@H]2O)[NH+](C)C[C@](O)C[C@@H](C)C(=N)OCOCOC[C@H](C)[C@@H](O)[C@]1(C)O
C955	CacoP	CacoP+	13	O=C1N[C@@]2[C[C@H]2/C=C/CCCCNC(=O)[C@H]2[C@H]1C[C@H](C2)Oc1nc(nc2c1ccc(c2C)OC)c1ccc(cc1)F)C(=O)[N-]S(=O)(=O)C1CC1
C956	CacoP	CacoP+	13	C[NH+](C)CCCN1c2c(cccc2)Se2ccc(cc12)Cl
C957	CacoP	CacoP+	12	C/C=N/C[C@H]1CN(C(=O)O1)c1cc(c(cc1)c1nnc(s1)C[NH3+])F)/S
C958	CacoP	CacoP+	13	O=S(=O)(c1ccc(cc1)N)Nc1ncccc1
C959	CacoP	CacoP+	13	CC(=O)N(C)[C@@H](Cc1cccc1)C(=O)N(C)[C@H](Cc1cccc1)C(=O)N(C)C(Cc1cccc1)C(=O)NC
C960	CacoP	CacoP+	10,8	COe1c(cc2c(nc(nc2c1)N1CCN(CC1)C(=O)c1ccc1)N)OC
C961	CacoP	CacoP+	13	O=S(=O)([O-])CCNC(=O)CC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3[C@H](O)CC4[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@]12C
C962	CacoP	CacoP+	13	O=C(NCCC[NH+])1CCOCC1[C@@H](Cc1cccc1)NC(=O)C1(CCCC1)NC(=O)c1cc2cccc2cc1
C963	CacoP	CacoP+	13	O=C(c1cc2c([nH]c(n2)SC)cc1Cl)N1CCCC(C)CC1
C964	CacoP	CacoP+	12	C[NH+]1CCC[C@H]1c1cccc1

C965	CacoP	CacoP+	13	CC1=NCCc2c1[nH]c1c2ccc(c1)OC
C966	CacoP	CacoP+	13	O=C1N2c3cccc3[C@@]34CC[NH+](C)CC5=CCO[C@@H](C1)[C@H]([C@@H]23)[C@@H]5CC4=O
C967	CacoP	CacoP+	13	O=c1oc2cccc2c(c1C(c1cccc1)CC(=O)C)O
C968	CacoP	CacoP+	13	O=C([N-]S(=O)(=O)c1ccc(cc1OC)C)C(c1cc2c(cc1)OCO2)c1cn(c2c1ccc(c2)F)C
C969	CacoP	CacoP+	13	C[NH+]1C2CC[C@@H]1C[C@H](OC(c1cc(ccc1)Cl)c1ccc(cc1)Cl)C2
C970	CacoP	CacoP+	10	CC1CC2C3CCC4=CC(=O)C=CC4(C)C3(F)C(O)CC2(C)C1(O)C(=O)CO
C971	CacoP	CacoP+	13	C[C@@H]1[C@H]2[C@@H]([C@H]3[C@@H](C(=O)C(=C([C@]3(C(=O)C2=C(c2c1cccc2O)O)O)O)C(=O)N)[NH+](C)C)O
C972	CacoP	CacoP+	12,2	[C@@H]12CC[C@](O)(C(=O)CO)[C@@]1(C)CC(=O)[C@H]1[C@H]2CCC2=CC(=O)CC[C@]12C
C973	CacoP	CacoP+	13	O=C([O-])Cc1ccc(cc1)Cn1cnc2c1cccc2
C974	CacoP	CacoP+	13	c[C@@H]1/C=C/C=C(C)\C(=O)NC2=C(O)c3c(c(c4c(c3C(=O)/C2=C\N[NH+]2CCN(C)CC2)C(=O)[C@](O)C=C/[C@@H](OC)[C@@H](C)[C@H](OC(=O)C)[C@H](C)[C@@H](O)[C@@H](C)[C@H]1O)(O)O4)C)O
C975	CacoP	CacoP+	12	COc1cc2c(cc1)N1C3C4C(CC1=O)OCC=C1C[NH+]5CCCC23C5CC41
C976	CacoP	CacoP+	13	O[C@@](C[N@@H+](Cc1ccc(cc1)c1cccc1)NC(=O)[C@@H](C(C)C)C)CC(=O)OC)(Cc1cccc1)C(=O)N[C@H]1c2cccc2C[C@@H]1O
C977	CacoP	CacoP+	12	[NH3+][C@@H](Cc1cccc1)C(=O)[O-]
C978	CacoP	CacoP+	13	O=C([O-])c1cn2[C@H](COc3c2c(cc(c3N2CC[NH+](CC2)C)F)c1=O)C
C979	CacoP	CacoP+	13	C/C=C\C(=O)OC(C)([C@@H]1Cc2c(ccc3c2oc(=O)cc3)O1)C/C
C980	CacoP	CacoP+	13	CC(C)[NH2+]CC(OC(=O)C1CC1)COc1cccc1OCC=C
C981	CacoP	CacoP+	13	NC(=O)c1cccc(c1)Cn1cnc1
C982	CacoP	CacoP+	13	O[C@@H]1[C@H](OC)C[C@H]2C(=O)C=C3C(CC[C@@]4(C)[C@@]3(O)CC[C@@H]4[C@@](C)(O)[C@H](OC)CCC(C)C)[C@]2(C)C1
C983	CacoP	CacoP+	13	Cc1nccc2c1[nH]c1c2ccc(c1)O
C984	CacoP	CacoP+	12,2	Oc1cc2c(cc1)C[C@H]1[NH+](CC3(O)CC3)CC[C@]2(CC)C1(C)C
C985	CacoP	CacoP+	13	O=C(N[C@H]1CC[N@@H+](CC2CCOCC2)CC1)[C@@H](Cc1cccc1)NC(=O)C1(CCCC1)NC(=O)c1cc2cccc2s1
C986	CacoP	CacoP+	13	O=C(Nc1cccc(c1)OCC)OCC[NH+]1CCCC1
C987	CacoP	CacoP+	10,11	CC(C)(C)[NH2+]CC(O)COc1nsnc1N1CCOCC1
C988	CacoP	CacoP+	13	O=C(OC1C[C@@H]2[NH+](C)[C@H](CC2)C1)C(c1cccc1)CO
C989	CacoP	CacoP+	13	Nc1nc2c(cc(c2)/C(=C/C(=O)N)/c2ccc(cc2)F)n1S(=O)(=O)C(C)C
C990	CacoP	CacoP+	13	O=c1c2c(cc(cc2O)oc(c1)c1cc(c(c1)OC)OC)OC
C991	CacoP	CacoP+	12	CO/N=C(N)\c1ccc(cc1)c1ccc(o1)c1ccc(cc1)/C(=N/OC)/N
C992	CacoP	CacoP+	12	COc1cc(ccc1)[C@@]1(O)CCCC[C@@H]1C[NH+](C)C
C993	CacoP	CacoP+	13	Oc1ccc(cc1)C(=O)OCCCCCCC
C994	CacoP	CacoP+	10	CC12CCC3C(CCC4=CC(=O)CCC34C)C1CCC2O
C995	CacoP	CacoP+	13	C=CCc1cccc1OCC(O)C[NH2+]C(C)C
C996	CacoP	CacoP+	13	CCCCCCCCC(=O)Nc1cnc1
C997	CacoP	CacoP+	13	O=C([C@@H](C)NC(=O)C)NCCc1cccc1
C998	CacoP	CacoP+	13	O=C([O-])c1cc2c(cc1)Sc1c(ccc1)N2CCC[NH+]1CC[NH+](c2cc(=O)n(C)c(=O)n2C)CCC1
C999	CacoP	CacoP+	13	O=C1c2c(cc(cc2OC(c2cc(c(cc2)OC)O)C1)O)O
C1000	CacoP	CacoP+	13	[NH3+]Cc1cccc(c1)Cc1nccn1
C1001	CacoP	CacoP+	13	CCCCCCCCC(=O)OCc1cccc1
C1002	CacoP	CacoP+	12	O[C@H]1CC[C@H]2C[NH+]3CCc4c([nH]c5cccc45)[C@@H]3C[C@@H]2[C@H]1C(=O)OC
C1003	CacoP	CacoP+	13	O=c1[nH]c(=O)n(cc1F)[C@H]1O[C@@H](COC(=O)CNC(=O)C(Cc2cccc2)[NH3+])[C@H](O)C1
C1004	CacoP	CacoP+	13	Nc1nc2ccc(cc2n1C(C)C)C(C(=O)N)c1cccc(c1F)F
C1005	CacoP	CacoP+	13	CCCCCCCCC(=O)Oc1cc(ccc1)F
C1006	CacoP	CacoP+	13	Nc1nc2ccc(cc2n1S(=O)(=O)C(C)C)/C(=C/C(=O)NC)/c1ccc(c(c1F)F)F
C1007	CacoP	CacoP+	13	O=C1C[C@@H]([N@H+]2CCC[N@@H+](CCCN3c4c(ccc(c4)CC(=O)[O-])CCc4c3cccc4)CC2)N(C)C(=O)N1C
C1008	CacoP	CacoP+	13	C[C@H]1C[C@H]2[C@@H]3CC[C@@](C(=O)CO)(O)[C@@]3(C)C[C@H](O)[C@@H]2[C@]2(C)C1=CC(=O)C=C2
C1009	CacoP	CacoP+	13	O[C@@H]1[C@H](O)C[C@H]2C(=O)C=C3C(CC[C@@]4(C)[C@@]3(O)CC[C@@H]4[C@@](C)(O)[C@H](OCC)CCC(C)(O)C)[C@]2(C)C1
C1010	CacoP	CacoP+	13	C[NH+]1CCC23C4C1Cc1c2c(cc1)OC)OC3C(C=C4)O





C1057	CacoP	CacoP-	13	[O-]C(=O)Cc1ccc(cc1)Cn1cnc1
C1058	CacoP	CacoP-	13	O=S1(=O)c2c(cccc2)C(c2ccc(cc2)O)(c2ccc(cc2)O)O1
C1059	CacoP	CacoP-	13	Ce1c([nH]c(c1CCC(=O)O)Cc1c(c(c([nH]1)/C=C/1/C(=C)C(C(=O)N1)C=C)C)CCC(=O)[O-])/C=C\1/C(=C(C=C)C(=O)N1)C
C1060	CacoP	CacoP-	13	CC(C)c1nc(nc(c1/C=C/C(CC(CC(=O)[O-])O)O)c1ccc(cc1)F)N(C)S(=O)(=O)C
C1061	CacoP	CacoP-	13	Fe1cc(ccc1N1CCS(=O)CC1)N1C[C@H](CNC(=O)C)OC1=O
C1062	CacoP	CacoP-	13	CS(=O)(=O)Nc1cc2c(cc1)N/C(=C\1/C(=O)[C@@H]3[C@H]4CC[C@H](C4)[C@@H]3N(C1=O)Cc1ccc(cc1)F)/NS2(=O)=O
C1063	CacoP	CacoP-	13	c1ccc(cc1)CC1Nc2c(cc(c2)C(F)(F)F)S(=O)(=O)N)S(=O)(=O)N1
C1064	CacoP	CacoP-	10,12,5	CC[NH+]1CCCC1CNC(=O)c1c(ccc(c1)S(=O)(=O)N)OC
C1065	CacoP	CacoP-	13	Ne1nenc2e1n2[C@H]1[C@@H](O)[C@H](O)[C@@H](CO)O1
C1066	CacoP	CacoP-	13	O=C(C1=C(CS[C@@H]2N1C(=O)[C@H]2NC(=O)C(NC(=O)N1C(=O)C(=O)N(CC)CC1)c1ccc(cc1)O)CSc1nmmn1CC)[O-]
C1067	CacoP	CacoP-	13	Oc1cc(cc(c1O)O)C(=O)OCCC
C1068	CacoP	CacoP-	13	CC(C)(C)NC(=O)[C@H]1C[C@H]2CCCC[C@@H]2[C@@H]1C[C@H](C(C)[C@@H](C1)N(=O)[C@@H](CC(=O)N)N(=O)c1nc2ccccc2cc1)O
C1069	CacoP	CacoP-	13	o=c1(c@@H)CSSCC(=O)N[C@@H](C2ccc(cc2)O)C(=O)N[C@@H](C2ccc(c2)C(=O)N[C@@H](CCC(=O)N)C(=O)N1)[C@H](C(=O)N)C(=O)NCCC(=O)N)CCCN=C(N)N)CCCC1
C1070	CacoP	CacoP-	13	N=c1ccc2c(c3ccccc3C(=O)OC)c3c(cc(cc3)N)oc2c1
C1071	CacoP	CacoP-	13	O=c1c(c(Cc2ccccc2O)n(CCO)cc1)O
C1072	CacoP	CacoP-	13	O=C1OC[C@H](Cc2cc3c([nH]cc3CC[NH+](C)C)cc2)N1
C1073	CacoP	CacoP-	13	O=C([C@H](OCc1ccccc1)[C@H](O)[C@@H](O)[C@@H](OCc1ccccc1)C(=O)N[C@@H](C)C)C(=O)N)N[C@@H]1[C@H](O)Cc2c1cccc2
C1074	CacoP	CacoP-	12,7	Ce1cnc2c1nc([nH]2)Cc1nc2c([nH]1)cc(cc2)/C(=N/O)/N
C1075	CacoP	CacoP-	13	Cn1cnc1CN(CCN(CC1CCN(C(=O)OC(C)C)CC1)S(=O)(=O)c1cn(en1)C)c1ccc(cc1)C#N
C1076	CacoP	CacoP-	13	O=C1OC[C@@H]2[C@H](O[C@H]3[C@H](O)[C@@H](O)[C@@H]4O[C@H](C)OC[C@H]4O3)c3c(cc4c(c3)OCO4)[C@H](C(C)[C@@H]12)c1cc(c(c1)OC)O)OC
C1077	CacoP	CacoP-	13	O=C(OC(C)O)N1[C@H](C(=O)N[C@@H](C2ccc(c2)C(=O)N([C@@H](C2c[nH]n2)C(=O)N[C@@H](C(C)[C@@H](O)C)C)C(=O)N[C@@H](C(C)C)C(=O)N)C2cccc2)CC(C)C)CCCC1
C1078	CacoP	CacoP-	13	O=C(c1cc(nn1c1cccc(c1)C(=N)N)C(F)(F)F)Nc1c(cc(c1)C)1ccccc1S(=O)(=O)C)F
C1079	CacoP	CacoP-	13	C[NH+]1C(CNc2ccc(cc2)C(=O)N[C@H](C(=O)[O-])CCC(=O)[O-])CNe2c1c(=O)nc(N)[nH]2
C1080	CacoP	CacoP-	13	O=C(C1=C(CS[C@@H]2N1C(=O)[C@]2(NC(=O)Cc1ccs1)OC)COC(=O)N)[O-]
C1081	CacoP	CacoP-	13	O[C@@H]1[C@H](COC(=O)[C@H](C2ccc(c2)[NH3+])O[C@H]([C@H]1O)n1c(=O)nc(O)cc1
C1082	CacoP	CacoP-	13	NC(=N)c1ccc2c(c1)[nH]c(n2)c1cccc1
C1083	CacoP	CacoP-	13	O=c1[nH]c(=O)n(cc1F)[C@H]1O[C@@H](COC(=O)[C@H]([C@@H](C)CC)N)[C@H](OC(=O)[C@H]([C@@H](C)CC)[NH3+])C1
C1084	CacoP	CacoP-	10	C[C@@H]1O[C@@H](O[C@H]2CC[C@]3(C)[C@H]4CC[C@]5(C)[C@H](CC[C@]5(O)[C@@H]4CCC3=C2)c2coc(=O)cc2)[C@H](O)[C@H](O)[C@H]1O
C1085	CacoP	CacoP-	13	CCNC(=O)[C@H]1CCCNC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]1CCC(=O)N1)Cc1nc[nH]1)Cc1c[nH]e2ccccc12)CO)C1ccc(cc1)O)CC(C)C)C)CCCN=C(N)N
C1086	CacoP	CacoP-	12	NC(=N)c1ccc(cc1)CNC(=O)[C@@H]1CCN1C(=O)[C@H]([NH2+])CC(=O)[O-])C1CCCCC1
C1087	CacoP	CacoP-	13	O=S(=O)(c1ccc(cc1)C([NH+])1CCN(C2CCC2)CCC1)c1nmmn1Cc1ccccc1)C
C1088	CacoP	CacoP-	13	O=c1c2c(n(en2)COC(CO)CO)nc(N)[nH]1
C1089	CacoP	CacoP-	13	O=C([O-])C(NC(=O)c1ccc(cc1)C)C1Cc1cc(=O)[nH]c2c1ccccc2
C1090	CacoP	CacoP-	13	COc1cc2c(c(cc2n2)c2csc(n2)NC(C)O)[C@H]2[C@H]3C(=O)N(CCCC/C=C[C@H]4[C@@](NC(=O)[C@@H]3C2)(C(=O)[N-]S(=O)(=O)C2CC2)C4)C)cc1
C1091	CacoP	CacoP-	13	O=C([O-])c1c(nc(n1Cc1ccc(cc1)c1ccccc1c1nmmn1)1)CCCCC1
C1092	CacoP	CacoP-	12	CCOC(=O)[C@H](CCc1ccccc1)[NH2+][C@@H](C)C(=O)N1CCC[C@H]1C(=O)[O-]
C1093	CacoP	CacoP-	13	[O-]C(=O)[C@H](NC(=O)C(C)C)[NH3+])C(C)C
C1094	CacoP	CacoP-	12	[O-]C(=O)C[C@H](NC(=O)[C@@H]1CCCN(C1)C(=O)CCCC1CC[NH2+][CC1)c1cccc1
C1095	CacoP	CacoP-	13	O=S(=O)(N(CCN1cccc1)C1CN(Cc2en2)C)c2ccc(cc2C1)C#N)c1cn(en1)C
C1096	CacoP	CacoP-	13	O=C([C@H]1[N@H+]([C@@H](O)[C@@H](O)[C@@H](NC(=O)c2ccccc2)O)CSc2ccccc2)C[C@H]2CCCC[C@@H]2C1)N(C)C)C O=C([O-
C1097	CacoP	CacoP-	13	][C@@H](NC(=O)c1ccc(cc1)N(Cc1nc2c(nc(nc2nc1)N)N)C)CCC(=O)O CC(C)[C@H]([NH3+])C(=O)OCCOCn1cnc2c1[nH]c(nc2=O)N
C1098	CacoP	CacoP-	13	[NH3+][C@@H](C(=O)N[C@H]1[C@H]2SCC(=C(N2C1=O)C(=O)[O-])CSc1n[nH]nc1)c1ccc(cc1)O
C1099	CacoP	CacoP-	12	C1c1c(c(cc1)C)C(=O)N[C@@H](Cc1ccc(cc1)c1c(c2ccc(cc2)F)enn(C)c1=O)C(=O)[O-]
C1100	CacoP	CacoP-	13	O=c1cc([NH2+])CCC[NH+]2CCC(CN3c4ccccc4Sc4c3cc(cc4)C(=O)[O-])CC2)n(C)c(=O)n1C
C1101	CacoP	CacoP-	13	CCOC1nc2ccccc2n1Cc1ccc(cc1)c1ccccc1c1n[nH]nn1)C(=O)[O-]
C1102	CacoP	CacoP-	13	





C1195	CacoP	CacoP+	13	O=C(C[NH3+])CCC(=O)[O-]
C1196	CacoP	CacoP+	13	CCCCOe1cc2c(cc1)[C@H](c1ccc3c(c1)OCO3)[C@@H](C(=O)[O-])[C@@H]2c1c(cc(cc1)OC)OCC(=O)O
C1197	CacoP	CacoP+	13	CCC(=O)N(c1cccc1)C1(CC[NH+])(CC1)CCn1c(=O)n(nn1)CC)COC
C1198	CacoP	CacoP+	13	CC1=C(N2[C@H](SC1)[C@@H](C2=O)NC(=O)C(c1cccc1)[NH3+])C(=O)[O-]
C1199	CacoP	CacoP+	10,11	CN1C(=C(O)c2c(cccc2)S1(=O)=O)C(=O)Nc1ncc(s1)C
C1200	CacoP	CacoP+	13	c[C@H]1/C=C/C(=O)N2=C3C(=NC4(N3)CC[NH+](CC4)CC(C)C)3c4c(c(c3C2=O)O)C)O[C@@](C4=O)(O/C=C/[C@H]([C@H]([C@H]([C@H]([C@H]([C@H]1O)C)O)C)OC(=O)C)OC)C)OC(=O)C)OC)C
C1201	CacoP	CacoP+	13	c1(ccccc1)Cn1c(nnn1)C([NH+])1CCN(C2CCC2)CCC1)c1ccc(cc1)n1cncn1
C1202	CacoP	CacoP+	13	OC[C@@H]1CC[C@H](n2cnc3c2nnc3O)O1
C1203	CacoP	CacoP+	13	[NH3+][C@@H](CCCCCCCC)C(=O)N[C@@H](Cc1ccc(cc1)O)C(=O)NCC(=O)NCC(=O)N[C@@H](Cc1cccc1)C(=O)N[C@@H](CC(C)C)C(=O)N
C1204	CacoP	CacoP+	12,2	c1cn(cn1)C[C@@]1(OC[C@@H](O1)COc1ccc(cc1)N1CCN(C(=O)C)CC1)c1c(cc(cc1)Cl)Cl
C1205	CacoP	CacoP+	13	CC(=O)c1ccc(cc1)N1CC(CNC(=O)C)[NH+](C)S1=O
C1206	CacoP	CacoP+	13	CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)NC(=O)C(c1cccc1)[NH3+])C(=O)OCOC(=O)C(C)C)C
C1207	CacoP	CacoP+	13	O[C@@H]1[C@@H](O)[C@@H](Cc2cccc2)N(Cc2cccc(c2)N)C(=O)N(Cc2cc(ccc2)N)[C@@H]1Cc1cccc1
C1208	CacoP	CacoP+	12,5,2	CC1Nc2cc(c(cc2C(=O)N)c1c1ccc1)C(S(=O)(=O)N)Cl
C1209	CacoP	CacoP+	13	O=C(c1cenn1CCc1ccncc1)Nc1ccc(cc1)OC(F)(Cl)F
C1210	CacoP	CacoP+	13	[NH3+][C@H](CC(=O)OCc1cccc1)C(=O)NC(C(=O)[O-])C
C1211	CacoP	CacoP+	13	CC[NH+]1CCCC1CNC(=O)c1cc(c(cc1OC)N)S(=O)(=O)CC
C1212	CacoP	CacoP+	13	O=C1C(Cn2cnc2C)CCc2n(c3c(c12)cccc3)C
C1213	CacoP	CacoP+	13	Oc1cccc(c1)c1ncc(o1)c1ccc(cc1)O
C1214	CacoP	CacoP+	13	Oc1ccc(cc1)C(=O)OC
C1215	CacoP	CacoP+	13	O=C([O-])CC[C@@H](NC(=O)c1ccc(c(c1)Cl)Cl)C(=O)N(CCCOC)CCCC
C1216	CacoP	CacoP+	13	C[C@H]1CN(c2c(c3c(c(c2F)N)c(=O)c(n3C2CC2)C(=O)[O-])F)C[C@@H](C)[NH2+]1
C1217	CacoP	CacoP+	13	FC(c1cc(ccc1)C1=CC[NH+](CCc2ccc3cccc3c2)CC1)(F)F
C1218	CacoP	CacoP+	13	O=C(c1nsec1[NH2+]Cc1c2cccc2ncc1)Nc1cccc(c1)Br
C1219	CacoP	CacoP+	12,4	Fc1c2c(ccc1)O[C@@H]1[C@@H]1(O2)C[NH2+]C1
C1220	CacoP	CacoP+	13	CC[C@H]1[C@@H]2[C@@H]([C@H](C)C(=O)O2)C2C3C1CCCC[NH+]3CC2
C1221	CacoP	CacoP+	13	CCCCNC(=O)[N-]S(=O)(=O)c1ccc(cc1)C
C1222	CacoP	CacoP+	13	O=C1N([C@H](c2cc3cccc3nc2)CC(=O)[O-])CC[C@H]1CCCc1ccc2c(n1)NCCC2
C1223	CacoP	CacoP+	13	O=C(N(C)C(Cc1cc(c(cc1)O)C(C)C)C(=O)N)C(C(C)N(C)C(=O)[C@@H]([NH3+])Cc1cccc1
C1224	CacoP	CacoP+	13	O=CNc1cc(ccc1O)C(O)C[NH2+]C(C)Cc1ccc(cc1)OC
C1225	CacoP	CacoP+	13	NC(=NCC1COc2cccc2O1)N
C1226	CacoP	CacoP+	13	O=C1N2c3cc(ccc3CCC2CO1)C(=O)C
C1227	CacoP	CacoP+	13	O=C([O-])CC1=C(C)/C(=C/c2ccc(cc2)S(=O)C)/c2c1cc(cc2)F
C1228	CacoP	CacoP+	12	C[C@]12CCC[C@](C)(C1CC[C@]13CC(=C)[C@](O)(C1)CCC23)C(=O)[O-]
C1229	CacoP	CacoP+	13	[C@@H]12[C@]3(O)CCC(=O)[C@H]4[C@]3(CC[NH+]1CC=C)c1c(c(ccc1C2)O)O4
C1230	CacoP	CacoP+	13	[n+]12c(cc3ccc4c(c3c1)OCO4)c1cc3c(cc1CC2)OCO3
C1231	CacoP	CacoP+	13	O=C([O-])c1ccc(cc1OCC)CC(=O)N[C@H](c1cccc1N1CCCC1)CC(C)C
C1232	CacoP	CacoP+	13	O=c1oe2c(ccc2)cc1
C1233	CacoP	CacoP+	13	[O-]C(=O)c1cc2c(cc1)C(=O)OC12c2c(cc(cc2)O)Oc2c1ccc(c2)O
C1234	CacoP	CacoP+	13	C[C@@]12CC[C@@H]3[C@H](CCC4=Cc5c(cno5)C[C@@]34C)[C@H]1CC[C@]2(O)C#C
C1235	CacoP	CacoP+	13	COc1c2c(c(c3c1ccc3)OCC1C(C)(O1)C)oc(=O)cc2
C1236	CacoP	CacoP+	13	C1CN(CC[NH+]1CC/C=C\1/c2cccc2Se2c1cc(cc2)C(F)(F)F)CCO
C1237	CacoP	CacoP+	13	c1(ccccc1)C1(CCCCC1)[NH+]1CCCCC1
C1238	CacoP	CacoP+	13	COc1ccc(c2c1cccc2)CCCN1CC[NH+](C2CCCC2)CC1
C1239	CacoP	CacoP+	13	O=C([O-])C1=CC(C(C(O1)C(C(O)CO)OC1(C(C)C1)CNC(=O)C(C(C)C)[NH3+])NC(=O)C)N=C(N)N
C1240	CacoP	CacoP+	13	[O-]C(=O)c1ccc(cc1)Cc1nccc1



C1287	CacoP	CacoP+	10	CC(C)(C)[NH2+]C[C@@H](COc1nsnc1N1CCOCC1)OC(=C)C1CC1
C1288	CacoP	CacoP+	13	OCC/C=C/c1ccc(c(c1)OC)OC
C1289	CacoP	CacoP+	13	CC(C)[NH2+]CC(OC(=O)C1CC1)COc1cccc2cccc12
C1290	CacoP	CacoP+	13	O=c1n(C)c(=O)n(C)c(c1)C1=CC[NH+](CCCN2c3cccc3Sc3e2ce(cc3)CC(=O)[O-])CC1
C1291	CacoP	CacoP+	13	C[NH+]1CCN(CC1)c1c(cc2c(c1F)n(cc2=O)C(=O)[O-])CCF)F
C1292	CacoP	CacoP+	13	CC(Cc1ccc(cc1)C(C(=O)[O-])C)C
C1293	CacoP	CacoP+	13	O=C(NCCC[NH+]1CCOCC1)[C@@H](Cc1cccc1)NC(=O)C1(CCCC1)NC(=O)c1cc2cccc2o1
C1294	CacoP	CacoP+	13	O=c1c(ccc2c1ccc(c2)O)c1ccc(cc1)O
C1295	CacoP	CacoP+	13	O[C@@](C[N@@H+](Cc1ccc(cc1)Br)NC(=O)[C@@H](C(C)(C)C)CC(=O)OC)(Cc1cccc1)C(=O)N[C@@H](Cc1cccc1)C(=O)NC
C1296	CacoP	CacoP+	13	O=C(c1cccc1OCC(O)C[NH2+])CCC)CCc1cccc1
C1297	CacoP	CacoP+	12	COc1ccc2c(c1)[C@@]13[C@@H]([C@@H](C2)[NH+](CC1)C)CCCC3
C1298	CacoP	CacoP+	13	O=C(NCC1CC[NH+](CC2CCOCC2)CC1)[C@@H](Cc1cccc1)NC(=O)C1(CCCC1)NC(=O)c1cc2ccc(cc2s1)N(CC)CC
C1299	CacoP	CacoP+	12	CC(CCC(=O)NCC(=O)[O-])C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CC(O)C12C
C1300	CacoP	CacoP+	13	CC(=O)c1ccc(cc1)N1CC(C[NH3+])OC1=O
C1301	CacoP	CacoP+	13	COc1ccc(cc1OC)OC)C(=O)N1CC[C@@](c2ccc(c(c2)Cl)Cl)(CC[NH+]2CCC(C(=O)N3CCOCC3)(c3cccc3)CC2)C1
C1302	CacoP	CacoP+	13	C[NH2+]CCCN1c2cccc2CCc2cccc12
C1303	CacoP	CacoP+	13	O=c1[nH]c(=O)n(cc1F)[C@H]1O[C@@H](COC(=O)C(C)C)[NH3+][C@H](O)C1
C1304	CacoP	CacoP+	13	O=C1CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](C(=O)C)CC[C@H]4[C@@H]3CCC2=C1
C1305	CacoP	CacoP+	13	O=c1n(C)c(=O)n(C)c(c1)[NH+]1CC[NH+](CC1)CCCN1c2cccc2Se2c1cc(cc2)CCC(=O)[O-]
C1306	CacoP	CacoP+	12	O=C1C[C@@H]2OCC=C3C[NH+]4CC[C@@]56[C@@H]4C[C@@H]3[C@@H]2[C@@H]5N1c1cccc61
C1307	CacoP	CacoP+	12	C[NH+](C)[C@H]1[C@@H]2C[C@H]3C(=C(O)c4c(cccc4O)[C@@]3(C)O)C(=O)[C@]2(O)C(=O)/C(=C(N)\O)/C1=O
C1308	CacoP	CacoP+	13	O=C1C(c2cccc2)(c2cccc2)C(=O)NC(=O)N1
C1309	CacoP	CacoP+	13	O[C@@H]([C@@H](O)CC(C)C)[C@@H](NC(=O)/C=C/c1cccc1)CC1CCCCC1
C1310	CacoP	CacoP+	13	CCCCCCCCC(=O)NC1CCCCC1
C1311	CacoP	CacoP+	13	O=C(c1cc2c([nH]c(n2)SC)cc1)N1CCCCC1
C1312	CacoP	CacoP+	13	Oc1c(ccc(c1)O)C(=O)/C=C/c1ccc(cc1)O
C1313	CacoP	CacoP+	13	O=c1cc(c2cccc2)oc2c1c(c(c(c2)O)O)O
C1314	CacoP	CacoP+	13	O=C1CC([NH+]2CCC[NH+](CC/C=C/3v4c(ccc(c4)C(=O)[O-])CCc4c3cccc4)CC2)N(C)C(=O)N1C
C1315	CacoP	CacoP+	13	Nc1nc2c(cc(cc2)/C(=C/C(=O)N)/c2cccc(c2F)F)n1C(C)C
C1316	CacoP	CacoP+	12	Cc1c2[nH]c3cc(=O)ccc3c2cc[nH]1
C1317	CacoP	CacoP+	13	CC(=O)N[C@@H](Cc1cccc1)C(=O)N[C@@H](Cc1cccc1)C(=O)N(C)C(Cc1cccc1)C(=O)N
C1318	CacoP	CacoP+	13	Nc1nc2ccc(cc2n1S(=O)(=O)[N-]C(=O)N1CCOCC1)/C(=C/C(=O)NC)/c1cccc(c1)F
C1319	CacoP	CacoP+	13	Oc1ccc(cc1)C(=O)OCCC
C1320	CacoP	CacoP+	13	Oc1ccc(cc1)/C=C/c1ccc(cc1)O)O
C1321	CacoP	CacoP+	12	CC[C@@]1(O)C(=O)OCc2c1cc1n(Cc3c(c4cccc4nc13)CC[NH2+]C(C)C)c2=O
C1322	CacoP	CacoP+	12	CC(=CC(=O)O)[C@H]1Cc2c(cc3c(c2)ccc(=O)o3)OC1(C)C)C
C1323	CacoP	CacoP+	13	O[C@H]1[C@@H](O)[C@@H](Cc2cccc2)N(Cc2ccc3[nH]nc(c3e2)N)C(=O)N(Cc2cccc2)[C@@H]1Cc1cccc1
C1324	CacoP	CacoP+	13	O=C(NCCC[NH+]1CCOCC1)[C@@H](Cc1cccc1)NC(=O)C1(CCCC1)NC(=O)c1ccc(s1)c1cccc1
C1325	CacoP	CacoP+	13	N#Cc1cccc(c1)Cc1nccn1
C1326	CacoP	CacoP+	13	O=C1C[C@@H]([N@@H+]2CC[N@@H+](CCCN3c4c(ccc(c4)C(=O)[O-])OCc4c3cccc4)CC2)N(C)C(=O)N1C
C1327	CacoP	CacoP+	13	O=C([C@@H](CC(C)C)NC(=O)C)NCCc1cccc1
C1328	CacoP	CacoP+	13	COc1e(e2c(c(cc(n2)e2nc(cs2)C(C)C)O)[C@H]2C[C@H]3C(=O)N(CCCC/C=C/[C@H]4[C@@](NC(=O)[C@@H]3C2)(C(=O)[N-S(=O)(=O)C2CC2)C4)C)cc1)Cl
C1329	CacoP	CacoP+	13	Nc1cccc(c1)Cn1cnc2c1cccc2
C1330	CacoP	CacoP+	12	C[C@@H]1O[C@H](OC[C@H]1)NC(=O)Cc1cccc1)c1ccc(cc1)Cl
C1331	CacoP	CacoP+	13	CC(=O)CCCC/C=C/CC#C/C=C\C
C1332	CacoP	CacoP+	13	O=C1CC([NH+]2CCC[NH+](CC/C=C/3v4c(ccc(c4)CC(=O)[O-])OCc4c3cccc4)CC2)N(C)C(=O)N1C

C1333	CacoP	CacoP+	13	Fe1c(ccc(c1)N1C[C@H](CNC(=S)C)OC1=O)c1nnc(s1)[C@@H]1[NH2+]CCCC1
C1334	CacoP	CacoP+	13	CCCCCCCCC(=O)Nc1c(ccc(c1)C)C
C1335	CacoP	CacoP+	13	Oc1ccc2c3c1O[C@@H]1[C@@H]43CC[NH+][C@H](C2)[C@@H]4C=C[C@@H]1O)C
C1336	CacoP	CacoP+	13	CCCCCCC/C=C/C=C/C(=O)NCC(C)C
C1337	CacoP	CacoP+	13	O=c1cc(e2ccccc2)oc2c1c(cc(c2)OC)OC
C1338	CacoP	CacoP+	13	Fe1c(ccc(c1)N1C[C@H](CNC(=S)C2CC2)OC1=O)N1CCN(C(=O)CO)CC1
C1339	CacoP	CacoP+	13	O=c1n(C)c(=O)n(C)c(e1)[NH+]1CC[NH+](CCC1)CCCN1c2ccccc2Sc2c1cc(cc2)C(C)(C)C(=O)[O-]
C1340	CacoP	CacoP+	13	O=S(=O)(N(CC1CCN(C(=O)OCC)CC1)C1CN(Ce2cncn2C)c2ccc(cc2C1)C#N)c1ncccc1
C1341	CacoP	CacoP+	13	O=C(c1nsec1[NH2+])Cc1ccccc1)Nc1ccc(c(c1)C(F)(F)F)C
C1342	CacoP	CacoP+	13	Clc1ccc(cc1)C[C@@H](C)C(=O)N1CCN(c2c(cc(cc2)C)[C@@H](NC(=O)CC[NH3+])C(C)C)CC1
C1343	CacoP	CacoP+	13	O=c1[nH]c(=O)n(cc1F)[C@H]1O[C@@H](COC(=O)CNC(=O)C(C)C)[NH3+][C@H](O)C1
C1344	CacoP	CacoP+	13	Oc1cc2c(c(c1)O)C(=O)OCC(CCC(CCC/C=C\2)O)C
C1345	CacoP	CacoP+	13	COc1cc2c(c(cc(n2)c2ccccc2)O[C@H]2[C@H]3C(=O)N(CCCC/C=C\C[CH]4[C@@H](NC(=O)[C@@H]3C2)(C(=O)[N-]S(=O)(=O)C2CC2)C4)C)cc1
C1346	CacoP	CacoP+	10	CC12CC(O)C3C(CCC4=CC(=O)CCC34C)C1CCC2C(=O)CO
C1347	CacoP	CacoP+	13	O=c1c(en(C2CC2)c2c1cc(c(c2)N1CC[NH+](CCC)C(C)C1)F)C(=O)[O-]
C1348	CacoP	CacoP+	13	O[C@@H](C[N@@H+])(Cc1ccc(cc1)Br)NC(=O)[C@@H](C(C)(C)C)CC(=O)OC)(Cc1ccccc1)C(=O)NCc1ccccc1
C1349	CacoP	CacoP+	13	Nc1nc2c(cc(c2)/C=C/C(=O)N)/c2ccccc2)n1S(=O)(=O)C(C)C
C1350	CacoP	CacoP+	13	CCCCCCCCC(=O)OC(C)C
C1351	CacoP	CacoP+	13	CCCCCCCCC(=O)Nc1ccc(cc1)OC
C1352	CacoP	CacoP+	13	Oc1ccc2c(c1)CC[C@@H]1[C@@H]2CC[C@]2(C)[C@@H](O)CC[C@@H]12
C1353	CacoP	CacoP+	13	Nc1nc2ccc(cc2n1S(=O)(=O)[N-]C(=O)N(C)C)/C=C/C(=O)N/c1ccccc1)F
C1354	CacoP	CacoP+	13	O=C(c1en(CC)c2c(cc(c(c2F)N2CC(C)[NH2+]CC2)F)c1=O)[O-]
C1355	CacoP	CacoP+	13	C#CC#CCCC/C=C/C(=O)NCC(C)C
C1356	CacoP	CacoP+	13	O=c1c2c(cc(c(c2O)OC)O)oc(c1)c1ccc(cc1)O
C1357	CacoP	CacoP+	13	CC(C(=C)CCC(C(=O)[O-])[C@H]1[C@H](O)C[C@]2(C)[C@]1(C)CC=C1C2=CC[C@@H]2[C@]1(C)CC[C@H](C2(C)C)O)C
C1358	CacoP	CacoP+	13	O=c1c(c(c2ccc(c(c2)O)O)oc2c1c(cc(c2)O)O)O
C1359	CacoP	CacoP+	13	Nc1nc2ccc(cc2n1S(=O)(=O)C(C)C)/C=C/C(=O)NCC/c1ccccc1)F)F
C1360	CacoP	CacoP+	13	O=C1CN=C(c2ccccc2)c2cc(ccc2N1)Cl
C1361	CacoP	CacoP+	13	O=C(c1cnn1CCc1ccccc1)Nc1ccc(cc1)C(C)(C)C
C1362	CacoP	CacoP+	13	Clc1ccc(c(c1)F)C[C@@H](C)C(=O)N1CCN(c2c(cc(cc2)C)[C@@H](NC(=O)CC[NH+](C)C)C(C)C)CC1
C1363	CacoP	CacoP+	13	O=C(N)c1ccccc1)Cc1ncccc1
C1364	CacoP	CacoP+	13	[NH3+]Cc1ccccc1)Cn1cnc2c1ccccc2
C1365	CacoP	CacoP+	13	CCCCCCCCC(=O)Oc1ccc(cc1)Cl
C1366	CacoP	CacoP+	13	O=C1[C@@H]2C[C@@H](O)c3nc(nc4c3cccc4C)OC)c3cc(ccc3)F)C[C@H]2C(=O)N(CCCC/C=C\C[CH]2[C@@H](N1)(C(=O)[N-]S(=O)(=O)C1CC1)C2)C
C1367	CacoP	CacoP+	13	O=C([N-]S(=O)(=O)c1ccc(cc1OC)C)C(c1cc2c(cc1)OCO2)c1cn(c2c1ccc(c2)C#N)C
C1368	CacoP	CacoP+	13	CC#CC#CCC/C=C\C=C(=O)NCC(C)CC
C1369	CacoP	CacoP+	12	CC[C@@]1(O)C(=O)OCc2c1cc1n(Cc3cc4ccccc4nc13)c2=O
C1370	CacoP	CacoP+	13	O=C(Nc1ccccc1)OCCCC)OCC[NH+]1CCCC1
C1371	CacoP	CacoP+	13	O=C1c2c(cc(cc2OC(c2ccc(cc2)O)C1)O)O
C1372	CacoP	CacoP+	13	O=c1c(c(c2ccc(cc2)OC)oc2c1c(cc(c2)O)O)O
C1373	CacoP	CacoP+	13	C[NH+]1C2CC[C@@H]1C[C@H](OC(c1ccc(cc1)Cl)c1ccccc1)C2
C1374	CacoP	CacoP+	13	O=C(NCC1CC[NH+](CC2CCOCC2)CC1)[C@@H](Cc1ccccc1)NC(=O)C1(CCCC1)NC(=O)c1cc2ccccc2s1
C1375	CacoP	CacoP+	13	CCCCCCCCC(=O)OCCCC
C1376	CacoP	CacoP+	13	O=c1c(en(C2CC2)c2c1cc(c(c2)N1CC[NH+](C)C(C)C1)F)C(=O)[O-]
C1377	CacoP	CacoP+	13	O[C@H]1[C@@H](OC)C[C@@]2(C)[C@H](C(=O)C=C3C2CC[C@@]2(C)[C@@]3(O)CC[C@@H]2[C@@](C)(O)[C@H](O)CCC(C)C)C1
C1378	CacoP	CacoP+	13	O=C1C=C[C@]2(C)[C@H]3C(O)C[C@]4(C)[C@](C(=O)CO)(O)CC[C@@H]4[C@@H]3CCCC=C1

C1379	CacoP	CacoP+	13	Ne1nc2ccc(cc2n1S(=O)(=O)C(C)C)/C(=C/C(=O)N)/c1cc(c(cc1)F)F
C1380	CacoP	CacoP+	13	O=c1c2c(cc(cc2oc(c1)c1cc(c(cc1)OC)O)O)O
C1381	CacoP	CacoP+	13	O[C@@H]1[C@H](O)C[C@H]2C(=O)C=C3C(CC[C@@]4(C)[C@@]3(O)CC[C@@H]4[C@@](C(O)[C@H](OC)CCC(C)(O)C)[C@]2(C)C)1
C1382	CacoP	CacoP+	13	O=c1n(C)c(=O)n(C)c(c1)[NH+]1CC[NH+](CCC1)CCCN1c2ccc2Se2c1cc(cc2)CC(=O)[O-]
C1383	CacoP	CacoP+	13	OC([C@@H]1[NH+]2CC[C@H]([C@H](C2)C=C)C1)c1ccnc2ccc(cc12)OC
C1384	CacoP	CacoP+	13	C/C=C\C=C/CC/C=C/C=C/C(=O)NCC(C)C
C1385	CacoP	CacoP+	13	Ne1nc2c(cc(cc2)/C(=C/C(=O)NC)/c2cccc(c2F)F)n1S(=O)(=O)C(C)C
C1386	CacoP	CacoP+	13	O=C1N[C@@]2[C[C@H]2/C=C/CCCCN(C)C(=O)[C@H]2[C@H]1C[C@H](C2)Oc1nc(nc2c1ccc(c2C)OC)c1cccc1C(=O)[N-]S(=O)(=O)C1CC1
C1387	CacoP	CacoP+	13	CC#CC#CCC/C=C\C=C(=O)NCC(C)C
C1388	HIA	HIA-	24	c(=O)[C@H](CCN)O)N[C@@H]1C[C@@H]([C@H]([C@@H]([C@H]1O[C@H]1[C@H]([C@@H]([C@H]([C@H]([C@H]([C@H](CO)O1)O)N)O)O)[C@@H]1[C@H](CC[C@H](CN)O1)N)N
C1389	HIA	HIA-	24	c1ccc(cc1)C(C(=O)NC1C(=O)N2C(C(=O)O)C(C)(C)SC12)NC(=O)N1C(=O)NCC1
C1390	HIA	HIA-	24	c1(csc(n1)N)/C(=N/OC)/C(=O)NC1C(=O)N2C(=C(CSC12)CSc1nc(c(CC(=O)O)s1)C)C(=O)O
C1391	HIA	HIA-	24	CC1(C(C(C(OC1)OC1C(CC(C(C1O)OC1C(CCC(C(C)NC)O1)N)N)O)NC)O
C1392	HIA	HIA-	24	CCC1CCC(C(OC2C(CC(C(C2O)OC2C(C(C(C)(CO2)O)NC)O)N)O1)N
C1393	HIA	HIA-	24	c12c3cc(cc1c(=O)n(c(=O)c2cc(c3N)S(=O)(=O)O)NNC(=O)NN)S(=O)(=O)O
C1394	HIA	HIA-	24	C1(=C(C(C)C2C(C(=O)N12)C(C)O)SC1CCC(C(=O)N(C)C)N1)C(=O)O
C1395	HIA	HIA-	24	c1ccc(cc1)C(C(=O)NC1C(=O)N2C(C(=O)O)C(C)(C)SC12)NC(=O)N1C(=O)N(CC1)S(=O)(=O)C
C1396	HIA	HIA-	24	C1=C(CN)OC(CC1N)OC1C(CC(C(C1O)OC1C(C(C(C)(CO1)O)NC)O)NCC)N
C1397	HIA	HIA-	24	c1cc(ccc1C(=N)N)OCCCCOC1ccc(cc1)C(=N)N
C1398	HIA	HIA-	24	C1(C(C(CO)(OC1CO)OC1C(C(C(C(COC2C(C(C(C(CO)O2)O)O)O)O1)O)O)O)O)O
C1399	HIA	HIA-	24	C(=O)(NC1C(C(C(CO)OC1O)O)O)N(C)N=O
C1400	HIA	HIA-	24	C1C(C(C(C(C1N)OC1C(C(C(C(CO)O1)O)N)O)O)OC1C(CC(C(CN)O1)O)N)N
C1401	HIA	HIA-	24	c1(csc(n1)N)/C(=N/OC(C(=O)O)(C)C)/C(=O)NC1C(=O)N(C1C)S(=O)(=O)O
C1402	HIA	HIA-	24	c1(csc(n1)N)/C(=N/OC)/C(=O)NC1C(=O)N2C(=C(CSC12)CSc1nc(=O)c(nm1C)O)C(=O)O
C1403	HIA	HIA-	24	C1(C(C(C(OC2C(C(CO)(O)OC2CO)O)OC1CO)O)O)O
C1404	HIA	HIA-	24	C1=C(C(C(C(C1NC1C(C(C(OC1C)OC1C(C(C(OC1CO)OC1C(C(C(O)OC1CO)O)O)O)O)O)O)O)O)O)CO
C1405	HIA	HIA-	24	c1c2c(c(c3c1c(=O)cc(C(=O)O)o3)CCC)n(c(cc2=O)C(=O)O)CC
C1406	HIA	HIA-	24	C1C(C(C(C(C1N)O)OC1C(C(C(CO)O1)OCC1C(C(C(C(CN)O1)O)O)N)O)OC1C(C(C(C(CN)O1)O)O)N)N
C1407	HIA	HIA-	24	C(#N)C(c1cccc1)OC1C(C(C(C(COC2C(C(C(C(CO)O2)O)O)O1)O)O)O
C1408	HIA	HIA-	24	c1(csc(n1)N)/C(=N/OC)/C(=O)NC1C(=O)N2C(=C(COC(=O)C)CSC12)C(=O)O
C1409	HIA	HIA-	24	c1cc(ccc1NC(=N)NC(=N)NCCCCNC(=N)NC(=N)Ne1ccc(cc1)Cl)Cl
C1410	HIA	HIA-	24	c1(c(c(c(c(c1I)NC(=O)C)I)NC(=O)C)I)C(=O)O
C1411	HIA	HIA-	24	C(=O)(CN(CC(=O)O)CCN(CC(=O)O)CC(=O)O)O
C1412	HIA	HIA-	24	C1(=C(CC2C(C(=O)N12)C(C)O)SCC/N=C/N)C(=O)O
C1413	HIA	HIA-	24	c1(c(c(c(c(c1I)N(C(=O)C)CC(CO)O)I)C(=O)NCC(CO)O)I)C(=O)NCC(CO)O
C1414	HIA	HIA-	24	c1c(c(c(c(c1I)NC(=O)COCCOCCOCC(=O)Ne1c(cc(c(c1I)C(=O)O)I)I)I)C(=O)O)I
C1415	HIA	HIA-	24	c1ccc(c(c1)C(=O)Ne1ccc(cc1)S(=O)(=O)Ne1nccs1)C(=O)O
C1416	HIA	HIA-	24	c1cc(ccc1NC(=O)CCC(=O)O)S(=O)(=O)Ne1nccs1
C1417	HIA	HIA-	24	C1(=O)CC2N1C(C(=O)O)C(C)(C)S2(=O)=O
C1418	HIA	HIA-	24	c1c(csc1)C(C(=O)NC1C(=O)N2C(C(=O)O)C(C)(C)SC12)C(=O)O
C1419	HIA	HIA-	24	C(#N)SCC(=O)NC1(C(=O)N2C(=C(CSC12)CSc1nmm1C)C(=O)O)OC
C1420	HIA	HIA-	24	C(=O)(C)NCCCS(=O)(=O)O
C1421	HIA	HIA-	24	c1ccc(cc1)CCC(C(=O)O)NC1C(=O)N2C(C(=O)O)CCCN2CCC1
C1422	HIA	HIA-	24	C(=O)(C1CC(CCC)CN1C)NC(C(C)O)C1C(C(C(C(O1)SC)O)O)O
C1423	HIA	HIA-	24	C(#C)c1cn(c(=O)[nH]c1=O)C1C(C(C(CO)O1)O)O)C
C1424	HIA	HIA+	24	c1(en2c(nc1=N)OC1C(C(CO)OC21)O)F



C1425	HIA	HIA+	24	c1cc2c(c(c1)OCC(CNC(C)(C)C)O)CC(C(C2)O)O
C1426	HIA	HIA+	24	c1c(c(ccc1S(=O)(=O)N)OC)C(=O)NCC1CCN(CC)C1
C1427	HIA	HIA+	24	c1(csc(n1)N=C(N)N)CSCC/C(=N/S(=O)(=O)N)/N
C1428	HIA	HIA+	24	c1c(cc(cc1O)O)C(CNC(C)C)O
C1429	HIA	HIA+	24	C=CC12CCC(CC1(CCC1C2CCC2(C)C(C3=CC(=O)OC3)CCC12O)O)OC1CC(C(C(C)O1)O)OC
C1430	HIA	HIA+	24	c1cc(c(cc1C(C1CCCN1)O)O)O
C1431	HIA	HIA+	24	c1cc(ccc1CC(=O)N)OCC(CNC(C)C)O
C1432	HIA	HIA+	24	c1ccc2c(c1)OCC(CNC(=N)N)O2
C1433	HIA	HIA+	24	C(=N)(N)NC(=N)N(C)C
C1434	HIA	HIA+	24	C(=O)(C(CCCN)(C(F)F)N)O
C1435	HIA	HIA+	24	c1ccc(c(c1)c1ccc(cc1)CN(C(=O)CCCC)C(C(=O)O)C(C)C)c1[nH]nnn1
C1436	HIA	HIA+	24	c12c(c(nc(n1)N(CCO)CCO)N1CCCCC1)nc(nc2N1CCCCC1)N(CCO)CCO
C1437	HIA	HIA+	24	c1cc2c(c(c1)O)C(=C1C(=O)C3(C(=O)C(=C(C(C3C(C1C2(C)O)O)N(C)C)O)C(=O)N)O)O
C1438	HIA	HIA+	24	c1ccc(cc1)CCC(C(=O)OCC)NC1C(=O)N2C(C(=O)O)CCCN2CCC1
C1439	HIA	HIA+	24	c1cc(ccc1CC(C)NC(Cc1cc(cc1)O)O)O
C1440	HIA	HIA+	24	c1cc(c2c3e1CC1C4(CCC(=O)C(C34CCN1C)O2)O)OC
C1441	HIA	HIA+	24	c1cc(C(CNC(C)(C)C)O)nc(c1O)CO
C1442	HIA	HIA+	24	c1ccc(cc1)CCC(C(=O)OCC)NC(C(=O)N1C(C(=O)O)CC2CCCC12)C
C1443	HIA	HIA+	24	c12c(cccc1)snc2N1CCN(CCc2cc3c(cc2Cl)NC(=O)C3)CC1
C1444	HIA	HIA+	24	c1cc(CNc2cc(cc(c2C(=O)O)S(=O)(=O)N)Cl)oc1
C1445	HIA	HIA+	24	c1ccnc(c1)NS(=O)(=O)c1ccc(cc1)/N=N/c1cc(c(cc1)O)C(=O)O
C1446	HIA	HIA+	24	c1c(cc(cc1O)O)C(CNC(C)C)C)O
C1447	HIA	HIA+	24	c1ccc2c(c1)C(=O)NC2(c1ccc(c(c1)S(=O)(=O)N)Cl)O
C1448	HIA	HIA+	24	c12c(cc(cc1)OC)c(ccc2C(=S)N(CC(=O)O)C)C(F)(F)F
C1449	HIA	HIA+	24	c1c(c(cc2c1NCNS2(=O)=O)S(=O)(=O)N)C(F)(F)F
C1450	HIA	HIA+	24	c12c(ccc(c1)CS(=O)(=O)NC)[nH]cc2CCN(C)C
C1451	HIA	HIA+	24	c1cc(c(c2c1N=C1NC(=O)CN1C2)Cl)Cl
C1452	HIA	HIA+	24	c1cc(c(c(c1CNNC(=O)C(CO)N)O)O)O
C1453	HIA	HIA+	24	c1c(c(c(cc1Br)Br)N)CN(C1CCCCC1)C
C1454	HIA	HIA+	24	c1cc(c2c(c1)C1CCOC(CC(=O)O)(CC(=O)O)C1N2)CC
C1455	HIA	HIA+	24	c12c(nc(nc1)N)n(en2)CCC(COC(=O)C)COC(=O)C
C1456	HIA	HIA+	24	c1ccc(cc1)CNNC(=O)c1cc(C)on1
C1457	HIA	HIA+	24	c1ccc2c(c1)Cc1cccc1N1C2CN(CC1)C
C1458	HIA	HIA+	24	c1c(c(cc(c1OC(=O)C)C)OCCN(C)C)C(C)C
C1459	HIA	HIA+	24	c1ccc2c(c1)n(c(=O)[nH]2)C1CCN(CCC(c2ccc(cc2)F)c2ccc(cc2)F)CC1
C1460	HIA	HIA+	24	c1cc(c(c(c1)C)NC(=O)NCCCNC(C)C)C
C1461	HIA	HIA+	24	c1(csc(n1)N)/C(=N/OC)/C(=O)NC1C(=O)N2C(=CCSC12)C(=O)O
C1462	HIA	HIA+	24	C1(=O)C(CON1)N
C1463	HIA	HIA+	24	c12c(cccc1)oc(c2C(=O)c1cc(c(c1)Br)O)Br)CC
C1464	HIA	HIA+	24	c1ccc2c(c1)C(=Nc1cccc1S2)N1CCN(CC1)CCOCCO
C1465	HIA	HIA+	24	c12c(ccc(c1)CS(=O)(=O)N1CCCCC1)[nH]cc2CCN(C)C
C1466	HIA	HIA+	24	C(=C\1/C(C(=O)O)N2C(=O)CC2O1)\CO
C1467	HIA	HIA+	24	C(CS(=O)(=O)O)S
C1468	HIA	HIA+	24	C1=C(C(=O)OCC)CC(C(C1OC(CC)CC)NC(=O)C)N
C1469	HIA	HIA+	24	c1ccc(cc1)C1(C(=O)NCNC1=O)CC
C1470	HIA	HIA+	24	C1=CC2CC3C4C=CC(C5C4(CCN3CC)C2C(=C1O)O5)O

C1471	HIA	HIA+	24	<chem>c12c(cc(cc1)OC(F)F)nc([nH]2)S(=O)Cc1c(c(ccn1)OC)OC</chem>
C1472	HIA	HIA+	24	<chem>c1ccc(cc1)C1(CCC1)C(CC(C)C)N(C)C)Cl</chem>
C1473	HIA	HIA+	24	<chem>c1ccc(cc1)C(c1ccc(cc1)O)C)CCN(C(C)C)C(C)C</chem>
C1474	HIA	HIA+	24	<chem>c1cc(c(c(c1)Cl)/C=N/NC(=N)N)Cl</chem>
C1475	HIA	HIA+	24	<chem>c12c(c(ccc1)C(F)(F)F)nc(cc2C(C1CCCCN1)O)C(F)(F)F</chem>
C1476	HIA	HIA+	24	<chem>c1ccc(c(c1)N1CCN(CCCNc2cc(=O)n(c(=O)n2C)C)CC1)OC</chem>
C1477	HIA	HIA+	24	<chem>c1cc(ccc1C(=O)C)S(=O)(=O)/N=C(/NC1CCCCC1)O</chem>
C1478	HIA	HIA+	24	<chem>c12c([nH]nc1)nc[nH]c2=O</chem>
C1479	HIA	HIA+	24	<chem>c12c3c(cccc3COC(CNCCO)c3ccccc3OC)O[nH]c1cccc2</chem>
C1480	HIA	HIA+	24	<chem>c1ccnc(c1)N(c1ccc(cc1)Cl)CCN(C)C</chem>
C1481	HIA	HIA+	24	<chem>c1ccc(c(c1)C1=NCC(=O)Nc2c1cc(cc2)[N+](=O)[O-])Cl</chem>
C1482	HIA	HIA+	24	<chem>c1cc(ccc1c1ccc(/C=N/N2C(=O)NC(=O)C2)o1)[N+](=O)[O-]</chem>
C1483	HIA	HIA+	24	<chem>c1cc(ccc1C(=O)c1c(C)[nH]c(=O)[nH]1)SC</chem>
C1484	HIA	HIA+	24	<chem>c1cc(c(c(c1)Cl)c1c(c(C)on1)C(=O)NC1C(=O)N2C(C(=O)O)C(C)(C)SC12)F</chem>
C1485	HIA	HIA+	24	<chem>c1ccc(cc1)CCCN1CCN(C(c2ccc(cc2)F)c2ccc(cc2)F)CC1</chem>
C1486	HIA	HIA+	24	<chem>c1ccc(cc1)C(CCNC)Oc1ccc(cc1)C(F)(F)F</chem>
C1487	HIA	HIA+	24	<chem>C(=N)(N)NCC1COC2(CCCCC2)O1</chem>
C1488	HIA	HIA+	24	<chem>c1c(ccnc1)C(=O)NN</chem>
C1489	HIA	HIA+	24	<chem>c1c(c(ccc1N)O)C(=O)O</chem>
C1490	HIA	HIA+	24	<chem>c1ccc(cc1)C(c1ccccc1)(C(=O)CC)CC(C)N(C)C</chem>
C1491	HIA	HIA+	24	<chem>c1cc(cc(c1)OC)CC(C)N</chem>
C1492	HIA	HIA+	24	<chem>c1ccc(cc1)C(C(=O)OC)C1CCCCN1</chem>
C1493	HIA	HIA+	24	<chem>c1ccc(cc1)C(c1ccccc1)S(=O)CC(=O)N</chem>
C1494	HIA	HIA+	24	<chem>c12c(ccc(c1)CCC(=O)C)cc(cc2)OC</chem>
C1495	HIA	HIA+	24	<chem>c12c(cc(cc1)OC)nc([nH]2)S(=O)Cc1c(c(cn1)C)OC)C</chem>
C1496	HIA	HIA+	24	<chem>c1c(c(cc2c1CCC(CNC(C)C)N2)[N+](=O)[O-])CO</chem>
C1497	HIA	HIA+	24	<chem>c12c(CC(CC1)NCCC)sc(n2)N</chem>
C1498	HIA	HIA+	24	<chem>c12c(ccc(c1)OC)nc2c(C1CC2CCN1CC2C=C)O</chem>
C1499	HIA	HIA+	24	<chem>c1c(c(cc2c1nc1c(nc(=O)[nH]c1=O)n2CC(C(C(CO)O)O)O)C)C</chem>
C1500	HIA	HIA+	24	<chem>C(#CC(C)C)C/C=C/CN(Cc1c2c(ccc1)cccc2)C</chem>
C1501	HIA	HIA+	24	<chem>c1ccc(c(c1)CN1Cc2csc2CC1)Cl</chem>
C1502	HIA	HIA+	24	<chem>c1ccc2c(c1)N(c1ccccc1S2)CC(C)CN(C)C</chem>
C1503	HIA	HIA+	24	<chem>c1ccc2c(c1)CCc1ccccc1N2CC(C)CN(C)C</chem>
C1504	HIA	HIA+	24	<chem>C(=C\C(C(=C\CO)\C)/C=C(/C=C/C1=C(C)CCCC1(C)C)\C</chem>
C1505	HIA	HIA+	24	<chem>c1c(c(ccc1OCC(F)(F)F)OCC(F)(F)F)C(=O)NCC1CCCCN1</chem>
C1506	HIA	HIA+	24	<chem>c1ccc(c(c1)C(=O)O)OC(=O)C</chem>
C1507	HIA	HIA+	24	<chem>c1cc(ccc1C(CCCN(CC)CCCCCCC)O)NS(=O)(=O)C</chem>
C1508	HIA	HIA+	24	<chem>C1=CC2(C(=CC1=O)C(C)CC1C3CCC(C(=O)CO)(C3(C)CC(C21)O)O)C</chem>
C1509	HIA	HIA+	24	<chem>c1cc(ccc1C(CP(=O)(OC)OC)P(=O)(OC)OC)Cl</chem>
C1510	HIA	HIA+	24	<chem>c1cc(c(cc1C(CNC(C)C)C)O)C(=O)O)O</chem>
C1511	HIA	HIA+	24	<chem>C(#N)c1cc(c2cnc2)c(C)[nH]c1=O</chem>
C1512	HIA	HIA+	24	<chem>c1ccc(cc1)CC(C(=O)O)NC(=O)C1CCC(CC1)C(C)C</chem>
C1513	HIA	HIA+	24	<chem>c1ccnc(c1)C1=NCC(=O)Nc2c1cc(cc2)Br</chem>
C1514	HIA	HIA+	24	<chem>c1c(c(ccc1NC(=O)CCC)OCC(CNC(C)C)O)C(=O)C</chem>
C1515	HIA	HIA+	24	<chem>c1cc(ccc1NC(=O)C)O</chem>
C1516	HIA	HIA+	24	<chem>c1cc(ccc1NC(=N)NC(=N)NC(C)C)Cl</chem>

C1517	HIA	HIA+	24	c12c(cccc1)[nH]cc2C(=O)OC1CC2CC3C(=O)CN2C(C3)C1
C1518	HIA	HIA+	24	c1cc(c(cc1C(NC(C)C)O)O)O
C1519	HIA	HIA+	24	c12c(cccc1)nc([nH]2)S(=O)Cc1cc(c(en1)C)OCC(F)(F)F
C1520	HIA	HIA+	24	c1ccc(cc1)C(C(C)NCCC(=O)c1cccc(c1)OC)O
C1521	HIA	HIA+	24	c1ccc(cc1)Oc1c(cc(cc1S(=O)(=O)N)C(=O)O)N1CCCC1
C1522	HIA	HIA+	24	c1cc(ccc1N)S(=O)(=O)Nc1nnc(C)s1
C1523	HIA	HIA+	24	c1ccc(c(c1)c1c2cc(ccc2n2c(en1)[nH]nc2C)Cl)Cl
C1524	HIA	HIA+	24	c1cn(c(=O)nc1N)C1CCC(CO)O1
C1525	HIA	HIA+	24	C1(=NC(=O)N(CC1)C1CSC(CO)O1)N
C1526	HIA	HIA+	24	c12c(cccc1)n(Cc1ccccc1)nc2OCCCN(C)C
C1527	HIA	HIA+	24	c1cc(ccc1C(=O)C(C)NC(C)(C)C)Cl
C1528	HIA	HIA+	24	C(#N)N/C(=N/C)/NCCSCc1c(C)[nH]en1
C1529	HIA	HIA+	24	C(=O)(C1CC(CCC)CN1C)NC(C1C(C(C(C(O1)SC)O)O)O)C(C)Cl
C1530	HIA	HIA+	24	c1cc(/C=C/C(=O)O)nc(c1)/C(=C/CN1CCCC1)/c1ccc(cc1)C
C1531	HIA	HIA+	24	C(=S)(N(CC)CC)SSC(=S)N(CC)CC
C1532	HIA	HIA+	24	c1c(c(cc(c1Cl)N)OC)C(=O)NCCN(CC)CC
C1533	HIA	HIA+	24	C(=C\C1C(C(=O)CC1O)CCCCCCC(=O)OC)/CC(C)(CCCC)O
C1534	HIA	HIA+	24	c1ccc2c(c1)N(c1cc(ccc1S2)NC(=O)OCC)C(=O)CCN1CCOCC1
C1535	HIA	HIA+	24	c1(c(nc(C)nc1Cl)OC)NC1=NCCN1
C1536	HIA	HIA+	24	c1cc(cc(c1)[N+](=O)[O-])C1C(=C(C)NC(=C1C(=O)OCC)C)C(=O)OC
C1537	HIA	HIA+	24	c1c2c(nc(c1F)N1CC3C(C3N)C1)n(c1ccc(cc1F)F)cc(c2=O)C(=O)O
C1538	HIA	HIA+	24	c1cc(c2c3e1CC1C4CCC(C(C34CCN1C)O2)O)OC
C1539	HIA	HIA+	24	c1c(c(ccc1S(=O)(=O)CC)OC)C(=O)NCC1CCCN1CC
C1540	HIA	HIA+	24	C1(c2cc(ccc2N(C1=O)C(=O)N)Cl)C(=O)c1ccs1
C1541	HIA	HIA+	24	c1cc(ccc1C(c1ccc(cc1)F)N1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)F
C1542	HIA	HIA+	24	C1C2CC3CC1CC(C2)(C3)N
C1543	HIA	HIA+	24	c1ccc(cc1)CC(C)N
C1544	HIA	HIA+	24	c1ccc2c(c1)C(=C1CCN(CC1)C)c1c(cccn1)CC2
C1545	HIA	HIA+	24	c1cc(ccc1CCOCC1CC1)OCC(CNC(C)C)O
C1546	HIA	HIA+	24	c1cc(ccc1COCCOC(C)C)OCC(CNC(C)C)O
C1547	HIA	HIA+	24	c1c2c(ccc1Cl)oc(=O)[nH]2
C1548	HIA	HIA+	24	c1cc(ccc1N)S(=O)(=O)c1ccc(cc1)O
C1549	HIA	HIA+	24	C1=CC2(C(=CC1=O)CCC1C3CC(C)C(C(=O)CO)(C3(C)CC(C21F)O)O)C
C1550	HIA	HIA+	24	c1cc(ccc1/C(=C(\c1ccc(cc1)O)/CC)/CC)O
C1551	HIA	HIA+	24	c1cc(c(cc1c1ccc(cc1F)F)C(=O)O)O
C1552	HIA	HIA+	24	c1cc(ccc1N(C(=O)C(Cl)Cl)C)O
C1553	HIA	HIA+	24	c1cc(c(c(c1C(=O)C(=O)CC)Cl)Cl)OCC(=O)O
C1554	HIA	HIA+	24	c1ccc(cc1)C(COC(=O)N)COC(=O)N
C1555	HIA	HIA+	24	C1(C(=O)N(c2ccccc2)N(c2ccccc2)C1=O)CC=C(C)C
C1556	HIA	HIA+	24	c1c(c(ccc1NC(=O)C(C)C)[N+](=O)[O-])C(F)(F)F
C1557	HIA	HIA+	24	c1cc(ccc1/C(=N/OCCN)/CCCCOC)C(F)(F)F
C1558	HIA	HIA+	24	C1=CC2C3CCC(C(=O)C)(C3(C)CCC2C2(C1=CC(=O)CC2)C)OC(=O)CCCC
C1559	HIA	HIA+	24	C12C(C(CO1)O)[N+](=O)[O-]OCC2O[N+](=O)[O-]
C1560	HIA	HIA+	24	c1ccc2c(c1)C(=C1CCN(CC1)C)c1ccsc1C(=O)C2
C1561	HIA	HIA+	24	c1cc2c(C(=C3CCN(C(=O)OCC)CC3)c3ccc(cc3CC2)Cl)nc1
C1562	HIA	HIA+	24	c1ccc(c(c1)C(=O)O)Nc1ccccc(c1)C

C1563	HIA	HIA+	24	c1ccc2c(c1)C(=C(C(=O)Nc1ncc(C)s1)N(C)S2(=O)=O)O
C1564	HIA	HIA+	24	c1cc(c2c3c1CC1C4C=CC(C(C34CCN1C)O2)O)O
C1565	HIA	HIA+	24	c1cc(C)nc2c1C(=O)C(C(=O)O)CN2CC
C1566	HIA	HIA+	24	c1ccc(c(c1)C1C(=C(C)NC(=C1C(=O)OCC(C)C)C)C(=O)OC)[N+](=O)[O-]
C1567	HIA	HIA+	24	c12c(cc(c(c1)OC)OC)c(Cc1ccc(c(c1)OC)OC)ncc2
C1568	HIA	HIA+	24	c1ccc(cc1)/N=N/c1ccc(nc1N)N
C1569	HIA	HIA+	24	c1ccc(cc1)C1(c2ccccc2)C(=O)NNC1=O
C1570	HIA	HIA+	24	c1c(cc(CCC)nc1)C(=S)N
C1571	HIA	HIA+	24	C=CCC1(C(=C)NC(=NC1=O)O)C(C)CCC
C1572	HIA	HIA+	24	c12c(cccc1)nc([nH]2)S(=O)Cc1c(c(ccn1)OCCCCOC)C
C1573	HIA	HIA+	24	c12c(cc(cc1)OC(F)(F)F)sc(n2)N
C1574	HIA	HIA+	24	c12c(c(c(c(c1n(cc(c2=O)C(=O)O)C1CC1)F)N1CC(C)NC(C)C1)F)N
C1575	HIA	HIA+	24	c1cc(ccc1N)S(=O)(=O)Nc1cc(C)nc(C)n1
C1576	HIA	HIA+	24	c1cc(ccc1/C=C\1/c2ccc(cc2C(=C1C)CC(=O)O)F)S(=O)C
C1577	HIA	HIA+	24	C1(C(=O)OC(CC)C2(C)C(C(C(=O)C(C)CC(C)(C(C(C1=O)C)OC1C(C(CC(C)O1)N(C)C)O)OC)C)N(C(=O)O2)CCCCn1cc(c2ccnc2)nc1)C
C1578	HIA	HIA+	24	c12c(cccc1)nc(c1csen1)[nH]2
C1579	HIA	HIA+	24	c1c(c(C(=CCCN2CCCC(C(=O)O)C2)c2c(ccs2)C)sc1)C
C1580	HIA	HIA+	24	C#CC1(CCC2C3C(C4=C(CC(=O)CC4)CC3C)CCCC12C)O
C1581	HIA	HIA+	24	c1ccc(cc1)CC1=NCCN1
C1582	HIA	HIA+	24	C1=CC2C(=CC1=O)CCC1C3CC4C(C(=O)CO)(C3(C)CC(C21F)O)OC(C)(C)O4
C1583	HIA	HIA+	24	C1=C2CC(CCC2(C)C2CCC3(C)C(CCC3C(C)CCCC(C)C)C2C1)O
C1584	HIA	HIA+	24	c1cc(c2c3c1CC1C4(CCC(=O)C(C34CCN1CC=C)O2)O)O
C1585	HIA	HIA+	24	c12c(cc(c(c1)OC)OC)nc(nc2N)N1CCN(C(=O)C2CCCO2)CC1
C1586	HIA	HIA+	24	c12c(c(ccc1)C1C(=C(C)NC(=C1C(=O)OC(C)C)C)C(=O)OC)non2
C1587	HIA	HIA+	24	c1ccc(c(c1)CC=C)OCC(CNC(C)C)O
C1588	HIA	HIA+	24	c1c(ccnc1)c1cc(c(=O)[nH]c1)N
C1589	HIA	HIA+	24	c1ccc(cc1)C(C(=O)OC1CC2C3C(C(C1)N2C)O3)CO
C1590	HIA	HIA+	24	c1c(cc(c2c1OC(C)(C)C1CCC(=CC21)C)O)CCCCC
C1591	HIA	HIA+	24	c1ccc(cc1)C(C(=O)OC1CC2CCC(C1)N2C)CO
C1592	HIA	HIA+	24	c1ccc2c(c1)C(=Nc1cc(ccc1N2)Cl)N1CCN(CC1)C
C1593	HIA	HIA+	24	c1cc(c(c(c1)Cl)Cl)C1C(=C(C)NC(=C1C(=O)OCC)C)C(=O)OC
C1594	HIA	HIA+	24	c1cc(cc(c1C(Cn1cncn1)(Cn1cncn1)O)F)F
C1595	HIA	HIA+	24	c1cc(cnc1)C(=O)O
C1596	HIA	HIA+	24	c1c(C(=O)O)ncc(C)[n+][O-]
C1597	HIA	HIA+	24	c1ccc2c(c1)C(=CCCN(C)C)c1ccccc1CC2
C1598	HIA	HIA+	24	C1(=NC(=NC(=O)C1(CC)CCC(C)C)O)O
C1599	HIA	HIA+	24	c1ccc2c(c1)N=C(c1cc(ccc1O2)Cl)N1CCNCC1
C1600	HIA	HIA+	24	c1cc(ccc1C(CCC(=O)O)N)Cl
C1601	HIA	HIA+	24	c1cn(C(=O)OCC)c(=S)n1C
C1602	HIA	HIA+	24	c1cc2c(c(c1)OCC(CNC(C)(C)C)O)CCC(=O)N2
C1603	HIA	HIA+	24	C1=CCC(=CC1)C(C(=O)NC1C(=O)N2C(=C(C)CSC12)C(=O)O)N
C1604	HIA	HIA+	24	c1cc(ccc1S(=O)(=O)NC(=O)NCCC)Cl
C1605	HIA	HIA+	24	c1(c(CCCl)sen1)C
C1606	HIA	HIA+	24	c1ccc2c(c1)CCc1ccc(cc1N2CCCN(C)C)Cl
C1607	HIA	HIA+	24	c1cc(c(c(c1)Cl)N=C1NCCN1)Cl
C1608	HIA	HIA+	24	c1ccc2c(c1)/C(=C\CCN1CCN(CC1)CCO)/c1cc(ccc1S2)Cl

C1609	HIA	HIA+	24	c1ccc(cc1)C(=O)C(C)N(CC)CC
C1610	HIA	HIA+	24	c1ccc(cc1)C(c1ccnc1)(C(=O)N)CCN(C(C)C)C(C)C
C1611	HIA	HIA+	24	c1ccc2c(c1)n(c(=O)[nH]2)CCCN1CCC(CC1)Nn1c2ccc(cc2[nH]c1=O)C1
C1612	HIA	HIA+	24	c1ccc2e(c1)/C(=C/CCN(C)C)/c1ccccc1SC2
C1613	HIA	HIA+	24	C1=C2CCC3C4CCC(C(=O)COC(=O)C)(C4(C)CC(C3(C2(C)CCC1=O)F)O)O
C1614	HIA	HIA+	24	c1c2c(ccc1F)n1c(c(C(=O)OCC)nc1)CN(C2=O)C
C1615	HIA	HIA+	24	c1cc(cc(c1F)c1ccc(cc1)C(C(=O)O)C
C1616	HIA	HIA+	24	c1cc(e2c3c1CN(CCC13C=CC(CC1O2)O)C)OC
C1617	HIA	HIA+	24	c1ccc(cc1)S(=O)(=O)Nc1ncc(en1)OCCOC
C1618	HIA	HIA+	24	C1=C(CCCC1)C1(C(=O)N=C(N(C1=O)C)O)C
C1619	HIA	HIA+	24	c1ccc(cc1)C(=O)c1cccc(c1)C(C(=O)O)C
C1620	HIA	HIA+	24	c1ccc(cc1)C(=O)c1ccc2C(C(=O)O)CCn12
C1621	HIA	HIA+	24	c1ccc(cc1)C1CN2C(=N1)SCC2
C1622	HIA	HIA+	24	c1ccc(c(c1)C1=NC(C(=O)Nc2c1cc(cc2)Cl)O)Cl
C1623	HIA	HIA+	24	c1cn(c(=S)[nH]1)C
C1624	HIA	HIA+	24	c1c([N+](=O)[O-])n(c(C)n1)CCO
C1625	HIA	HIA+	24	c1ccc(cc1)C1=NCC(=O)Nc2c1cc(cc2)[N+](=O)[O-]
C1626	HIA	HIA+	24	c1cc([N+](=O)[O-])oc1/C=N/N1C(=O)NC(=O)C1
C1627	HIA	HIA+	24	c1(csc(CN(C)C)n1)CSCCN/C(=C/[N+](=O)[O-])/NC
C1628	HIA	HIA+	24	c1cc(cc2c1CC1C(C)C2(C)CCN1CC=C(C)C)O
C1629	HIA	HIA+	24	c12c(nen1C)n(c(=O)n(c2=O)CCCC(=O)C)C
C1630	HIA	HIA+	24	C(=O)(C(C)NC(C(=O)OCC)CCC)N1C(C(=O)O)CC2CCCCC12
C1631	HIA	HIA+	24	c1ccc(cc1)C(C(C)N)O
C1632	HIA	HIA+	24	c1cc(ccc1C(CNC(C)C)O)NC(=O)C
C1633	HIA	HIA+	24	c1ccc2c(c1)N(c1ccccc1S2)CC(C)N(C)C
C1634	HIA	HIA+	24	c1ccc(cc1)CCC(=O)c1ccccc1OCC(CNCCC)O
C1635	HIA	HIA+	24	c12c(cccc1)c(ccc2)C(C(C)NC(C)C)O
C1636	HIA	HIA+	24	c1ccc2c(c1)C=Cc1ccccc1C2CCCNC
C1637	HIA	HIA+	24	c1cc(ccc1CCNC(C)C(c1ccc(cc1)O)O)O
C1638	HIA	HIA+	24	c1cc(cc(c1)OCC(CNC(C)C)O)NS(=O)(=O)C
C1639	HIA	HIA+	24	c1cc(ccc1N)S(=O)(=O)Nc1c(c(C)ns1)C
C1640	HIA	HIA+	24	c12c(cccc1)nc1c(c2N)CCCC1
C1641	HIA	HIA+	24	c1ccc(cc1)C1=NC(C(=O)N(c2c1cc(cc2)Cl)C)O
C1642	HIA	HIA+	24	c1(c(nsn1)OCC(CNC(C)C)C)O)N1CCOCC1
C1643	HIA	HIA+	24	c12c(cccc1)n(cc2C(=O)OC1CC2CCC(C1)N2C)C
C1644	HIA	HIA+	24	c1cc(ccc1C(C1(CCCC1)O)CN(C)C)OC
C1645	HIA	HIA+	24	c1cc(ccc1c1c(CC(=O)N(CCC)CCC)n2c(ccc(c2)C)n1)C
C1646	HIA	HIA+	24	c1ccc(cc1)Oc1c(cc(cc1S(=O)(=O)N)C(=O)O)NCCCC
C1647	HIA	HIA+	24	c1cc(ccc1OC(C(=O)OCC)(C)C)Cl
C1648	HIA	HIA+	24	c1c2c(c(c(c1F)N1CC(C)NCC1)OC)n(cc(c2=O)C(=O)O)C1CC1
C1649	HIA	HIA+	24	c1cc(ccc1CCOC)OCC(CNC(C)C)O
C1650	HIA	HIA+	24	c1c[n+](c(nc1N1CCCC1)N)[O-]
C1651	HIA	HIA+	24	C1=C2CCC3C4CCC(C(=O)C)C4(C)CCC3C2(C)CCC1=O
C1652	HIA	HIA+	24	c1cc(cc(c1)Nc1ccncc1S(=O)(=O)NC(=O)NC(C)C)C
C1653	HIA	HIA+	24	c1c(C)nc2n(c1N(CC)CC)ncn2
C1654	HIA	HIA+	24	c1cc(cnc1)C1CCC(=O)N1C

C1655	HIA	HIA+	24	C(#N)C(c1cc(c(c1)OC)OC)OC)(CCCN(CCc1ccc(c(c1)OC)OC)C)C(C)C
C1656	HIA	HIA+	24	c1ccc(ccc1C)S(=O)(=O)NC(=O)NN1CC2CCCC2C1
C1657	HIA	HIA+	24	c1ccc(cc1)C1=NC(C(=O)Nc2c1cc(cc2)Cl)O
C1658	HIA	HIA+	24	c12c(cc(cc1)F)onc2C1CCN(CCc2c(C)nc3CCCCn3c2=O)CC1
C1659	HIA	HIA+	24	c1ccc(cc1)n1c(=O)cc(C)n1C
C1660	HIA	HIA+	24	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCN(C)C
C1661	HIA	HIA+	24	c1c(c(cc(c1Cl)N)OC)C(=O)NC1CCN(CCCOe2ccc(cc2)F)CC1OC
C1662	HIA	HIA+	24	C1=C2C(=CC3C4CCC(C(=O)C)(C4(C)CCC3C2(C)C2CC2C1=O)OC(=O)C)Cl
C1663	HIA	HIA+	24	c1ccc(ccc1C)S(=O)(=O)NC(=O)NC1C2CCC(C)(C2(C)C)C1O
C1664	HIA	HIA+	24	c1ccc(ccc1CCNC(=O)c1ccc(ccc1OC)Cl)S(=O)(=O)NC(=O)NC1CCCCC1
C1665	HIA	HIA+	24	c1ccc2c(c1)C(=O)c1ccc(ccc1OC2)CC(=O)O
C1666	HIA	HIA+	24	c1cc(c(c(c1)Cl)Cl)c1c(nc(nn1)N)N
C1667	HIA	HIA+	24	c1ccc(c(c(c1)C)NC(=O)CN(CC)CC)C
C1668	HIA	HIA+	24	c1ccc(c(c(c1)C)OCC(C)N)C
C1669	HIA	HIA+	24	c1ccc(cc1)C1c2ccccc2CN(CCO1)C
C1670	HIA	HIA+	24	c1ccc(cc1)c1c(c2ccccc2)oc(CCC(=O)O)n1
C1671	HIA	HIA+	24	C(#N)c1c(nc(C)[nH]c1=O)NCc1ccnc1
C1672	HIA	HIA+	24	c1cc(cc(c1)OC(=O)N(CC)C)C(C)N(C)C
C1673	HIA	HIA+	24	c1cc(c2c(c1)NC(=O)C2)CC(NCCC)NCCC
C1674	HIA	HIA+	24	c1c(c(cc(c1OC)OC)S(=O)C)C
C1675	HIA	HIA+	24	C(=O)(C(CCC)CCC)O
C1676	HIA	HIA+	24	c1cc(ncc1Cl)N1C(=O)c2c(C1OC(=O)N1CCN(CC1)C)ncn2
C1677	HIA	HIA+	24	c12c(nen1C)n(c(=O)n(c2=O)C)C
C1678	HIA	HIA+	24	c1ccc(cc1)C1=[N+](CC(=Nc2c1cc(cc2)Cl)NC)[O-]
C1679	HIA	HIA+	24	c1ccc(ccc1C1CC1(C1)Cl)OC(C(=O)O)(C)C
C1680	HIA	HIA+	24	c1ccc(cc1)C1=NCC(=O)N(c2c1cc(cc2)Cl)C
C1681	HIA	HIA+	24	c1ccc2c(c1)C(=O)OC12c2ccc(cc2O)c2cc(ccc12)O)O
C1682	HIA	HIA+	24	c1c2c(c(c(c1F)N1CC(C)NCC1)F)n(cc(c2=O)C(=O)O)CC
C1683	HIA	HIA+	24	c1ccc(cc(c1C(Cn1cnc1)OCc1ccc(cc1Cl)Cl)Cl)Cl
C1684	HIA	HIA+	24	c1ccc(cc1)C(c1cccen1)CCN(C)C
C1685	HIA	HIA+	24	C1=CC2(C(=CC1=O)CCC1C3CCC(C(=O)CO)(C3(C)CC(C21)O)O)C
C1686	HIA	HIA+	24	c1c2c(ccc1SC)ncn(/C=C/C(=O)O)c2=O
C1687	HIA	HIA+	24	c1ccc2c(c1)N(c1ccc(cc1S(=O)(=O)N2C)Cl)CCCCCCC(=O)O
C1688	HIA	HIA+	24	c1ccc(c(c1)OCC)OCC1COCCN1
C1689	HIA	HIA+	24	c1ccc(cc1)NC(=O)C
C1690	HIA	HIA+	24	c1(NC(=O)C)nnc(s1)S(=O)(=O)N
C1691	HIA	HIA+	24	C=C1/C(=C\C=C\2/CCCC3(C)C2CCC3C(C)CCCC(C)C)/CC(CC1O)O
C1692	HIA	HIA+	24	c1ccc(cc1)n1c(=N)c(c(C)n1C)N(C)C
C1693	HIA	HIA+	24	c1ccc(c(c1)OC)OCCNCC(c1ccc(cc1S(=O)(=O)N)C)O
C1694	HIA	HIA+	24	C(#N)C(c1cc(cc(c1)Cn1cnc1)C(C#N)(C)C)C
C1695	HIA	HIA+	24	c1cc(ccc1c1ccc(/C=N/N2C(=O)N(C(=O)C2)CCCCN2CCN(CC2)C)o1)Cl
C1696	HIA	HIA+	24	c1ccc(cc1)CC1NS(=O)(=O)c2cc(c(cc2N1)C(F)(F)F)S(=O)(=O)N
C1697	HIA	HIA+	24	c1ccc(c(c1)C(=O)O)c1ccc(cc1)NC(=O)C)OC(=O)C
C1698	HIA	HIA+	24	c1ccc(cc1)CN(c1cccen1)C(CN1CCCC1)COCC(C)C
C1699	HIA	HIA+	24	c1ccc(cc1)C(=O)NCCc1ccc(cc1)OC(C(=O)O)(C)C
C1700	HIA	HIA+	24	c1ccc(cc1)C(CCN1CCCCC1)(C1CC2C=CC1C2)O

C1701	HIA	HIA+	24	c1ccc(cc1)C1(C(=O)OCCCN(CC)CC)CC2CCC1C2
C1702	HIA	HIA+	24	c1ccc(cc1)C1=NC(C(=O)N(c2c1cc(cc2)Cl)C)OC(=O)N(C)C
C1703	HIA	HIA+	24	c1ccc2c(c1)C=Cc1cccc1N2C(=O)N
C1704	HIA	HIA+	24	C(=O)(NCCCl)N(CCCl)N=O
C1705	HIA	HIA+	24	C(C(Cl)(Cl)Cl)(O)O
C1706	HIA	HIA+	24	c12c(cc(cc1)Cl)ncce2N(CCCCN(CC)CC)C
C1707	HIA	HIA+	24	c1cc(ccc1OCC(CO)O)Cl
C1708	HIA	HIA+	24	C(#CCC(C)C(C#CC1C2C/C(=C\C0CC(=O)O)/CC2CC1O)O)CC
C1709	HIA	HIA+	24	C(#N)C1(c2ccc(c(c2)OC2CCCC2)OC)CCC(C(=O)O)CC1
C1710	HIA	HIA+	24	C(#N)c1ccc2c(c1)COC2(c1ccc(cc1)F)CCCN(C)C
C1711	HIA	HIA+	24	C1=C2CCC3C4CCC(C(=O)CO)C4(C)CC(C3C2(C)CCC1=O)O
C1712	HIA	HIA+	24	c1ccc2c(c1)ccc(=O)o2
C1713	HIA	HIA+	24	c1c2c(cc(c1Cl)S(=O)(=O)N)S(=O)(=O)NC(CN1CCCC1)N2
C1714	HIA	HIA+	24	c1cc(c2c3c1CC1C4C=CC(C(C34CCCN1C)O2)OC(=O)C)OC(=O)C
C1715	HIA	HIA+	24	C(=O)(C1(CCCCC1)C1CCCC1)OCCN(CC)CC
C1716	HIA	HIA+	24	c1cc(ccc1CCN(CCOc1ccc(cc1)NS(=O)(=O)C)C)NS(=O)(=O)C
C1717	HIA	HIA+	24	c12c(cc(c(c1)OC)OC)nc(nc2N)N1CCN(C(=O)C2COc3cccc3O2)CC1
C1718	HIA	HIA+	24	C#CC1(CCC2C3CCc4cc(ccc4C3CCC12C)O)O
C1719	HIA	HIA+	24	CCO
C1720	HIA	HIA+	24	C#CC1(CCC2C3CCC4=CC(CCC4C3CCC12C)OC(=O)C)OC(=O)C
C1721	HIA	HIA+	24	c1ccc(c(c1)CC(=O)O)Oc1ccc(cc1Cl)Cl
C1722	HIA	HIA+	24	C1=CC2(C)C3CCC4(C)C(C(=O)NC(C)(C)C)CCC4C3CCC2NC1=O
C1723	HIA	HIA+	24	c1(c[nH]c(=O)nc1N)F
C1724	HIA	HIA+	24	c1ccc2c(c1)/C(=C\CCN1CCN(CC1)CCO)/c1cc(ccc1S2)C(F)(F)F
C1725	HIA	HIA+	24	c12c(cccc1)n(c(c2c1ccc(cc1)F)/C=C/C(CC(CC(=O)O)O)O)C(C)C
C1726	HIA	HIA+	24	C(=C(C)C)CC/C(=C\1/C2CC(C3C4(C)CCC(C(C)C4CCC3(C)C2(C)CC1OC(=O)C)O)/C(=O)O
C1727	HIA	HIA+	24	c1cc(cc(c1C(C)S(=O)(=O)C)(Cn1cncn1)O)F)F
C1728	HIA	HIA+	24	c1cc(ccc1CCNC(=O)c1cnc(cn1)C)S(=O)(=O)NC(=O)NC1CCCCC1
C1729	HIA	HIA+	24	c12c(cccc1)n(C)nc2C(=O)NC1CC2CCCC(C1)N2C
C1730	HIA	HIA+	24	c1cc(cc(c1)Cl)C1(CCN(CCCC(=O)c2ccc(cc2)F)CC1)O
C1731	HIA	HIA+	24	c12c(cccc1)c(nnc2)NN
C1732	HIA	HIA+	24	c1ccc2c(c1)C(=O)N(c1ccc(cc1)C(C(=O)O)CC)C2
C1733	HIA	HIA+	24	c12c(ccc(c1)OC)n(cc2CC(=O)O)C(=O)c1cccc1
C1734	HIA	HIA+	24	c1ccc(c(c1)c1ccc(cc1)CN1C(=NC2(C1=O)CCCC2)CCCC)c1n[nH]nn1
C1735	HIA	HIA+	24	C1(C2C(C(CO2)O[N+](=O)[O-])OC1)O
C1736	HIA	HIA+	24	c1ccc2c(c1)C(=C(C(=O)Nc1cc(C)on1)C(C)S2(=O)=O)O
C1737	HIA	HIA+	24	c1ccc2c(c1)c(=O)n(c(=O)[nH]2)CCN1CCC(C(=O)c2ccc(cc2)F)CC1
C1738	HIA	HIA+	24	C(#N)c1ccc(cc1)C(c1ccc(C#N)cc1)n1cncn1
C1739	HIA	HIA+	24	C(=O)(C(CC)N1C(=O)CCC1)N
C1740	HIA	HIA+	24	c1cc2c(c(c1)OCC(CNC(C)(C)C)O)CCCC2=O
C1741	HIA	HIA+	24	C#CC1(CCC2C3CCC4=CC(=O)CCC4C3CCC12CC)O
C1742	HIA	HIA+	24	c12c3cccc1C1=CC(CN(C1C2c[nH]3)C)NC(=O)N(CC)CC
C1743	HIA	HIA+	24	c1ccc(c(c1)C1=NC(C(=O)N(c2c1cc(cc2)Cl)C)O)Cl
C1744	HIA	HIA+	24	c1ccnc(c1)NC(=O)C1=C(c2c(cc(s2)Cl)S(=O)(=O)N1C)O
C1745	HIA	HIA+	24	C#CC1(CCC2C3CCC4=CCCC4C3CCC12C)O
C1746	HIA	HIA+	24	c1ccc(c(c1)C(=O)O)Nc1c(ccc(c1Cl)C)Cl

C1747	HIA	HIA+	24	C1=C2C(=CC3C4CCC(C(=O)C)(C4(C)CCC3C2(C)CCC1=O)OC(=O)C)C
C1748	HIA	HIA+	24	c1ccc(cc1)OC1(CC)CCCCN(C1)C
C1749	HIA	HIA+	24	c1ccc(cc1)C1(C(=O)N(C(=O)C1)C)C
C1750	HIA	HIA+	24	c12e3cccc1C1=CC(C(=O)NC(CC)CO)CN(C1Cc2cn3C)C
C1751	HIA	HIA+	24	c1ccc(c1)C1=NCc2n(c3c1cc(cc3)Cl)c(nc2)CF
C1752	HIA	HIA+	24	c1ccc(c2c3c1CC1C4(CCC(C(C34CCN1CC1CCC1)O2)O)O)O
C1753	HIA	HIA+	24	c1ccc(nc1)C(=O)NCCO[N+](=O)[O-]
C1754	HIA	HIA+	24	c1ccc(nc1)C1CCCN1C
C1755	HIA	HIA+	24	C(#N)C1=C(C(=O)OC)C(c2cccc(c2)[N+](=O)[O-])C(=C(C)N1)C(=O)OC(C)C
C1756	HIA	HIA+	24	c12c(c(ccc1[N+](=O)[O-])O)nccc2
C1757	HIA	HIA+	24	C#CC1(CCC2C3CCC4=CC(=O)CCC4C3CCC12C)O
C1758	HIA	HIA+	24	C#CC1(CCC2C3CCC4=C/C(=N/O)/CCC4C3CCC12CC)OC(=O)C
C1759	HIA	HIA+	24	c1ccc2c(c1)C(=CCNC)c1cccc1CC2
C1760	HIA	HIA+	24	c1c2c3c(c1F)N1CCN(CC1)C)OCC(C)n3cc(c2=O)C(=O)O
C1761	HIA	HIA+	24	c12c(ccc1)n(c1c2C(=O)C(CC1)Cn1ccnc1)C
C1762	HIA	HIA+	24	c1ccc(cc1)C(c1cccc1C)OCCN(C)C
C1763	HIA	HIA+	24	c1ccc2c(c1)C(=N)Cc1cccc1N2C(=O)N
C1764	HIA	HIA+	24	C(#CCOC(=O)C(c1cccc1)(C1CCCC1)O)CN(CC)CC
C1765	HIA	HIA+	24	C1(C(=O)N(c2cccc2)N(c2ccc(cc2)O)C1=O)CCCC
C1766	HIA	HIA+	24	c1cc(ccc1C1CCNCC1COc1ccc2c(c1)OCO2)F
C1767	HIA	HIA+	24	C1(=O)C(C(=O)NC(=O)N1)(CC)C(C)CCC
C1768	HIA	HIA+	24	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCN1CCN(CC1)CCO
C1769	HIA	HIA+	24	c1ccc(cc1)C1(C(=O)NC(=O)CC1)CCN(CC)CC
C1770	HIA	HIA+	24	C1(c2cccc2)C(=O)c2cccc2C1=O
C1771	HIA	HIA+	24	c1ccc2c(c1)C(=C(C(=O)Nc1cccc1)N(C)S2(=O)=O)O
C1772	HIA	HIA+	24	c1c2c(cc(c1Cl)S(=O)(=O)N)S(=O)(=O)N(C(CSCC(F)(F)F)N2)C
C1773	HIA	HIA+	24	c1cc(ccc1C(=O)O)S(=O)(=O)N(CCC)CCC
C1774	HIA	HIA+	24	c1cc(ccc1C(=O)NC(C)C)CNNC
C1775	HIA	HIA+	24	c1ccc(c(c1)C(C)C)OC(C)C
C1776	HIA	HIA+	24	c12c(nen1CC(C)O)n(c(=O)n(c2=O)C)C
C1777	HIA	HIA+	24	c1ccc(cc1)C(C(C)NC)O
C1778	HIA	HIA+	24	c1cnc(en1)C(=O)N
C1779	HIA	HIA+	24	c1ccc(c(c1OC)C(=O)NCC1CCCN1CC)OC)Br
C1780	HIA	HIA+	24	c1ccc(c(c1)C(=O)O)OC(=O)c1cccc1O
C1781	HIA	HIA+	24	C#CCN(C(C)Cc1cccc1)C
C1782	HIA	HIA+	24	c1ccc2c(c1)C(=C(C(=O)Nc1nccs1)N(C)S2(=O)=O)O
C1783	HIA	HIA+	24	c1cc(ccc1N)S(=O)(=O)Nc1cc(C)on1
C1784	HIA	HIA+	24	C1(C(=O)N(c2cccc2)N(c2cccc2)C1=O)CCS(=O)c1cccc1
C1785	HIA	HIA+	24	c1ccc(cc1)/C(=C(/c1cccc1)\CC)/c1ccc(cc1)OCCN(C)C
C1786	HIA	HIA+	24	c1cnc(c1)NC(=O)C1=Cc2c(ccs2)S(=O)(=O)N1C
C1787	HIA	HIA+	24	c1ccc(cc1)C(c1cccc1)(C1CCN(CCCC(c2ccc(cc2)C(C)(C)C)O)CC1)O
C1788	HIA	HIA+	24	c1cc(ccc1CC(C(=O)O)OCC)OCCc1ccc(cc1)OS(=O)(=O)C
C1789	HIA	HIA+	24	C1=C2CCC3C4CCC(C4(C)CCC3C2(C)CCC1=O)O
C1790	HIA	HIA+	24	c1c([N+](=O)[O-])n(c(C)n1)CCS(=O)(=O)CC
C1791	HIA	HIA+	24	c1ccc(c(c1)C)NC(=O)C(C)N)C
C1792	HIA	HIA+	24	c1ccc(cc1)/C(=C(/c1cccc1)\CCCl)/c1ccc(cc1)OCCN(C)C



C1793	HIA	HIA+	24	<chem>C1=CC2(C(=CC1=O)CCC1C3CC(C(C(=O)CO)(C3(C)CC(C21F)O)O)O)C</chem>
C1794	HIA	HIA+	24	<chem>c1ccc(cc1)C(CCN1CCCC1)(C1CCCC1)O</chem>
C1795	HIA	HIA+	24	<chem>C1CN(CCC1)P(=O)(N(CCC1)CC1)OC1</chem>
C1796	HIA	HIA+	24	<chem>c12e(cccc1)sc(c2)C(C)N(C(=O)N)O</chem>
C1797	HIA	HIA+	24	<chem>c1cc(ccc1C(=O)c1c(cc(CC(=O)O)n1C)C)Cl</chem>
C1798	HIA	HIA+	24	<chem>c12c(cccc1)onc2CS(=O)(=O)N</chem>
C1799	HIA	HIA+	24	<chem>c1ccc2c(c1)C=C(c1cc(ccc1S2)Cl)OCCN(C)C</chem>
C1800	HIA	HIA-	24	<chem>c1ccc2e(c1)C13CC[N+](C1CC(/C(=C/CO)/C4)C1=CN4e5ccccc5C56CC[N+](C5CC(/C(=C/CO)/C7)C(=CN2C31)C46)CC=C)CC=C</chem>
C1801	HIA	HIA-	24	<chem>c1cc[n+](cc1)CC1=C(C(=O)O)N2C(=O)C(C2SC1)NC(=O)/C(=N\OC)/c1csc(n1)N</chem>
C1802	HIA	HIA-	24	<chem>c1cc[n+](cc1)CC1=C(C(=O)O)N2C(=O)C(C2SC1)NC(=O)/C(=N\OC(C(=O)O)(C)C)/c1csc(n1)N</chem>
C1803	HIA	HIA-	24	<chem>c1cc(cc(c1)O)[N+](CC)(C)C</chem>
C1804	HIA	HIA-	24	<chem>C(=O)(C)OC1C2(C)CCC3C(CCC4CC(C(CC34C)[N+](C3)CCCC3)C)OC(=O)C2CC1[N+](C)CCCC1)C</chem>
C1805	HIA	HIA-	24	<chem>c1cc(e2cc1CC1c3e(cc(c3O3ccc(cc3)CC3c4cc(e(cc4CC[N+](C)C)OC)O2)O)OC)CC[N+](C)C)O</chem>
C1806	HIA	HIA-	24	<chem>C(=O)(C)OC1C2(C)CCC3C(CCC4CC(C(CC34C)N3CCCC3)OC(=O)C)C2CC1[N+](C)CCCC1)C</chem>
C1807	HIA	HIA-	24	<chem>c1cc(cc(c1)OC(=O)N(C)C)[N+](C)(C)C</chem>
C1808	HIA	HIA-	24	<chem>c1ccc(cc1)C[N+](CCOe1ccccc1)(C)C</chem>
C1809	HIA	HIA-	24	<chem>C(=O)(N)OC(C)C[N+](C)(C)C</chem>
C1810	HIA	HIA-	24	<chem>c1cc(c(c1)OCC[N+](CC)(CC)OCC[N+](CC)(CC)OCC[N+](CC)(CC)CC</chem>
C1811	HIA	HIA-	24	<chem>c1c(cc[n+](c1)COC[n+](c1)C)C=C/N/O/C=N/O</chem>
C1812	HIA	HIA-	24	<chem>C(CC[N+](C)CCCC1)C(CC[N+](C)CCCC1)C</chem>
C1813	HIA	HIA-	24	<chem>c1ccc(cc1)C(=C1CC[N+](CC1)(C)C)c1ccccc1</chem>
C1814	HIA	HIA-	24	<chem>C(=O)(CC(C[N+](C)C)C)OC(=O)C)O</chem>
C1815	HIA	HIA-	24	<chem>c1ccc(cc1)C(C(=O)OC1CC2C3C(C(C1)[N+](C)C)O3)CO</chem>
C1816	HIA	HIA-	24	<chem>c1ccc(cc1)C(C(=O)OC1CC[N+](C1)(C)C)(C1CCCC1)O</chem>
C1817	HIA	HIA-	24	<chem>c1ccc(c(c1)C[N+](CC)(C)C)Br</chem>
C1818	HIA	HIA-	24	<chem>c1cc[n+](c(c1)/C=N/O)C</chem>
C1819	HIA	HIA+	24	<chem>c1c(c(c(c(c1OC)C)C)/C=C/C(=C/C=C/C(=C\C(=O)O)/C)/C)C</chem>
C1820	HIA	HIA+	24	<chem>c1ccc(cc1)C1=NCe2n(c3c1cc(cc3)Cl)c(C)nn2</chem>
C1821	HIA	HIA+	24	<chem>c1cc(ccc1C1(C(=O)NC(=O)CC1)CC)N</chem>
C1822	HIA	HIA+	24	<chem>c1ccc2c(c1)C(=O)N(C1CCCN(CC1)C)NC2Cc1ccc(cc1)Cl</chem>
C1823	HIA	HIA+	24	<chem>c1ccnc(c1)CCNC</chem>
C1824	HIA	HIA+	24	<chem>C(#N)c1ccc(cc1C(F)(F)F)NC(=O)C(C)(CS(=O)(=O)c1ccc(cc1)F)O</chem>
C1825	HIA	HIA+	24	<chem>c1ccc(cc1)Cc1ccccc1OCCCCNC</chem>
C1826	HIA	HIA+	24	<chem>c1(cn(c(=O)nc1NC(=O)OCCCC)C1C(C(C(C)O1)O)O)F</chem>
C1827	HIA	HIA+	24	<chem>c1cc(ccc1C(C(CO)NC(=O)C(C)C)O)[N+](=O)[O-]</chem>
C1828	HIA	HIA+	24	<chem>c12e(cccc1)nc2C(C1CC2CCN1CC2C=C)O</chem>
C1829	HIA	HIA+	24	<chem>c1e2c(cc3e1OCCO3)n(CC)nc(c2=O)C(=O)O</chem>
C1830	HIA	HIA+	24	<chem>C1C(=O)N(c2ccccc2)c2cc(ccc2N(C1=O)C)Cl</chem>
C1831	HIA	HIA+	24	<chem>c1cc(e2c3e1CC1C4C=CC(C(C34CCN1C)O2)O)OC</chem>
C1832	HIA	HIA+	24	<chem>c1ccc2c(c1)C=Cc1ccccc1C2=C1CCN(CC1)C</chem>
C1833	HIA	HIA+	24	<chem>CCCC(CCC)CCCC1COCCN1CCO</chem>
C1834	HIA	HIA+	24	<chem>c1ccc2e(c1)CCc1ccccc1N2CCCN</chem>
C1835	HIA	HIA+	24	<chem>c1ccc(cc1)C1=NCC(=O)Nc2c1cc(cc2)Cl</chem>
C1836	HIA	HIA+	24	<chem>C#CC1(CCC2C3CCC4=CCCC4C3C(=C)CC12CC)O</chem>
C1837	HIA	HIA+	24	<chem>c1ccc(cc1)C(c1ccccc1)(C(=O)N1CCCC1)C(C)CN1CCOCC1</chem>
C1838	HIA	HIA+	24	<chem>c1cc(cc2c1N=C(C)NS2(=O)=O)Cl</chem>

C1839	HIA	HIA+	24	c1ccc(c(e1)CC(=O)O)Nc1ccc(cc1Cl)Cl
C1840	HIA	HIA+	24	C(#N)CC1(CCC2C3C(=C4C(=CC(=O)CC4)CC3)CCC12C)O
C1841	HIA	HIA+	24	c1ccc2c(c1)C(c1ccccc1OC2)CCCN(C)C
C1842	HIA	HIA+	24	C1(=O)C(C)CC(C)(C(C)C(C(C(=O)OC(C)C(C(C1C)O)O)C)OC1CC(C)(C(C(C)O1)O)OC)OC1C(C(C(C)O1)N(C)C)O)O
C1843	HIA	HIA+	24	c1cc(cc2c1C1CCC3(C)C(CCC3O)C1CC2)OC(=O)N(CCC1)CCCC1
C1844	HIA	HIA+	24	CCC(CO)NCCNC(C)CO
C1845	HIA	HIA+	24	c1c(cc(CC)nc1)C(=S)N
C1846	HIA	HIA+	24	c1cc(ccc1c1cc(c[n+](c1c1ccc(C)nc1)[O-])Cl)S(=O)(=O)C
C1847	HIA	HIA+	24	c1cc(cc(e1)C(F)(F)F)C(C)CNCC
C1848	HIA	HIA+	24	c1ccc(cc1)Oc1cccc(c1)C(C(=O)O)C
C1849	HIA	HIA+	24	C1=CC2(C(=CC1=O)C(CC1C3CC4C(C(=O)CO)(C3(C)CC(C21)O)OC(C)(C)O4)F)C
C1850	HIA	HIA+	24	c1ccc(c(e1)C1=NCC(=O)N(e2c1cc(cc2)Cl)CCN(CC)CC)F
C1851	HIA	HIA+	24	C#CC1(C=CC2C3CCC4=CC(=O)CCC4C3CCC12CC)O
C1852	HIA	HIA+	24	c1cc(c(e1)Cl)CC(=O)N=C(N)N)Cl
C1853	HIA	HIA+	24	c1c2c(cc(e1Cl)S(=O)(=O)N)S(=O)(=O)NCN2
C1854	HIA	HIA+	24	c12c(cc(cc1)Cl)ncce2NC(C)CCN(CC)CCO
C1855	HIA	HIA+	24	c1ccc2c(c1)CCc1cccc1N2CCCN(C)C
C1856	HIA	HIA+	24	c1ccc2c(c1)C(=O)N(c1ccc(cc1)C(C(=O)O)C)C2
C1857	HIA	HIA+	24	c1ccc(cc1)C12c3cc(ccc3N(C(=O)CN1C(=O)C=C(C)O2)C)Cl
C1858	HIA	HIA+	24	c1ccc(cc1)CCC(C)NCC(c1ccc(c(e1)C(=O)N)O)O
C1859	HIA	HIA+	24	C(#N)C(=NNc1ccc(cc1)C1=NNC(=O)CC1C)C#N
C1860	HIA	HIA+	24	c1c(c(ccc1N1C(=O)OC(CNC(=O)C)C1)N1CCOCC1)F
C1861	HIA	HIA+	24	c1ccc(c(e1)c1ccc(cc1)Cn1c(c(nc1CCCC)Cl)CO)c1[nH]nnn1
C1862	HIA	HIA+	24	c1ccc2c(c1)C1c3ccccc3C2(CC1)CCNC
C1863	HIA	HIA+	24	c12c(ccc(c1)C(=O)c1cccc1)nc([nH]2)NC(=O)OC
C1864	HIA	HIA+	24	C#CC1(CCC2C3CCc4cc(ccc4C3CCC12C)OC)O
C1865	HIA	HIA+	24	c1ccc(c(e1)OC)OCC(COC(=O)N)O
C1866	HIA	HIA+	24	c1ccc(c(e1)C)N1C(=O)e2cc(c(cc2NC1C)Cl)S(=O)(=O)N
C1867	HIA	HIA+	24	c1cc(cnc1)C(=O)C(c1ccnc1)(C)C
C1868	HIA	HIA+	24	c1cc(ccc1C(=O)NCCN1CCOCC1)Cl
C1869	HIA	HIA-	24	c1cc(ccc1C(C(=O)NC1(C(=O)N2C(=C(COC12)CSc1nnn1C)C(=O)O)OC)C(=O)O)O
C1870	HIA	HIA+	24	c12c(cccc1)cc(cc2)CC(C(=O)OCCN(CC)CC)CC1CCCCO1
C1871	HIA	HIA+	24	c12c(ccc(c1)C(C(=O)O)C)cc(cc2)OC
C1872	HIA	HIA+	24	c12c(ccc(c1)CCS(=O)(=O)NC)[nH]c(c2)C1CCN(CC1)C
C1873	HIA	HIA+	24	c1ccc(c(e1)C1C(=C(C)NC(=C1OC(=O)C)C)C(=O)OC)[N+](=O)[O-]
C1874	HIA	HIA+	24	c1c(c(ccc1N1C(=O)C(C)(C)NC1=O)[N+](=O)[O-])C(F)(F)F
C1875	HIA	HIA+	24	C#CC1(CCC2C3CCC4=CC(=O)CCC4C3C=CC12CC)O
C1876	HIA	HIA+	24	c1ccc(cc1)C(c1ccccc1)N1CCN(CCCn2c3ccccc3[nH]e2=O)CC1
C1877	HIA	HIA+	24	c1ccc(c(e1)OCC=C)OCC(CNC(C)C)O
C1878	HIA	HIA+	24	c1ccc(c(e1)C1CCCC1)OCC(CNC(C)(C)C)O
C1879	HIA	HIA+	24	c1ccc(cc1)C1(C(=O)NC(=O)NC1=O)CC
C1880	HIA	HIA+	24	c1ccc(cc1)C(c1c(c2ccccc2oc1=O)O)CC
C1881	HIA	HIA+	24	c1ccc(cc1)N1C(=O)C(=O)C(CCCC)N1c1ccccc1
C1882	HIA	HIA+	24	c12c(cccc1OCC(CNC(C)C)O)[nH]cc2
C1883	HIA	HIA+	24	c1c(ccnc1)C(=O)c1c(CC)[nH]c(=O)[nH]1
C1884	HIA	HIA+	24	c1ccc2c(c1)C(=C1CCN(CC1)C)c1ccsc1CC2

C1885	HIA	HIA+	24	c1ccc2c(c1)CCN1C(=O)CN(C(=O)C3CCCC3)CC21
C1886	HIA	HIA+	24	c1ccc(cc1)C(CCN1CCCC1)(C1CCCC1)O
C1887	HIA	HIA+	24	c1ccc(cc1)C(c1ccc1)(C(=O)OC1CCN(CC1)C)OCCC
C1888	HIA	HIA+	24	c1c(CCC)[nH]c(=S)[nH]c1=O
C1889	HIA	HIA+	24	c1cc2c(c(c1)O)CC1CC(CN(C1C2)CCC)NS(=O)(=O)N(CC)CC
C1890	HIA	HIA+	24	c1c(cc(cc1O)O)C(CNCCCn1c2c(nc1)n(c(=O)n(c2=O)C)C)O
C1891	HIA	HIA+	24	c12c(ccc(c1)Cn1cncn1)[nH]cc2CCN(C)C
C1892	HIA	HIA+	24	c1ccc2c(c1)C(=O)NS2(=O)=O
C1893	HIA	HIA+	24	C(=C\Br)/C1C(=O)NC(=O)N(C1)C1C(C(C(CO)O1)O)O
C1894	HIA	HIA+	24	C1=CC(n2cc(c(nc2=O)N)C)OC1CO
C1895	HIA	HIA+	24	c1cc(ccc1N)S(=O)(=O)Nc1nc(cc(C)n1)C
C1896	HIA	HIA+	24	c1ccc(c(c1)OCC)OCCNC(C)Cc1ccc(c(c1)S(=O)(=O)N)OC
C1897	HIA	HIA+	24	c12c(cccc1)n(c(C1C=c3c(=C(C)C1)nc(CCC)n3Cc1ccc(cc1)c1ccccc1C(=O)O)n2)C
C1898	HIA	HIA+	24	c1c2c(cc(c1OC)OC)C1CC(=O)C(CC(C)C)CN1CC2
C1899	HIA	HIA+	24	c1cc(ccc1C)S(=O)(=O)NC(=O)NCCCC
C1900	HIA	HIA+	24	c1cc(ccc1C)C(=O)c1ccc(CC(=O)O)n1C
C1901	HIA	HIA+	24	CC1(C)OC2C(COC3(C2OC(C)(C)O3)COS(=O)(=O)N)O1
C1902	HIA	HIA+	24	c1cc(cc(c1)OC)C1(CCCCC1CN(C)C)O
C1903	HIA	HIA+	24	C(=O)(C1CCC(CC1)CN)O
C1904	HIA	HIA+	24	c1cc(cc(c1)Cl)N1CCN(CCCn2c(=O)n3ccccc3n2)CC1
C1905	HIA	HIA+	24	c1c(cc(c(c1OC)OC)OC)Cc1enc(nc1N)N
C1906	HIA	HIA+	24	c1cc(ccc1C(C(=O)O)C)C1C/C(=N/O)/CCCC1
C1907	HIA	HIA+	24	C(#N)c1c2n(c(ccn2)c2cccc(c2)N(C(=O)C)CC)nc1
C1908	HIA	HIA-	24	C1=C(C(=O)O)OC(C1NC(=N)N)NC(=O)C)C(C(CO)O)O
C1909	HIA	HIA-	18	CN(C)C(=O)Oe1ccc[n+](C)c1
C1910	HIA	HIA+	14	CCN1CCC[C@@H]1CNC(=O)c1c(OC)ccc(c1)S(=O)(=O)CC
C1911	HIA	HIA+	14	Cc1cn([C@@H]2O[C@@H](CO)C=C2)c(=O)[nH]c1=O
C1912	HIA	HIA-	15,22	OC[C@H]1O[C@H](O[C@@H]2[C@@H](O)[C@H](O)[C@H]3O[C@H](CN)[C@@H](O)[C@H](O)[C@H]3O)[C@@H](N)CC2N)[C@H](O)[C@@H](N)C1O
C1913	HIA	HIA+	14,20	Nc1ccc(cc1)S(=O)(=O)Nc1ccc1
C1914	HIA	HIA+	15,18,21,22	COc1ccc(CCN(C)CCCC(C#N)(C(C)C)c2cc(OC)c(OC)cc2)cc1OC
C1915	HIA	HIA+	20	C(=C\CN1CCN(CC1)C(c1ccc(F)cc1)c1ccc(F)cc1)/c1ccccc1
C1916	HIA	HIA+	15,16,19,22	CC(NC(C)(C)C)C(=O)c1ccccc1)c1
C1917	HIA	HIA+	18	CN(C)CCC(c1ccc(Cl)cc1)c1ccccc1
C1918	HIA	HIA+	20	ON1C(=c2cc(Cl)ccc2=N/C(=N\C)/C1)c1ccccc1
C1919	HIA	HIA-	15	NC(=S)N/N=C/c1ccc(NC(=O)C)cc1
C1920	HIA	HIA+	20	N/C(=N\C(C)C)/N=C(\N)/Nc1ccc(Cl)cc1
C1921	HIA	HIA+	15,16,18,19,22	OCC(C(=O)OC1C[C@@H]2N(C)[C@@H](C1)[C@@H]1O[C@H]21)c1ccccc1
C1922	HIA	HIA+	15,22	COc1cc2c(cc1)nc([nH]2)S(=O)Cc1ccc(C)c(OC)c1C
C1923	HIA	HIA+	15	O/C(=C\1/N(C)S(=O)(=O)c2ccccc2C1=O)/Nc1ncs1
C1924	HIA	HIA+	14,15	COc1cc(ccc1)[C@@]1(O)CCCC[C@@H]1CN(C)C
C1925	HIA	HIA+	14	CC(C)[C@H](N)C(=O)OCCOCn1cnc2c1[nH]c(N)nc2=O
C1926	HIA	HIA+	15,22	OC1=C(O)C(=O)[C@H](O1)[C@@H](O)CO
C1927	HIA	HIA-	14,22	CC(=O)N(O)CCCCCN(C(=O)CCC(=O)N(O)CCCCCN(C(=O)CCC(=O)N(O)CCCCCN
C1928	HIA	HIA+	14	CC(C)(C)NC[C@H](O)c1cc(CO)c(O)cc1
C1929	HIA	HIA+	15,16,19	NCC1(CC(=O)O)CCCC1
C1930	HIA	HIA+	14,20	CCCN(CCC)CCc1c2CC(=O)Nc2ccc1

C1931	HIA	HIA+	20	OC(=O)[C@@H]1N2C(=O)[C@@H](NC(=O)c3c(oc3c3c(F)cccc3Cl)C)[C@H]2SC1(C)C
C1932	HIA	HIA-	23,15,16,19,21	OC(=O)C1=C/C(=N\Nc2cc(C(=O)O)c(O)cc2)/C=CC1=O
C1933	HIA	HIA+	15,16,19	OC(=O)C1=C(CSc2n[nH]nc2)CS[C@H]2N1C(=O)[C@H]2NC(=O)C(N)c1ccc(O)cc1
C1934	HIA	HIA-	17	oc[C@H]1o[C@@H](O[C@@H]2[C@@H](O)[C@H](N)C[C@H](N)[C@H]2O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2N)[C@H](O)C1O[C@H]1O[C@@H](CN)[C@@H](O)[C@H](O)[C@H]1N
C1935	HIA	HIA+	5,16,18,19,21,2	[C@@H]12C[C@@H](C)[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]1(F)[C@H]2CCC2=CC(=O)C=C[C@@]12C
C1936	HIA	HIA+	15,22	C1=C2C(=C[C@H]3[C@@H]4CC[C@](OC(=O)C)(C(=O)C)[C@@]4(C)CC[C@@H]3[C@@]2(C)[C@H]2C[C@H]2C1=O)C1
C1937	HIA	HIA+	15,18,22	Oc1c2O[C@H]3C(=O)CC[C@@]4(O)[C@H]5Cc(cc1)c2[C@@]34CCN5CC=C
C1938	HIA	HIA-	15,21,22	OC(=O)C1=C(CSc2nc(=O)c(=O)[nH]n2C)CS[C@H]2N1C(=O)[C@H]2NC(=O)/C(=NOC)/c1csc(n1)N
C1939	HIA	HIA-	16,19,22	O[C@H]1[C@@H](O[C@@H]2[C@@H](O)[C@H](O[C@H]3O[C@H](CN)CC[C@H]3N)[C@@H](N)CC2N)OC[C@@](O)(C)[C@@H]1NC
C1940	HIA	HIA+	14,20	CC(=O)c1ccc(cc1)S(=O)(=O)NC(=O)NC1CCCCC1
C1941	HIA	HIA+	14	CCC1(CCC(C)C)C(=O)NC(=O)NC1=O
C1942	HIA	HIA-	15	OC(COc1cccc2c1c(=O)cc(o2)C(=O)[O-])COc1c2c(=O)cc(oc2ccc1)C(=O)[O-]
C1943	HIA	HIA+	14	CNC(=C[N+](=O)[O-])NCCSCc1ccc(CN(C)C)o1
C1944	HIA	HIA+	15,22	COP(=O)(OC)OC(c1ccc(Cl)cc1)P(=O)(OC)OC
C1945	HIA	HIA-	18	COc1cc2c(Sc3cccc3N2CC(C)CN(C)C)cc1
C1946	HIA	HIA+	15,16,19,22	CC(C)(C)NCC(O)COc1c2C[C@H](O)[C@H](O)Cc2ccc1
C1947	HIA	HIA-	15	CNC(=O)c1c(I)c(NC(=O)C)c(I)c(C(=O)[O-])c1I
C1948	HIA	HIA+	14	COCCCOc1c(C)c(C[S@@])(=O)c2nc3cccc3[nH]2)nc1
C1949	HIA	HIA+	20	N(N=C(C#N)C#N)c1ccc(cc1)C1=NNC(=O)C[C@H]1C
C1950	HIA	HIA+	15,16,19,21,22	OC[C@@H](NC(=O)C(Cl)Cl)[C@H](O)c1ccc(cc1)[N+](=O)[O-]
C1951	HIA	HIA+	16	O[C@H](COc1nsnc1N1CCOCC1)CNC(C)(C)C
C1952	HIA	HIA+	15	OC(=O)[C@@H](N)Cc1cc(O)c(O)cc1
C1953	HIA	HIA+	17	N1c2cccc2N=c2sc(cc2=C1N1CCN(C)CC1)C
C1954	HIA	HIA-	14	Nc1nc(S)c2nc[nH]c2n1
C1955	HIA	HIA-	15	OC(=O)C(O/N=C(\C(=O)N[C@@H]1C(=O)N([C@H]1C)S(=O)(=O)O)/c1csc(n1)N)(C)C
C1956	HIA	HIA+	15,22	O/C(=C/1\N(C)S(=O)(=O)c2c(scc2)C1=O)/Nc1cccc1
C1957	HIA	HIA+	15	OC(=O)CN1c2cccc2CC[C@H](N[C@H](C(=O)OCC)CCc2cccc2)C1=O
C1958	HIA	HIA+	14,15,17,22	NC(=N)NC(=O)c1nc(Cl)c(N)nc1N
C1959	HIA	HIA+	14,20	CCN(C)C(=O)Oc1cccc(c1)[C@H](C)N(C)C
C1960	HIA	HIA+	15,17,22	NC(=Nc1nc(CSCC/C(=N\S(=O)(=O)N)/N)cs1)N
C1961	HIA	HIA+	15,18,22	COc1cc2c(cc1)n(C(=O)c1ccc(Cl)cc1)c(C)c2CC(=O)O
C1962	HIA	HIA+	14,16,19,21,22	OC(=O)c1cccc1O
C1963	HIA	HIA+	14	CC1(C)OC2CC3C4CCC5=CC(=O)C=CC5(C)C4(F)C(O)CC3(C)C2(O1)C(=O)CO
C1964	HIA	HIA+	18	c1ccc(cc1)[C@@](OCC[C@@H]1N(C)CCC1)(c1ccc(Cl)cc1)C
C1965	HIA	HIA-	20	O[C@H]1[C@H](O[C@H]2OC(=CC[C@H]2N)CN)[C@@H](N)C[C@@H](NCC)[C@@H]1O[C@H]1OC[C@@](O)(C)[C@H](NC)[C@H]1O
C1966	HIA	HIA+	15,22	CCOc1cccc1OCC1CNCCO1
C1967	HIA	HIA+	15	CC(N)(Cc1cc(O)c(O)cc1)C(=O)O
C1968	HIA	HIA+	14,18	CN(C)C(=O)Cc1c(nc2ccc(C)cn12)c1ccc(C)cc1
C1969	HIA	HIA+	15,16,19,21	CC1=C(N2[C@H](SC1)[C@H](NC(=O)[C@H](N)c1cccc1)C2=O)C(=O)O
C1970	HIA	HIA+	15,16,19,22	CC(C)NCC(O)c1ccc(NS(=O)(=O)C)cc1
C1971	HIA	HIA+	14,15,21,22	Cn1c2c([nH]cn2)c(=O)n(C)c1=O
C1972	HIA	HIA+	18	CN(C)CCCN1c2cccc2Sc2cccc12
C1973	HIA	HIA+	15,22	On1c(=N)nc(cc1N)N1CCCCC1
C1974	HIA	HIA+	20,22	N1c2c(N=c3cccc3=C1N1CCN(C)CC1)ccc(Cl)c2
C1975	HIA	HIA+	15,16,17,19,22	NS(=O)(=O)c1cc(C(=O)O)c(NCc2ccco2)cc1Cl
C1976	HIA	HIA+	18	CN(C)CCOC(c1cccc1)c1cccc1

C1977	HIA	HIA+	14	Cn1nnc2c(ncn2c1=O)C(=O)N
C1978	HIA	HIA+	14	CC1(C)S[C@H]2[C@H](NC(=O)[C@@H](N)c3ccccc3)C(=O)N2[C@@H]1C(=O)O
C1979	HIA	HIA-	14	CN(C)C(=O)OC1=CN(C)C=C=C1
C1980	HIA	HIA+	14	CC1=CN=C[C@H](N1O)C(=O)O
C1981	HIA	HIA+	14	Nc1nc2c(ncn2[C@@H]2C[C@@H](CO)C=C2)c(N)n1
C1982	HIA	HIA+	14	CC(=CC(=O)O)c1nc(ccc1)C(=CCN1CCCC1)c1ccc(C)cc1
C1983	HIA	HIA+	14	CC[C@H]1OC(=O)[C@@H](C)C(=O)[C@@H](O)[C@@H](O)[C@@H]2O[C@H](C)C[C@@H](C)[C@@H]2O)N(C)C[C@@H](C)C(=O)[C@@H](C)[C@H]2N(CCCn3cnc(c3)c3cnc3)C(=O)O[C@H]12C)OC
C1984	HIA	HIA+	14	CC(C)NC[C@H](O)c1cc(NS(=O)(=O)C)ccc1
C1985	HIA	HIA+	14	CC1(C)S[C@H]2[C@H](NC(=O)[C@@H](N)c3ccc(O)cc3)C(=O)N2[C@H]1C(=O)O
C1986	HIA	HIA-	14	COC1CC(CCC1O)C=C(C)C1OC(=O)C2CCCCN2C(=O)C(=O)C2(O)OC(C(CC2C)OC)C(CC(C)CC(=CC(CC=C)C(=O)CC(O)C1C)C)OC
C1987	HIA	HIA-	14	NC[C@@H]1O[C@@H](O)[C@H]2[C@@H](N)C[C@@H](N)[C@H](O)[C@H]3O[C@@H](CO)[C@H](O)[C@@H](N)[C@H]3O)[C@H]2O)[C@H](N)C[C@@H]1O
C1988	HIA	HIA-	14	OC[C@@H]1O[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](O)[C@H](O)[C@H]1O
C1989	HIA	HIA+	14	C[C@H]12CC[C@H]3[C@H](CCC4=CC(=O)CC[C@H]34C)[C@@H]1CC[C@H]2O
C1990	HIA	HIA+	14	COc1cc(C)c(cc1OC)[S@](=O)C
C1991	HIA	HIA+	14	CN1c2c(cccc2)[C@@H](NCCCCC(=O)O)c2c(cc(Cl)cc2)S1(=O)=O
C1992	HIA	HIA+	14	Cc1cc2c(cc1C)n(C[C@H](O)[C@@H](O)[C@H](O)CO)c1nc(=O)[nH]c(=O)c1n2
C1993	HIA	HIA+	14	CN1[C@H]2CC[C@@H]1CC(C2)OC(=O)c1c[nH]c2ccccc12
C1994	HIA	HIA+	14	Oc1ccc(cc1)c1c(C(=O)c2ccc(OCCN3CCCC3)cc2)c2c(s1)cc(O)cc2
C1995	HIA	HIA+	15,16,19,22	O=C1NC(=O)C(N1)(c1ccccc1)c1ccccc1
C1996	HIA	HIA+	15	CO/N=C(\C(=O)N[C@H]1[C@H]2SCC(=C(N2C1=O)C(=O)OCOC(=O)C(C)(C)C)/c1csc(N)n1
C1997	HIA	HIA+	14	N=C(Nc1ccccc1)Nc1ccccc1
C1998	HIA	HIA+	15,17,22	OC(=O)Cc1ccccc1Nc1c(Cl)ccccc1Cl
C1999	HIA	HIA+	14	CC1(OC(=CC1=O)C(=O)O)c1ccccc1
C2000	HIA	HIA+	14	N(N=Nc1ccccc1)c1ccccc1
C2001	HIA	HIA+	3,15,16,18,19,22	CC(C)NCC(O)COc1ccc(NC(=O)C)cc1
C2002	HIA	HIA+	18	c1cc(OC)c(OC)c2c1[C@H](OC2=O)[C@@H]1N(C)CCc2cc3c(OCO3)c(OC)c12
C2003	HIA	HIA+	18	NC(=O)CCCN/C(=C/\C=C(F)C=CC1=O)/c1ccc(Cl)cc1
C2004	HIA	HIA+	15,22	O/C(=C\1/N(C)S(=O)(=O)c2ccccc2C1=O)/Nc1ccc(s1)C
C2005	HIA	HIA-	15	OC(CNCCNC(=O)N1CCOCC1)COc1ccc(O)cc1
C2006	HIA	HIA+	15	N[C@H]1C(=O)NOC1
C2007	HIA	HIA+	20	OC(=O)c1cn(c2c(OC)c(N3C[C@H]4NCCC[C@H]4C3)c(F)cc2e1=O)C1CC1
C2008	HIA	HIA+	15,16,19,22	C[C@H](CS)C(=O)N1CCC[C@H]1C(=O)O
C2009	HIA	HIA+	15,16,18,19	CN(Cc1nc2c(nc1)nc(N)nc2N)c1ccc(cc1)C(=O)N[C@@H](CCC(=O)O)C(=O)O
C2010	HIA	HIA-	23,15,16,18,19	OC[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)CO
C2011	HIA	HIA+	15,16,19,22	c1cn(c(n1)C)CC1C(=O)c2c(n(c3ccccc23)C)CC1
C2012	HIA	HIA+	18	Clc1ccc2n(C3CCN(CCCn4c(=O)[nH]c5ccccc45)CC3)c(=O)[nH]c2c1
C2013	HIA	HIA-	14	CNC(=O)c1c(I)c(NC(=O)C)c(I)c(C(=O)O)c1I
C2014	HIA	HIA+	14,18	Nc1nc(N)c2nc(c(N)nc2n1)c1ccccc1
C2015	HIA	HIA-	16,19,22	OC(=O)c1cc(=O)c2c(o1)ccc(OCC(O)COc1ccccc3c1c(=O)cc(o3)C(=O)O)c2
C2016	HIA	HIA+	20	O/C(=C\1/C(=O)[C@@H](N(C)C)[C@@H]2[C@@H](O)[C@H]3C(=C(O)c4c(cccc4O)[C@]3(O)C)C(=O)[C@]2(O)C1=O)/N
C2017	HIA	HIA+	15	OC(=O)[C@H]1N(C(=O)C(N[C@@H](C(=O)OCC)CCc2ccccc2)C)CCC1
C2018	HIA	HIA+	15,16,19	OC[C@H]1O[C@@H](n2cc(/C=C/Br)c(=O)[nH]c2=O)[C@@H](O)C1O
C2019	HIA	HIA+	14,20	[C@@H]12C[C@@H](O)[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]1(F)[C@H]2CCC2=CC(=O)C=C[C@H]12C
C2020	HIA	HIA-	15	CN(CCCCCN(C)C(=O)O)c1ccc[n+](C)c1)C(=O)O)c1ccc[n+](C)c1
C2021	HIA	HIA-	14,22	OC(=O)CN(CCN(CC(=O)O)Cc1ccccc1O)Cc1ccccc1O
C2022	HIA	HIA+	14	Cc1cn([C@H]2C[C@H](N=[N+]=[N-])[C@H](CO)O2)c(=O)[nH]c1=O

C2023	HIA	HIA+	15	[nH]1c(nc2cccc12)CCCN(C)CC[C@@]1(OC(=O)COC)CCc2c(ccc(F)c2)[C@@H]1C(C)C
C2024	HIA	HIA+	15,16,17,19	Cc1cn([C@H]2[C@H](N=[N+]=[N-])[C@@H](CO)O2)c(=O)[nH]c1=O
C2025	HIA	HIA+	21	c1ccc2N(C(=O)[C@H](OC(=O)C)[C@@H](Sc2c1)c1ccc(OC)cc1)CCN(C)C
C2026	HIA	HIA+	14	CC(C)NC[C@@H](O)COc1cccc2cccc12
C2027	HIA	HIA+	16,17,18,19,21	CC(C)NCC(O)COc1c2cccc2ccc1
C2028	HIA	HIA+	15,16,18,19,22	CN/C(=N)CCSCc1c(C)[nH]cn1)/NC#N
C2029	HIA	HIA-	15	NS(=O)(=O)c1c(Cl)cc(NCc2cccs2)c(c1)c1nnn[nH]1
C2030	HIA	HIA+	20	NC(=NCC1OC2(OC1)CCCC2)N
C2031	HIA	HIA-	14	OC(=O)C1=C[C@H](N=C(N)N)[C@@H](NC(=O)C)[C@@H](O1)[C@H](O)[C@H](O)CO
C2032	HIA	HIA+	14	CCOc1c(OC[C@H]2CNCCO2)cccc1
C2033	HIA	HIA+	18,22	COc1ccc(cc1)C1Sc2c(cccc2)N(CC(N)C)C(=O)C1OC(=O)C
C2034	HIA	HIA+	14	NCCOCC1=C(C(=O)OCC)C(c2cccc2Cl)C(=C(N1)C)C(=O)OC
C2035	HIA	HIA+	14	COc1ccc(cc1)[C@H](CN(C)C)C1(O)CCCC1
C2036	HIA	HIA+	15,16,18,19	COc1cc2nc(nc(N)c2cc1OC)N1CCN(CC1)C(=O)c1cccc1
C2037	HIA	HIA+	20	O[C@H]1C=C[C@@]23c4c(ccc(OC)c4O[C@H]2C1)CN(C)CC3
C2038	HIA	HIA+	17	CO[C@H]1C=C(O[C@@]2(C)Oe3c(C2=O)e2c(c(O)c3C)C(=O)C(=C3)NC4(CCN(CC(C)C)CC4)N=C23)NC(=O)C(=C=C/[C@@H](C)[C@H](O)[C@@H](C)[C@H](O)[C@@H](C)[C@H](OC(=O)C)[C@@H]1C)/C
C2039	HIA	HIA+	14,15	O/N=C\1/CCCC(c2ccc(cc2)C(C(=O)O)C)C1
C2040	HIA	HIA-	15,16,19	Nc1nc2c(ncn2COC(CO)CO)c(=O)[nH]1
C2041	HIA	HIA+	14,15	OC[C@H]1O[C@@H](n2nc(nc2)C(=O)N)[C@H](O)C1O
C2042	HIA	HIA+	14,15,16,19,22	NC(=O)n1c(O)c(C(=O)c2cccs2)c2c1ccc(Cl)c2
C2043	HIA	HIA+	15,16,19	NC(C(=O)NC1C2CCC(=C(N2C1=O)C(=O)O)Cl)c1cccc1
C2044	HIA	HIA-	15,16,19	NS(=O)(=O)c1cc2c(cc1Cl)N=CNS2(=O)=O
C2045	HIA	HIA+	14	OC(=O)CCn1c2c(C[C@@H](CC2)NS(=O)(=O)c2ccc(F)cc2)c2c1cccc2
C2046	HIA	HIA-	23,15,22	OC[C@H]1O[C@](O)(CO)[C@H](O)C1O[C@H]1O[C@H](CO)[C@H](O)[C@H](O)C1O
C2047	HIA	HIA-	15,16,19	OC(=O)C1=C(COC(=O)N)CS[C@@H]2N1C(=O)[C@H]2NC(=O)/C(=N\OC)/c1cccc1
C2048	HIA	HIA-	15	[C@H]12SC(C)(C)[C@@H](N1C(=O)[C@H]2NC(=O)Cc1cccc1)C(=O)O
C2049	HIA	HIA+	14	Cc1nnc2CN=C(c3cccc3Cl)e3cc(Cl)ccc3n12
C2050	HIA	HIA+	20	OC(=O)[C@H]1N2N(CCC1)CCC[C@H](N[C@H](C(=O)OCC)CCc1cccc1)C2=O
C2051	HIA	HIA+	15,22	OC[C@@H]1O[C@H](n2ccc(nc2=O)N)CS1
C2052	HIA	HIA+	18	CN(C)CC/C=C\1/c2cccc2C=Cc2cccc12
C2053	HIA	HIA+	22	OC(=O)[C@H](N(C(=O)CCCC)Cc1ccc(cc1)c1cccc1c1n[nH]nn1)C(C)C
C2054	HIA	HIA+	15	CCN(CC)CCC1C(CC(=O)NC1=O)c1cccc1
C2055	HIA	HIA+	15,16	NC(=O)OCC1=C(N2C(=O)[C@@H](NC(=O)C(=N\OC)/c3cccc3)[C@H]2SC1)C(=O)OC(OC(=O)C)C
C2056	HIA	HIA+	19	CO/N=C(/C(=O)NC1C2SCC(=C(N2C1=O)C(=O)OC(C)OC(=O)C)COC(=O)N)\c1cccc1
C2057	HIA	HIA-	18	CC[C@@H](CO)NC(=O)[C@H]1CN(C)[C@@H]2Cc3en(C)c4cccc(c34)C2=C1
C2058	HIA	HIA+	14	CCCC(C)C1(CC=C)C(=O)NC(=O)NC1=O
C2059	HIA	HIA+	15,22	CN1/C(=C(O)Nc2cccn2)/C(=O)c2cccc2S1(=O)=O
C2060	HIA	HIA+	14	CC(C)(C)NC[C@H](O)c1cc(O)cc(O)c1
C2061	HIA	HIA+	14	OC(=O)Cc1cc2c(cc1)C(=O)c1cccc1CS2
C2062	HIA	HIA+	18,20	OC1(CCN(CCCC(=O)c2ccc(F)cc2)CC1)c1ccc(Cl)cc1
C2063	HIA	HIA+	15,16,18,19,22	COc1cc2c(ccnc2cc1)[C@H](O)[C@H]1C[C@@H]2CCN1C[C@@H]2C=C
C2064	HIA	HIA+	14	COc1cc2c(ccnc2cc1)[C@@H](O)[C@@H]1C[C@@H]2CCN1C[C@@H]2C=C
C2065	HIA	HIA+	15,22	CC(Cc1ccc(O)cc1)NCC(O)c1cc(O)cc(O)c1
C2066	HIA	HIA+	15,16,19	CC1(C)S[C@@H]2[C@H](NC(=O)[C@H](N)c3ccc(O)cc3)C(=O)N2[C@H]1C(=O)O
C2067	HIA	HIA+	14	CCOC(=O)[C@H](CCc1cccc1)N[C@@H](C)C(=O)N1Cc2cccc2C[C@H]1C(=O)O
C2068	HIA	HIA+	15,22	O[C@H]1[C@H](O)[C@H]2[C@@H](O)C1[C@H](O)[C@H]3[C@H](O)C1[C@H](O)C1[C@H]4CC[C@@]5(C)C@H(C)C1[C@H]6[C@H]5[C@@H](O)[C@]5(C)C7=CC(=O)OC7)CC(C)[6S(O)C4]OC3C)OC2C)O[C@H](C)[C@H]1O

C2069	HIA	HIA+	14	COc1ccc2c(cccc2c1C(F)(F)F)C(=S)N(C)CC(=O)O
C2070	HIA	HIA+	15,22	O/C(=C/1\N(C)S(=O)(=O)c2ccccc2C1=O)/Nc1noc(c1)C
C2071	HIA	HIA+	14,15	[C@@H]12CC[C@@]3(CCC(=O)O3)[C@@]1(C)CC[C@H]1[C@H]2[C@@H](CC2=CC(=O)CC[C@@]12C)SC(=O)C
C2072	HIA	HIA-	14	O[C@H](CNCCNC(=O)N1CCOCC1)COc1ccc(O)cc1
C2073	HIA	HIA-	15,16	C[C@H](N[C@H](CCc1ccccc1)C(=O)O)C(=O)N1CCCC[C@@H]1C(=O)O
C2074	HIA	HIA-	19	CC(NC(Cc1ccccc1)C(=O)O)C(=O)N1CCCC1C(=O)O
C2075	HIA	HIA+	14	CC(C)NC[C@@H](O)COc1ccc(CC(=O)N)cc1
C2076	HIA	HIA+	14	OCC1OC(C(O)C1O)n1cc(C=Br)c(=O)[nH]c1=O
C2077	HIA	HIA+	15,22	Cc1c(OCC(F)(F)F)ccnc1CS(=O)c1nc2c([nH]1)cccc2
C2078	HIA	HIA-	14,15,17	Nc1nc2c(nen2COCCO)c(=O)[nH]1
C2079	HIA	HIA+	15	O[C@H]1[C@H](OC2C(C)[C@H](O)[C@@H]3[C@@H](C)[C@H](O)[C@@](OC)(C)C3)[C@H](C=O)O[C@H](CC)[C@](O)(C)[C@H](O)[C@H](N(C)CC(C)[C@]2(O)C)C)O[C@H](C)[C@@H]1N(C)C
C2080	HIA	HIA+	17	Cc1ccccc(C)c1NC(=O)c1cc(c(Cl)cc1O)S(=O)(=O)N
C2081	HIA	HIA-	14,23,15,22	OC[C@H]1O[C@](O[C@H]2O[C@H](CO[C@H]3O[C@H](CO)[C@H](O)[C@H](O)C3O)[C@@H](O)[C@H](O)C2O)(CO)[C@@H](O)C1O
C2082	HIA	HIA+	20	CC(C)(C)NCC(O)c1ccc(O)c(CO)c1
C2083	HIA	HIA+	14	Cc1noc(NS(=O)(=O)c2ccc(N)cc2)c1C
C2084	HIA	HIA-	20	CC1(C)C(N2C(=O)CC2S1(=O)=O)C(=O)[O-]
C2085	HIA	HIA+	15	OC(=O)C1=CCS[C@H]2N1C(=O)[C@H]2NC(=O)/C(=N\OC)/c1csc(n1)N
C2086	HIA	HIA+	14,18	CCCC(C)(COC(=O)N)COC(=O)N
C2087	HIA	HIA+	23,15,21,22	CCN1CCCC1CNC(=O)c1c(OC)ccc(c1)S(=O)(=O)N
C2088	HIA	HIA+	14	CCN1CCC[C@@H]1CNC(=O)c1cc(ccc1OC)S(=O)(=O)N
C2089	HIA	HIA+	15,22	OC(=O)[C@@H]1N2C(=O)[C@@H](NC(=O)C(C(=O)Oc3ccccc3)c3ccccc3)[C@H]2SC1(C)C
C2090	HIA	HIA+	15	OC(=O)[C@H]1N(C(=O)CP(=O)(OC(OC(=O)CC)(C)C)CCCCc2ccccc2)[C@@H](C1)C1CCCC1
C2091	HIA	HIA-	18	CN(C)CC/C=C/1\c2c(COc3c1ccccc3)cccc2
C2092	HIA	HIA+	14,17	Oc1c2en[nH]c2nen1
C2093	HIA	HIA+	15,16,19	CCn1cc(C(=O)O)c(=O)c2cc(F)c(cc12)N1CCNCC1
C2094	HIA	HIA+	15,16,19,22	[C@@H]12CC[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@H]1[C@H]2CCCC2=CC(=O)C=C[C@]12C
C2095	HIA	HIA+	14	OC(=O)C1=CC(=N)Nc2ccc(cc2)S(=O)(=O)Nc2cccn2)C=CC1=O
C2096	HIA	HIA+	3,15,16,18,19,20	OC(=O)C1=C/C(=N)Nc2ccc(cc2)S(=O)(=O)Nc2cccn2)/C=CC1=O
C2097	HIA	HIA+	15,22	[C@@H]12Oc3c(OC)ccc4c3[C@]31CCN(C)[C@H](C4)[C@@H]3C=C[C@@H]2O
C2098	HIA	HIA+	14	CCN(CC)Cc1cc(Nc2c3ccc(Cl)cc3nec2)ccc1O
C2099	HIA	HIA+	14	CC[C@@]12CCCN3CCc4c([C@H]13)n(c1ccccc41)C(=C2)C(=O)O
C2100	HIA	HIA+	15,22	O/C(=C/1\N(C)S(=O)(=O)c2c(sc(Cl)c2)C1=O)/Nc1cccn1
C2101	HIA	HIA+	15	OC[C@H]1O[C@H]2n3cc(F)c(=N)nc3O[C@H]2C1O
C2102	HIA	HIA-	15	O[C@H]1CC(=O)O[C@H](CCC2[C@H](C=CC3=C[C@H](C)C[C@H](OC(=O)[C@@H](C)CC)[C@H]23)C)C1
C2103	HIA	HIA-	15	oc[C@H]1O[C@H](O[C@@H]2[C@H](O)[C@H](N)C[C@H](N)[C@H]2O)[C@H](CN)[C@@H](O)[C@H](O)[C@H]2N)[C@H](O)C1O[C@H]1O[C@H](CN)[C@@H](O)[C@H](O)[C@H]1N
C2104	HIA	HIA+	15	NC(CCC(=O)O)C=C
C2105	HIA	HIA+	22	CC(=O)CC(c1ccccc1)c1c(O)c2c(oc1=O)cccc2
C2106	HIA	HIA+	14	COc1c(OC)cc(CCN(C)CCC[C@@](C#N)(C(C)C)c2cc(OC)c(OC)cc2)cc1
C2107	HIA	HIA-	15,20	OC(COc1ccc(cc1)CCNC(=O)NC(C)C)CNC(C)C
C2108	HIA	HIA+	20	OCc1c(Cl)nc(n1)Cc1ccc(cc1)c1ccccc1c1n[nH]nn1)CCCC
C2109	HIA	HIA+	18	[nH]1cc(c2c1ccc(c2)CCS(=O)(=O)c1ccccc1)C[C@@H]1N(C)CCC1
C2110	HIA	HIA+	15	OC(=O)C1=C(C)CSC2N1C(=O)C2NC(=O)C(N)c1ccc(O)cc1
C2111	HIA	HIA+	15,16,19	[C@H]12SC(C)(C)[C@@H](N1C(=O)[C@H]2NC(=O)COc1ccccc1)C(=O)O
C2112	HIA	HIA+	14	Oc1c(c(=O)c2ccccc2o1)C(c1ccccc1)CC(=O)C
C2113	HIA	HIA+	15,16,18,19,21	CC(=O)CC(c1ccccc1)c1c(O)oc2ccccc2c1=O
C2114	HIA	HIA+	15,22	[C@@H]12Oc3c(O)ccc4c3[C@]31CCN(C)[C@H](C4)[C@@H]3C=C[C@@H]2O

C2115	HIA	HIA+	15,16,19,22	[C@@H]12CC[C@H](C(=O)C)[C@@]1(C)CC[C@H]1[C@H]2CCC2=CC(=O)CC[C@]12C
C2116	HIA	HIA+	15,22	OCC(C(=O)OC1C[C@H]2N(C)[C@H](CC2)C1)c1cccc1
C2117	HIA	HIA-	15,16	c1ccc(cc1)CC[C@@H](C(=O)[O-])[NH2+][C@H](C(=O)N1CCCC[C@H]1C(=O)[O-])CCCC[NH3+]
C2118	HIA	HIA-	19	NCCCCC(NC(CCc1cccc1)C(=O)O)C(=O)N1CCCC1C(=O)O
C2119	HIA	HIA-	18	CN1CCN(CC(=O)n2c3cccc3c(=O)[nH]c3e2nccc3)CC1
C2120	HIA	HIA+	14,15,22	CN(C)c1c(C)n(C)n(c1=O)c1cccc1
C2121	HIA	HIA+	14	CN1[C@H]2C[C@@H](C[C@@H]1)[C@H]1O[C@@H]21)OC(=O)[C@H](CO)c1cccc1
C2122	OB	OB-	27	[C@](c1cc(c(c1)OC)OC)OC)(C(C)C)(CCC[N@H+](CCc1cc(c(cc1)OC)OC)C)C#N
C2123	OB	OB+	27	c1(cc(c(cc1)O)C(=O)[O-])[C@@H](C[NH2+])C(C)(C)O
C2124	OB	OB+	27	C(c1cccc1)(C(=O)N)(C(=O)N)CC
C2125	OB	OB+	27	C1C(=O)C=C2[C@H](C1)[C@@H]1[C@@H](CC2)[C@H]2[C@](CC1=C)([C@](CC2)(O)C#C)CC
C2126	OB	OB+	27	c12c(n(cn1)[C@@H]1C[C@@H](C=C1)CO)nc(nc2NC1CC1)N
C2127	OB	OB-	27	S(=O)(=O)(CCCCN(=O)C)[O-]
C2128	OB	OB-	27	[C@@H]1([C@@H]([C@@H]([C@@H](O)C@H]1CO)O)O)O)O)O)[C@@H]1([C@@H]([C@@H]([C@@H](O1)C)[NH2+][C@@H]1[C@@H]([C@@H]([C@@H](C=C1)CO)O)O)O)O)O)O)O)O
C2129	OB	OB+	27	c1(c(ccc(c1)NC(=O)CCC)OC[C@@H](C[NH2+])C(C)O)C(=O)C
C2130	OB	OB+	27	[C@@H](c1c(c2c(cccc2)oc1=O)O)(c1ccc(cc1)[N+](=O)[O-])CC(=O)C
C2131	OB	OB+	27	c1c(ccc(c1)NC(=O)C)O
C2132	OB	OB+	27	S(=O)(=O)(c1sc(nm1)NC(=O)C)N
C2133	OB	OB+	26	ONC(=O)C
C2134	OB	OB-	27	[C@@H](C(=O)[O-])(NC(=O)C)CS
C2135	OB	OB+	27	c12c(nen1COCCO)c(=O)[nH]c(n2)N
C2136	OB	OB+	27	c1(c[n+](c(cn1)C)[O-])C(=O)[O-]
C2137	OB	OB+	27	c1(c(cc(c(c1)C)/C=C/C(=C/C(=O)[O-])C)/C)OC)C
C2138	OB	OB+	27	c1c(cc2c(c1)n1c(nnc1C[NH+])(C)C)CN=C2c1cccc1)Cl
C2139	OB	OB-	27	N(C1(CC[NH+](CC1)CCn1n(nnc1=O)CC)COC)(c1cccc1)C(=O)CC
C2140	OB	OB+	27	c12c(nc(nc1N)N(CCCN(=O)[C@@H]1OCCC1)C)cc(c(c2)OC)OC
C2141	OB	OB+	27	c1(c(cc2c(c1)nn[nH]2)OC)C(=O)NC[C@@H]1[NH+](CCC1)CC=C
C2142	OB	OB+	27	c12c([nH]nc1)nc[nH]c2=O
C2143	OB	OB+	27	C([NH+])1CCN(CC1)c1nc(nc(n1)NCC=C)NCC=C)(c1ccc(cc1)F)c1ccc(cc1)F
C2144	OB	OB+	27	S(=O)(=O)(N1CCCC1)C(c1cc2c(cc1)[nH]cc2CC[NH+](C)C
C2145	OB	OB+	27	c12c3c(nc1CCN(C2=O)C)c1c([nH]cn1)C)C)cccc3
C2146	OB	OB+	27	n12c(nnc1C)CN=C(c1c2ccc(c1)Cl)c1cccc1
C2147	OB	OB-	27	c1(c(ccc1)CC=C)OC[C@H](C[NH2+])C(C)O
C2148	OB	OB-	27	[C@H]1([C@H](C(=O)C[C@H]1O)CCCCC(=O)[O-])/C=C/[C@H](CCCC)O
C2149	OB	OB+	27	C12(CC3CC(C1)CC(C2)C3)[NH3+]
C2150	OB	OB+	27	c1(c(cc(cc1Br)Br)C[NH2+])C1CCC(CC1)O)N
C2151	OB	OB-	27	C(=N)[C@H]1[C@H]2N([C@@H](C(S2)(C)C)C(=O)[O-])C1=O)/N1CCCCC1
C2152	OB	OB-	27	C(=N)[C@H]1[C@H]2N([C@@H](C(S2)(C)C)C(=O)O)C(=O)C(C)(C)C1=O)/N1CCCCC1
C2153	OB	OB+	27	c1cc(ccc1)n1c(cc(=N)cn1)OC
C2154	OB	OB-	27	[C@H]1([C@H]([C@H]([C@H]([C@H]([C@H]1NC(=O)C@H](CCN)N)OC@H]1[C@@H]([C@H]([C@H]([C@H]([C@H]1CN)O)O)O)O)O)O)O)O)O)O)O)[C@@H]1([C@H]([C@H]([C@H]([C@H]([C@H]1CO)O)[NH3+])O
C2155	OB	OB+	27	c1(c(nc(c(n1)C1)N)N)C(=O)N=C(N)N
C2156	OB	OB+	27	c1cc(c2c(c1)nc1c(c2)Cn2c1cc1c(c2=O)CCC(=O)[C@@]1(CC)O)N
C2157	OB	OB+	27	[NH3+]CC(=O)CCC(=O)[O-]
C2158	OB	OB+	27	c1(c2c(oc1CCCC)cccc2)C(=O)c1cc(c(c1)I)OCC[NH+](CC)CC)I
C2159	OB	OB+	27	[C@@H]1([C@H](O)C[C@H]2[C@@H]1OC(O2)(C)C)[C@@H](CO)O)OCCC[NH+](C)C
C2160	OB	OB+	27	S(=O)(=O)(c1c(cc(c(c1)C(=O)NC[C@H]1[NH+](CCC1)CC)OC)N)CC





C2207	OB	OB+	27	c1(ccc(cc1)CCOCC1CC1)OC[C@@H](C[NH2+])C(C)C)O
C2208	OB	OB+	27	c1ccc(cc1)OC[C@H](C[NH2+])CCc1ccc(c1)OC)OC)O)C
C2209	OB	OB+	27	C(Oc1cccc(cc1)CCNC(=O)c1cccc1)(C(=O)[O-])(C)C
C2210	OB	OB-	27	c1(c(cccc1)OCCCC[NH2+])C)Cc1cccc1
C2211	OB	OB+	27	[C@@H]12[C@@H](NC(=O)N1)CS[C@H]2CCCCC(=O)[O-]
C2212	OB	OB+	27	[C@@]([C@H]1[C@H]2C[C@@H](C1)C=C2)(c1cccc1)(CC[NH+]1CCCCC1)O
C2213	OB	OB+	27	c1(ccc(cc1)COCCOC(C)C)OC[C@@H](C[NH2+])C(C)C)O
C2214	OB	OB+	27	c1(c(c(nc(n1)c1ncccn1)OCCO)Oc1c(cccc1)OC)NS(=O)(=O)c1ccc(cc1)C(C)C)C
C2215	OB	OB+	27	c1cccc(c1Br)C[N+](CC)(C)C
C2216	OB	OB+	27	Br1cc2c(cc1)NC(=O)CN=C2c1ncccc1
C2217	OB	OB+	27	c1(c(c(ccc1)CC(=O)[O-])N)C(=O)c1ccc(cc1)Br
C2218	OB	OB+	27	c1(c(c(cc(c1)Br)Br)N)C[NH+](C1CCCCC1)C
C2219	OB	OB+	27	[C@@H]12N(C(=O)[C@@H]([C@H]1C(C)C)NC(=O)[C@@H]1C=C3c4c5c(ccc4)N[C@H]([C@@H]5C[C@@H]3[NH+](C1)C)Br)[C@H](C(=O)N1[C@@H]2CCCC1)CC(C)C
C2220	OB	OB+	27	c1(c(cc(c(c1)Br)N)OC)C(=O)NCC[NH+](CC)CC
C2221	OB	OB+	27	Br1ccc(cc1)C(CC[NH+])(C)C)c1ncccc1
C2222	OB	OB+	27	n12c(nnc1C)CN=C(c1c2sc(c1)Br)c1c(cccc1)Cl
C2223	OB	OB+	27	c12c(c[nH]c1cccc2)CC([NH2+])C[C@H](COc1c(cccc1)C#N)O)(C)C
C2224	OB	OB+	27	[C@]12([C@]3([C@@H]([C@H]1[C@H]1[C@H]([C@H]([C@H](C2)O)[C@@]2(C(=CC(=O)C=C2)CC1)C)O[C@H](O3)CCC)C(=O)CO)C
C2225	OB	OB+	27	c1(c(cc(cc1OC)OC)OC)C(=O)CCC[NH+]1CCCC1
C2226	OB	OB+	27	c1ccc2c(c1CC)CC(=C2)[C@@H](O)C[NH2+])C(C)C)C
C2227	OB	OB+	27	c1(c(c(cc(c1)C(=O)[O-])NCCCC)Oc1cccc1)S(=O)(=O)N
C2228	OB	OB+	27	[C@]123[C@@]45[C@H]([NH+](CC1)CC1CC1)Cc1c2c(c(cc1)O)O[C@H]3[C@]([C@H](C4)[C@@](C(C)C)C)O)C(CC5)OC
C2229	OB	OB-	27	C12(CC(=O)N(C(=O)C1)CCCC[NH+]1CCN(CC1)c1ncccn1)CCCC2
C2230	OB	OB+	27	S(=O)(=O)(OCCCCOS(=O)(=O)C)C
C2231	OB	OB-	27	[C@]123[C@]([C@H]([NH+](CC1)CC1CC1)Cc1c2cc(cc1)O)(CCCC3)O
C2232	OB	OB-	27	[N+]1(C2C3C(C1CC(C2)OC(=O)C(c1cccc1)CO)O3)(CCCC)C
C2233	OB	OB+	27	c12c3cccc1[nH]cc2C[C@@H]1[C@@H]3C[C@H](C[NH+]1CC=C)C(=O)N(C(=O)NCC)CCCN(C)C
C2234	OB	OB+	27	c12c(nen1C)n(c(=O)n(c2=O)C)C
C2235	OB	OB+	27	[C@]12([C@H](/C=C/C=C/3)C=C)[C@H](C[C@@H](C3)O)O)/CCC1)CC[C@@H]2[C@H](CCCC(O)C)C)C
C2236	OB	OB+	27	c12n(c(nc1cccc2C(=O)[O-])OCC)Cc1ccc(cc1)c1c(cccc1)c1n[nH]nn1
C2237	OB	OB+	27	[C@H]1(n2c(=O)nc(c2)F)NC(=O)OCCCC[C@@H]([C@@H]([C@H](O1)C)O)O
C2238	OB	OB+	27	N1([C@@H](C(=O)[O-])CCC1)C(=O)[C@H](CS)C
C2239	OB	OB+	27	N1(c2c(cccc2)C=Cc2c1cccc2)C(=O)N
C2240	OB	OB+	27	N12[C@@H]([C@@H](C1=O)NC(=O)C(c1cccc1)C(=O)O)SC([C@@H]2C(=O)[O-])(C)C
C2241	OB	OB-	27	n1(c(=S)n(cc1)C)C(=O)OCC
C2242	OB	OB-	27	C1CCN(N=O)C(=O)NCCCC1
C2243	OB	OB-	27	[O-]C(=O)C[C@@H](OC(=O)C)C[N+](C)(C)C
C2244	OB	OB+	27	c1cc(c2c(c1)NC(=O)CC2)OC[C@@H](O)C[NH2+])C(C)C)C
C2245	OB	OB+	27	c12c3c([nH]c1cccc2CO[C@@H](C[NH2+])CCOc1c(cccc1)OC)O)cccc3
C2246	OB	OB-	27	N12[C@@H]([C@@H](C1=O)NC(=O)CC#N)SCC(=C2C(=O)[O-])COC(=O)C
C2247	OB	OB+	27	N12[C@@H]([C@@H](C1=O)NC(=O)C(c1cccc1)[NH3+])SCC(=C2C(=O)[O-])Cl
C2248	OB	OB+	27	N12[C@@H]([C@@H](C1=O)NC(=O)C(c1ccc(cc1)O)[NH3+])SCC(=C2C(=O)[O-])C
C2249	OB	OB+	27	N12[C@@H]([C@@H](C1=O)NC(=O)C(c1ccc(cc1)O)[NH3+])SCC(=C2C(=O)[O-])CSc1nn[nH]c1
C2250	OB	OB-	27	N12[C@@H]([C@@H](C1=O)NC(=O)Cn1nnc1)SCC(=C2C(=O)[O-])CSc1sc(nn1)C
C2251	OB	OB-	27	N12[C@@H]([C@@H](C1=O)NC(=O)/C=N/O)/c1sc(nc1)N)SCC(=C2C(=O)[O-])C=C
C2252	OB	OB+	27	N12[C@@H]([C@@H](C1=O)NC(=O)/C=N/C(=O)CC(=O)O)/c1sc(nc1)N)SCC(=C2C(=O)[O-])C=C

C2253	OB	OB-	27	N12[C@@H]([C@@H](C1=O)NC(=O)/C(=N/OC)/c1nc(sc1)N)SCC(=C2C(=O)[O-])CSc1sc(c(n1)C)CC(=O)O
C2254	OB	OB-	27	N12[C@@H]([C@@H]([C@@H](C1=O)NC(=O)[C@@H](c1ccc(cc1)O)NC(=O)N1C(=O)C(=O)N(CC1)CC)SCC(=C2C(=O)[O-])CSc1n(nnn1)C
C2255	OB	OB-	27	N12[C@@H]([C@@H]([C@@H](C1=O)NC(=O)/C(=N/OC)/c1nc(sc1)N)SCC(=C2C(=O)[O-])COC(=O)C
C2256	OB	OB-	27	[C@]1([C@@H]2N(C1=O)C(=C(CS2)COC(=O)N)C(=O)[O-])(NC(=O)Cc1csc1)OC
C2257	OB	OB+	27	N(=C(\C(=O)N[C@H]1[C@@H]2N(C(=C(CS2)COC)C(=O)O[C@@H](OC(=O)OC(C)C)C1=O)/c1nc(sc1)N)\OC
C2258	OB	OB+	27	N12[C@@H]([C@@H]([C@@H](C1=O)NC(=O)C(c1ccc(cc1)O)[NH3+])SCC(=C2C(=O)[O-])/C=C/C
C2259	OB	OB-	27	N(=C(\C(=O)N[C@H]1[C@@H]2N(C(=C(CS2)C[n+]2cccc2)C(=O)[O-])C1=O)/c1nc(sc1)N)\OC(C(=O)[O-])(C)C
C2260	OB	OB+	27	S1[C@H]2N(C(=O)[C@H]2NC(=O)/C(=C\CC(=O)O)/c2nc(sc2)N)C(=CC1)C(=O)[O-]
C2261	OB	OB-	27	N(=C(\C(=O)N[C@H]1[C@@H]2N(C1=O)C(=CCS2)C(=O)[O-])/c1nc(sc1)N)\OC
C2262	OB	OB-	27	N(=C(\C(=O)N[C@H]1[C@@H]2N(C1=O)C(=C(CS2)CSc1nc(=O)c(nn1)C)O)C(=O)[O-])/c1nc(sc1)N)\OC
C2263	OB	OB+	27	N(=C(\C(=O)N[C@H]1[C@@H]2N(C(=C(CS2)COC(=O)N)C(=O)[O-])C1=O)/c1occc1)\OC
C2264	OB	OB+	27	c1(c(cc(cc1)NC(=O)N(CC)CC)C(=O)C)OC[C@@H](O)C[NH2+][C(C)(C)C
C2265	OB	OB+	27	N12[C@H]([C@@H]([C@@H](C1=O)NC(=O)C(c1cccc1)[NH3+])SCC(=C2C(=O)[O-])C
C2266	OB	OB-	27	N12[C@@H]([C@@H]([C@@H](C1=O)NC(=O)Cc1csc1)SCC(=C2C(=O)[O-])COC(=O)C
C2267	OB	OB-	27	N12[C@H]([C@@H]([C@@H](C1=O)NC(=O)CSc1cnc1)SCC(=C2C(=O)[O-])COC(=O)C
C2268	OB	OB+	27	N12[C@@H]([C@@H]([C@@H](C1=O)NC(=O)C(C1=CCC=CC1)[NH3+])SCC(=C2C(=O)[O-])C
C2269	OB	OB+	27	C(=C\c1c(c(nc1C(C)C)C)COC)c1ccc(cc1)F/[C@H](C[C@H](CC(=O)[O-])O)O
C2270	OB	OB+	27	[C@H]([NH+])1CC[NH+](CC1)CCOCC(=O)[O-](c1ccc(cc1)Cl)c1cccc1
C2271	OB	OB+	27	c1(ccc(cc1)CCCC(=O)[O-])N(CCC1)CCCl
C2272	OB	OB+	27	c1c(ccc(c1)[N+](=O)[O-])C(O)C(COC(=O)CCCCCCCCCCCCC)NC(=O)C(Cl)Cl
C2273	OB	OB+	27	c12c(ccc(c1)Cl)N=C(C[N+](=C2c1cccc1)[O-])NC
C2274	OB	OB-	27	Clc1ccc(cc1)N/C(=N/C(=N/CCCCC)/N=C(N=C(Nc1ccc(cc1)Cl)N)N)/N
C2275	OB	OB+	27	Clc1ccc(cc1)C1S(=O)(=O)CCC(=O)N1C
C2276	OB	OB+	27	c12c(ccnc1cc(cc2)Cl)N(CCCC[NH+](CC)CC)C
C2277	OB	OB-	27	S1(=O)(=O)c2c(cc(c2)S(=O)(=O)N)Cl)N=CN1
C2278	OB	OB+	27	c1(cc(c2c(c1O)nc2)Cl)Cl
C2279	OB	OB+	27	N(c1ccc(cc1)Cl)(c1ncccc1)CC[NH+](C)C
C2280	OB	OB+	27	c12c(ccc(c1)Cl)Sc1c(cccc1)N2CCC[NH+](C)C
C2281	OB	OB+	27	c1c(ccc(c1)Cl)S(=O)(=O)[N-]C(=O)NCCC
C2282	OB	OB+	27	C(=C\1/c2c(ccc(c2)Cl)Sc2c1cccc2)\CC[NH+](C)C
C2283	OB	OB+	27	[C@@]12([C@H]([C@@H]([C@@H](C(=C(C1=O)C(=O)N)O)[NH+](C)C)C[C@H]1C(=C2O)C(=O)c2c(c(ccc2O)Cl)[C@]1(O)C)O
C2284	OB	OB+	27	c1ccc2c(c1)C(=O)N[C@]2(O)c1ccc(c(c1)S(=O)(=O)N)Cl
C2285	OB	OB+	27	C1([C@@H](C1)C1=NCCN1)(c1cccc1)c1cccc1
C2286	OB	OB+	27	C(=C\1/C[C@@H]2[C@H]([C@@H]([C@@H](C[C@@H]2C1)O)C#C[C@H]([C@H](CC#CCC)C)O)/COCC(=O)[O-]
C2287	OB	OB+	27	C1CC1COCCOc1ccc(cc1)OCC(CCC(C)C)O
C2288	OB	OB+	27	N12C(=O)[C@H]([NH2+][C@H](C(=O)OCC)CCc3cccc3)CCC[NH+]1CCC[C@H]2C(=O)[O-]
C2289	OB	OB+	27	c1cccc(c1)CC[C@H](N[C@@H]1C(=O)N2[NH+](CCC1)CCC[C@H]2C(=O)[O-])C(=O)[O-]
C2290	OB	OB+	27	C1(c2cc(c(cc2)OC)OC2CCCC2)(CCC(CC1)C(=O)[O-])C#N
C2291	OB	OB-	27	c1(c([nH]cn1)C)SCCN/C(=N/C)/NC#N
C2292	OB	OB-	27	[C@@H]12[C@@H]([C@@H]([C@@H]3CC(C[C@H]1[N+])3(CC1CC1)C)OC(=O)[C@@H](c1cccc1)CO)O2
C2293	OB	OB-	27	c1c(cc(cc1)CCC[NH2+][C@@H](c1ccc2c1cccc2)C)C(F)F
C2294	OB	OB+	27	Clc1cc2c(cc1)N(CCC#N)C(=O)C(O)N=C2c1c(ccc1)F
C2295	OB	OB+	27	C1([C@@H](C1)c1ccc(cc1)OC(C(=O)[O-])(C)C)(Cl)Cl
C2296	OB	OB+	27	c12c(cc(c(n1)N1CCCC1)F)c(=O)c(en2C1CC1)C(=O)[O-]
C2297	OB	OB+	27	c1(c(cc(c(c1)Cl)N)OC)C(=O)N[C@@H]1[C@@H](C[NH+](CC1)CCCOc1ccc(cc1)F)OC
C2298	OB	OB+	27	[C@]1(c2c(cc(cc2)C#N)CO1)(c1ccc(cc1)F)CCC[NH+](C)C







C2437	OB	OB+	27	Fe1cn([C@@H]2O[C@@H]([C@@H](O)C2)CO)c(=O)[nH]c1=O
C2438	OB	OB+	27	c1c(c(cc1)F)c1noc(c1C(=O)NC1C(=O)N2C1SC(C2(C(=O)[O-])C)(C)C)C1
C2439	OB	OB+	27	c1(c(cc(cc1)F)F)C(Cn1ncn1)(Cn1ncn1)O
C2440	OB	OB+	27	c1(nc(=O)[nH]cc1F)N
C2441	OB	OB-	27	c1c(cc2c(c1)n1c(c(nc1)C(=O)OCC)CN(C2=O)C)F
C2442	OB	OB-	27	[C@@]12([C@@]3([C@@H](C[C@H]1O(CO2)(C)C)[C@H]1[C@H]([C@H](C3)O)[C@@]2(C(=CC(=O)C=C2)[C@H](C1)F)C)C(=O)CO
C2443	OB	OB+	27	c12c(ccc(c1)[N+](=O)[O-])N(C(=O)CN=C2c1c(cccc1)F)C
C2444	OB	OB+	27	[C@@H]12[C@@]3(C(=CC(=O)C=C3)[C@H](C[C@H]1[C@H]1[C@])(C[C@@H]2O)([C@H]([C@@H](C1)C)C(=O)CO)C)F)C
C2445	OB	OB+	27	C12(c3c(cccc3)C(=O)O1)c1c(cc(cc1)O)Oc1c2ccc(c1)O
C2446	OB	OB+	27	c1(=O)c([nH]c(=O)[nH]1)F
C2447	OB	OB+	27	C(c1cccc(c1)O[C@H](c1cccc1)CC[NH2+]C)(F)(F)F
C2448	OB	OB+	27	F[C@@]12[C@H]([C@H]3[C@@])([C@@](O)(CC3)C)(C[C@@H]1O)C)CCC1=CC(=O)CC[C@@]21C
C2449	OB	OB+	27	C1(=C\CC[NH+]2CCN(CC2)CCO)/c2c(ccc(c2)C(F)(F)F)Sc2c1cccc2
C2450	OB	OB-	27	N1(c2c(ccc(c2)C(F)(F)F)Sc2c1cccc2)CCC[NH+]1CCN(CC1)CCO
C2451	OB	OB+	27	c1(c(nc(cc1)NCc1ccc(cc1)F)N)NC(=O)OCC
C2452	OB	OB+	27	c12c(ccc(c1)Cl)N(C(=O)CN=C2c1c(cccc1)F)CC[NH+](CC)CC
C2453	OB	OB+	27	c1(cc(ccc1)F)c1ccc(cc1)[C@H](C(=O)[O-])C
C2454	OB	OB+	27	C(c1c(ccc(c1)NC(=O)C(C)C)[N+](=O)[O-])(F)(F)F
C2455	OB	OB-	27	[C@]12([C@@]3(C(=CC(=O)C=C3)[C@H](C[C@H]1[C@H]1[C@])(C[C@@H]2O)([C@]([C@@H](C1)C)C(=O)SCF)OC(=O)CC)C)F)C)F
C2456	OB	OB+	27	c1(c(n(c2c1cccc2)C(C)C)/C=C/[C@H](C[C@H](CC(=O)[O-])O)O)c1ccc(cc1)F
C2457	OB	OB+	27	c1(ccc(cc1)C(=N/OCC[NH3+])/CCCCOC)C(F)(F)F
C2458	OB	OB+	27	N1([C@@H](C[C@H](C1)C1CCCC1)C(=O)[O-])C(=O)CP(=O)(O[C@H](OC(=O)CC)C(C)C)CCCCc1cccc1
C2459	OB	OB+	27	c12c3c([nH]c1ccc(c2)C(=O)N)CC[C@H](C3)[NH2+]C
C2460	OB	OB+	27	[C@]1([C@H]([C@H]([C@@H](CO1)O)O)O)(CO)O
C2461	OB	OB+	27	c1(c(cc(cc1)NCc1ccc1)Cl)S(=O)(=O)N)C(=O)[O-]
C2462	OB	OB+	27	C(=C1/[C@H]2[C@@]([C@@]3([C@@H]([C@@]4([C@@H](CC3)[C@@H]([C@@H](CC4)O)C)C)[C@@H](C2)O)C)(C[C@@H]1OC(=O)C)\(C(=O)[O-])/CCC=C(C)C
C2463	OB	OB-	27	c1c2c(cc3c1OCCO3)nc1c(c2C[NH+]2CCN(CC2)C)Cn2c1cc1c(c2=O)COC(=O)[C@@H]1CC
C2464	OB	OB+	27	C1(C(=O)[O-])(CCCC1)C[NH3+]
C2465	OB	OB+	27	c1(ccc2c3c1O[C@@H]1[C@@]3(CC[NH+](C2)C)C=C[C@@H](C1)O)OC
C2466	OB	OB-	27	c12c(ccn1COC(CO)CO)c(=O)[nH]c(n2)N
C2467	OB	OB+	27	c12c(cc(c(c1OC)N1C[C@H]([NH2+]CC1)C)F)c(=O)c(cn2C1CC1)C(=O)[O-]
C2468	OB	OB+	27	c1(c(cc2c(c1)c(nen2)Nc1ccc(c(c1)Cl)F)OC)OCCC[NH+]1CCOCC1
C2469	OB	OB+	27	c1(c(ccc(c1)C)C)OCCCC(C(=O)[O-])(C)C
C2470	OB	OB+	27	Fe1c(nc2c(c1)c(=O)c(cn2C1CC1)C(=O)[O-])N1CC(/C(=N\OC)/C1)C[NH3+]
C2471	OB	OB+	27	n1(cncn1)C[C@]([C@@H](C)S(=O)(=O)C)(c1c(cc(cc1)F)F)O
C2472	OB	OB-	27	[C@H]1([C@H]([C@@H]([C@H](C[C@H]1N)N)O)[C@@H]1[C@@H](CC[C@H](O1)[C@H](NC)C)N)O)[C@@H]1[C@@H]([C@H]([C@](CO1)(O)C)[NH2+]C)O
C2473	OB	OB-	27	[C@H]1([C@H]([C@@H]([C@H](C[C@H]1N)N)O)[C@@H]1[C@@H](CC[C@H](O1)CC)N)O)[C@@H]1[C@@H]([C@H]([C@](CO1)(O)C)[NH2+]C)O
C2474	OB	OB+	27	[C@@]12([C@@](C=C[C@H]1[C@H]1[C@H](CC2)[C@@H]2C(=CC(=O)CC2)CC1)(C#C)O)CC
C2475	OB	OB+	27	S(=O)(=O)(c1ccc(cc1)CCNC(=O)c1c(ccc(c1)Cl)OC)[N-]C(=O)NC1CCCCC1
C2476	OB	OB+	27	c1(ccc(cc1)C)S(=O)(=O)[N-]C(=O)N[NH+]1C[C@H]2[C@@H](C1)CCCC
C2477	OB	OB+	27	N1(C(=O)C(=C(C1)C)C)C(=O)NCCc1ccc(cc1)S(=O)(=O)[N-]C(=O)NC1CCC(CC1)C
C2478	OB	OB+	27	S(=O)(=O)(c1ccc(cc1)CCNC(=O)c1ncc(nc1)C)[N-]C(=O)NC1CCCCC1
C2479	OB	OB+	27	[C@@H]1([C@@H]([C@H](O[C@H]([C@@H]1[NH3+])O)CO)O)O
C2480	OB	OB+	27	OC[C@H](O)CO[N+](=O)[O-]
C2481	OB	OB-	27	C1([C@@](C(=O)O)[C@@H]2CC[N+](C2)(C)C)(O)c2cccc2)CCCC1
C2482	OB	OB+	27	c12c(nn(c1cccc2)C)C(=O)NC1C[C@@H]2[NH+](C[C@@H](C1)CCC2)C





C2529	OB	OB+	27	n12c(ccc1C(=O)c1cccc1)[C@H](CC2)C(=O)[O-]
C2530	OB	OB+	27	s1c2c(cc1)/C(=C\1/CC[NH+](CC1)C)c1c(ccc1)CC2=O
C2531	OB	OB+	27	c1cc2c(cc1O)c(c[nH]2)C[C@H](C(=O)[O-])[NH3+]
C2532	OB	OB+	27	[C@H](C(=O)[O-])(CCCN=C(N)N)[NH3+]
C2533	OB	OB+	27	c1(c(ccc1)[C@H](C[NH2+][C@H](CCc1cccc1)C)O)C(=O)N
C2534	OB	OB-	27	[C@]1([C@H]([C@@H]([C@H](O1)CO)O[C@H]1[C@@H]([C@H]([C@H]([C@H](O1)CO)O)O)O)(CO)O
C2535	OB	OB+	27	[C@H]1(N2C(=O)N=C(CC2)N)O[C@H](SC1)CO
C2536	OB	OB+	27	c1(c(nc(nn1)N)N)c1c(c(cc1)Cl)Cl
C2537	OB	OB+	27	c1([nH]c2c(n1)cccc2)S(=O)Cc1ccc(cen1)C)OCC(F)(F)F
C2538	OB	OB-	27	Clc1cc(ccc1OCc1cc(ccc1)F)Nc1ncnc2c1cc(cc2)c1oc(cc1)C[NH2+]CCS(=O)(=O)C
C2539	OB	OB-	27	[C@]1([C@@H]2N(C1=O)C=C(CO2)CSc1n(nnn1)C)C(=O)[O-](NC(=O)[C@@H](c1ccc(cc1)O)C(=O)O)OC
C2540	OB	OB+	27	FC(F)(F)c1ccc(cc1)NC(=O)c1c(oc1)C O(C(C[NH+](CCC(c1cccc1)c1cccc1)C)(C)C)C(=O)C1=C(NC(=C(C1c1ccc(cc1)[N+](=O)[O-
C2541	OB	OB-	27	)]C(=O)OC)C
C2542	OB	OB+	27	C(c1ccc(cc1)C#N)(c1ccc(cc1)C#N)n1nnc1
C2543	OB	OB+	27	[C@@H]1(c2cccc2)N=C2N(C1)CCS2
C2544	OB	OB+	27	N1(C(C(=O)N)CC)C(=O)CCC1
C2545	OB	OB+	27	O(c1c2c(ccc1)C(=O)CCC2)C[C@@H](O)C[NH2+]C(C)(C)C
C2546	OB	OB+	27	Fc1ccc(cc1)C1(CCC([NH+]2C[C@H]([C@](CC2)(c2cccc2)C(=O)[O-])C)CC1)C#N
C2547	OB	OB+	27	c12c3ccc(c1OCC(n2cc(c3=O)C(=O)[O-])C)N1CC[NH+](CC1)CF
C2548	OB	OB+	27	[C@]12([C@@](CC[C@H]1[C@H]1[C@H](CC2)[C@@H]2C(=CC(=O)CC2)CC1)(C#C)O)CC
C2549	OB	OB+	27	C12(c3c(ccc3)C(c3c1cccc3)CC2)C[C@H](C[NH2+]C)O
C2550	OB	OB+	27	c1(ccc(cc1)NN=C(C#N)C#N)C1=NNC(=O)C[C@H]1C
C2551	OB	OB+	27	c1(c(ccc1C)C)NC(=O)C[NH+](CC)CC
C2552	OB	OB+	27	[C@@H]1([C@H](NC(=O)[C@@H]2[NH+](C[C@@H](C2)CCC)C)[C@@H](O)C)[C@@H]([C@@H]([C@H]([C@H](O1)SC)O)O)O
C2553	OB	OB+	27	c1(cc(cc1)N1CCOCC1)F)N1C(=O)O[C@H](C1)CNC(=O)C
C2554	OB	OB+	26	S1SCC[C@H]1CCCCC(=O)[O-]
C2555	OB	OB+	27	N1(C(=O)[C@@H]([NH2+][C@@H](CCc2cccc2)C(=O)[O-])CCCCN)[C@@H](CCC1)C(=O)[O-]
C2556	OB	OB-	27	c12c3cccc1[nH]cc2C[C@H]1C3=C[C@@H](C[NH+]1C)NC(=O)N(CC)CC
C2557	OB	OB+	27	Clc1c(c(ccc1)Cl)OC(C1=NCCN1)C
C2558	OB	OB+	27	c12c(cc(c1F)N1C[C@H]([NH2+][CC1)C)F)c(=O)c(cn2CC)C(=O)[O-]
C2559	OB	OB+	27	ClCCN(N=O)C(=O)NC1CCCCC1
C2560	OB	OB+	27	C(c1cccc1)(c1cccc1)(C(=O)N(C)C)CC[NH+]1CCC(CC1)(c1ccc(cc1)Cl)O
C2561	OB	OB+	27	c1ccc(cc1)[C@@H]([NH3+])C[NH2+][C@@H]1C(=O)N2[C@@H]1CCC(=C2C(=O)[O-])Cl
C2562	OB	OB+	27	C1(=C2CCN(CC2)C(=O)OCC)c2c(cc(cc2)Cl)CCc2c1nccc2
C2563	OB	OB+	27	C1(=N[C@@H](C(=O)Nc2c1cc(cc2)Cl)O)c1c(ccc1)Cl
C2564	OB	OB+	27	c1cc(ccc1Cl)N(C(=O)Cc1cccc1)C1CC[NH+](CC1)C(C)C
C2565	OB	OB+	27	c12c(ccc(c1)Cl)N(C(=O)[C@H](N=C2c1c(ccc1)Cl)O)C
C2566	OB	OB+	27	n1(c(nc(c1CO)Cl)CCCC)Cc1ccc(cc1)c1c(ccc1)c1[n-]nnn1
C2567	OB	OB-	26	ClCOC(=O)[C@]1(OC(=O)OCC)[C@@]2([C@H]([C@H]3[C@H]([C@@H](O)C2)[C@@]2(C(=CC(=O)C=C2)CC3)C)CC1)C
C2568	OB	OB-	27	c12c3ccc(c1c1cc(cc2c(=O)n(c3=O)[NH2+][NC(=O)NN)S(=O)(=O)[O-])N)S(=O)(=O)[O-]
C2569	OB	OB+	27	c1(ccc(c1)CC(=O)[O-])Nc1c(ccc1Cl)F)C
C2570	OB	OB+	27	[C@]12([C@](CC[C@@H]1[C@@H]1[C@@H](CC2)[C@H]2C(=CCCC2)CC1)(O)C#C)C
C2571	OB	OB-	27	[C@H]([C@@H]([C@@H](CO)O)O)([C@@H](CO)O)O
C2572	OB	OB+	27	c1ccc2c(c1)C1(c3c(ccc3)C2CC1)CCC[NH2+]C
C2573	OB	OB+	27	FC1(F)CCC(C(=O)N[C@@H](CC[NH+]2[C@H]3CC(n4c(nnc4C)C(C)C)C[C@@H]2CC3)c2cccc2)CC1
C2574	OB	OB-	27	[C@@H]12c3c(cc(cc3O)CCCC)OC([C@@H]1CCC(=C2)C)(C)C

C2575	OB	OB+	27	C1c1cccc(cc1)C1(O)N2C(=NCC2)c2c1cccc2
C2576	OB	OB+	27	c12c(nc([nH]1)NC(=O)OC)ccc(c2)C(=O)c1cccc1
C2577	OB	OB+	26	C1c1c(c(ccc1C)Cl)Nc1c(cccc1)C(=O)[O-]
C2578	OB	OB+	27	c1cccc(c1)OC(C[NH+](C)C)Oc1cccc1
C2579	OB	OB+	27	c1c(ccc2c1OCO2)CC[C@@H]([NH2+][C[C@@H](c1cc(c(cc1)O)C(=O)N)O)C
C2580	OB	OB-	27	[C@]12([C@H]([C@H]3[C@H](CC1)[C@@]1(C(=CC(=O)CC1)[C@H](C3)C)C)CC[C@@]2(C(=O)C)O)C
C2581	OB	OB-	27	[C@]12([C@](CC[C@H]1[C@H]1[C@H](CC2)[C@@]2(C(=CC(=O)CC2)[C@H](C1)C)C)(C(=O)C)OC(=O)C)C
C2582	OB	OB+	26	[O-]C(=O)c1c(cccc1)Nc1c(ccc1)C)C
C2583	OB	OB+	27	c12c(c(ccn1)C(F)(F)F)[C@@H]([C@H]1[NH2+][CCCC1)O)cccc2C(F)(F)F
C2584	OB	OB-	27	N1([C@H](C(=O)NCc2ccc(cc2)C(=N)N)CC1)C(=O)[C@@H](C1CCCCC1)[NH2+][CC(=O)[O-]
C2585	OB	OB-	27	c12c(ccc(c1)OC)N=C[C@H]2CCNC(=O)C
C2586	OB	OB+	27	S1(=O)(=O)c2c(cccc2)C(=C(N1C)C(=O)Nc1sc(en1)C)O
C2587	OB	OB+	27	N(c1ccc(cc1)C[C@H](C(=O)[O-])[NH3+])(CCCC)CCCI
C2588	OB	OB+	27	[NH3+]C12CC3(CC(C1)(CC(C3)C2)C)C
C2589	OB	OB+	27	c1cccc(c1)C1(C(=O)OCC)CC[NH+](CC1)C
C2590	OB	OB+	27	c12c([nH]c(c1)C)cccc2OC[C@H](C[NH2+](C)C)O
C2591	OB	OB+	27	O=C(Nc1c(cccc1)C)C1[NH+](CCCC1)C
C2592	OB	OB-	27	[C@@]1(c2cc(ccc2)O)(C[NH+](CCCC1)C)CC
C2593	OB	OB-	27	c12c(nc[nH]1)[nH]cnc2=S
C2594	OB	OB-	27	[C@@H]12N(C=C([C@@H]1C)S[C@@H]1[NH2+][C@@H](CC1)C(=O)N(C)C)C(=O)[O-]C(=O)[C@@H]2[C@H](O)C
C2595	OB	OB+	27	c1c(ccc(c1C(=O)[O-])O)N
C2596	OB	OB+	27	C(S(=O)(=O)[O-])CS
C2597	OB	OB+	27	c12e3cccc1n(cc2C[C@@H]1[C@@H]3C[C@H](C[NH+](C)C)CNC(=O)OCc1cccc1)C
C2598	OB	OB+	27	C(=N)(N(C)C)NC(=N)N
C2599	OB	OB+	27	c1cc(c2c(c1)C(=C)[C@@H]1[C@@H](C2=O)[C@H]([C@]2([C@@H]([C@H]1C)[C@@H]([C@H]([C@@H](C2=O)C(=O)N)O)[NH+](C)C)O)O)O
C2600	OB	OB+	27	C(c1cccc1)(c1cccc1)(C(=O)CC)C[C@H]([NH+](C)C)C
C2601	OB	OB+	26	c1(ccccc1)C(c1cccc1)(CC([NH+](C)C)C)C(CC)OC(=O)C
C2602	OB	OB+	27	c1(ccccc1)C[C@@H]([NH2+])C
C2603	OB	OB-	27	N(c1ncccc1)(Cc1sccc1)CC[NH+](C)C
C2604	OB	OB+	27	n1(c(=S)[nH]cc1)C
C2605	OB	OB+	27	c12c(ncc(n1)CN(c1ccc(cc1)C(=O)N[C@H](C(=O)[O-])CCC(=O)O)C)nc(nc2N)N
C2606	OB	OB+	27	[C@@](C(=O)[O-])(Cc1cc(c(cc1)O)O)([NH3+])C
C2607	OB	OB+	27	c1cc2c3c(c1)C1=C[C@H](C[NH+])([C@@H]1Cc3c[nH]2)C)C(=O)N[C@@H](CC)CO
C2608	OB	OB+	27	C1CCC[C@@H]([NH2+])1[C@@H](c1cccc1)C(=O)OC
C2609	OB	OB+	27	c1(ccccc1)C1(C(=O)NC(=O)N(C1=O)C)CC
C2610	OB	OB+	27	[C@]12([C@H]([C@H]3[C@H]([C@H](C1)O)[C@@]1(C(=CC(=O)C=C1)[C@H](C3)C)C)CC[C@@]2(C(=O)CO)O)C
C2611	OB	OB-	27	c12c3cccc1n(cc2C[C@@H]1C3=C[C@H](C[NH+](C)C)C(=O)N[C@H](CO)CC)C
C2612	OB	OB-	27	S1[C@H]2N([C@H](C1(C)C)C(=O)[O-])C(=O)[C@H]2NC(=O)c1c(cccc1OC)OC
C2613	OB	OB+	27	c1(c(cc(c(c1)Cl)N)OC)C(=O)NCC[NH+](CC)CC
C2614	OB	OB+	27	c12c(cc(c(c1)S(=O)(=O)N)Cl)N[C@H](N(C2=O)c1c(cccc1)C)C
C2615	OB	OB-	27	N1(c2c(ccc(c2)S(=O)(=O)C)Sc2c1cccc2)CCC[NH+](C)CC(C1)C(=O)N
C2616	OB	OB+	27	c1(ccc(cc1)CCOC)OC[C@@H](C[NH2+](C)C)O
C2617	OB	OB+	27	n1(c(enc1C)[N+](=O)[O-])CCO
C2618	OB	OB+	27	c1(c(cccc1)C)OC[C@H]([NH3+])C
C2619	OB	OB+	27	N12[C@@H](c3c(cccc3)Cc3c1cccc3)C[NH+](CC2)C
C2620	OB	OB+	27	[C@H]1([C@@](CCc2c1ccc(c2)F)(OC(=O)CC)CC[NH+](CCCc1[nH]c2c(n1)cccc2)C)C)C



C2667	OB	OB+	27	<chem>n1(c2c(c(ccc2)C)[nH]c(=O)c2c1nccc2)C1CC1</chem>
C2668	OB	OB+	27	<chem>c12c(cccc1OC[C@H](C[NH2+]C(C)C)O)CCCN2C(=O)c1cnccc1</chem>
C2669	OB	OB+	27	<chem>c1(c(c(cc(c1C(=O)OC)C)[N+](=O)[O-])C(=O)OCC[NH+](Cc1cccc1)C)C1C=C(NC(=C1)C)C</chem>
C2670	OB	OB-	27	<chem>Br1cc(ene1)C(=O)OC[C@H]1C[C@@]2(OC)[C@H]([NH+](C1)C)Cc1c3e2cccc3n(c1)C</chem>
C2671	OB	OB+	27	<chem>c1(cnccc1)C(=O)NCCO[N+](=O)[O-]</chem>
C2672	OB	OB+	27	<chem>[C@H]1(c2cnccc2)[NH+](CCC1)C</chem>
C2673	OB	OB+	27	<chem>FC(F)(F)c1cc(cc(c1)NC(=O)c1cc(c(cc1)C)Ne1nc(cen1)c1cccnc1)n1cc(nc1)C</chem>
C2674	OB	OB+	27	<chem>FC(F)(F)c1cc(ccc1[N+](=O)[O-])N1C(=O)C(NC1=O)(C)C</chem>
C2675	OB	OB+	27	<chem>s1c(ncc1[N+](=O)[O-])NC(=O)c1c(cccc1)OC(=O)C</chem>
C2676	OB	OB+	27	<chem>FC(F)(F)c1cc(c(c1)C(=O)C1C(=O)CCCC1=O)[N+](=O)[O-] c12c(ccc(c1)[N+](=O)[O-])NC(=O)CN=C2c1cccc1 N1(C(=O)NC(=O)C1)/N=C/c1oc(cc1)[N+](=O)[O-]</chem>
C2677	OB	OB+	27	<chem>C(CO[N+](=O)[O-])(CO[N+](=O)[O-])O[N+](=O)[O-]</chem>
C2678	OB	OB+	27	<chem>c1(nc(sc1)C[NH+](C)C)CSCCN/C(=C/[N+](=O)[O-])/NC</chem>
C2679	OB	OB-	27	<chem>[NH+]1[C[C@H](c2c(c(ccc2)N)C1)c1cccc1)C</chem>
C2680	OB	OB+	27	<chem>c12c(ccc(c1)Cl)NC(=O)CN=C2c1cccc1</chem>
C2681	OB	OB+	27	<chem>c1(cc(c(cc1)O)O)[C@H](C[NH3+])O</chem>
C2682	OB	OB+	27	<chem>[C@]12([C@@H]([C@@H]3[C@@H](CC1)[C@H]1C(=CC(=O)CC1)CC3)CC[C@]2(C#C)O)C</chem>
C2683	OB	OB-	27	<chem>c1(cc(ccc1)O)[C@H](C[NH3+])O</chem>
C2684	OB	OB+	27	<chem>c1(cccc(c1)C(F)(F)F)CC(C)[NH3+]</chem>
C2685	OB	OB-	27	<chem>c12c(cc(c(c1)N1CC[NH2+]CC1)F)c(=O)c(en2CC)C(=O)[O-]</chem>
C2686	OB	OB+	27	<chem>[C@]12([C@@]([C@]1[C@H]1[C@H]1[C@H](C=C2)[C@@H]2C(=CC(=O)CC2)CC1)(C#C)O)CC</chem>
C2687	OB	OB+	27	<chem>c1ccc2c(c1)CCc1c(cccc1)C2=CCC[NH2+]C</chem>
C2688	OB	OB+	27	<chem>c1c(cccn1)/C(=C/C[NH2+]C)/c1ccc(cc1)Br</chem>
C2689	OB	OB+	27	<chem>[C@@H]1(c2c(c3c(cc2CC[NH+]1C)OCO3)OC)C1c2c(c(c(cc2)OC)OC)C(=O)O1</chem>
C2690	OB	OB+	27	<chem>O1C([C@H](OC)[C@@H](OC(=O)N)[C@H](O)[C@H]1O)c1c(c2c(cc1)c(=O)c(c(o2)O)NC(=O)c1cc(c(cc1)O)CC=C(C)C)(C)C</chem>
C2691	OB	OB+	27	<chem>e12c(c[nH]c1cccc2)C[C@H]1C(=O)N[C@@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C@H)(O)CO)CSSC[C@@H](C(=O)N[C@H](C(=O)N1)Cc1cccc1)NC(=O)[C@@H](Cc1cccc1)[NH3+])[C@H](O)C)CCCCN</chem>
C2692	OB	OB-	27	<chem>c12c3c(c(cc1c(=O)c(en2[C@H](CO3)C)C(=O)[O-])F)N1CC[NH+](CC1)C</chem>
C2693	OB	OB-	27	<chem>C1(=Ne2c(cccc2)Ne2c1cc(s2)C)N1CC[NH+](CC1)C</chem>
C2694	OB	OB+	27	<chem>c1(ccccc1c1nn[n-]n1)c1ccc(cc1)Cn1c(nc(c1C(=O)OCc1c(oc(=O)o1)C)C(O)(C)C)CCC</chem>
C2695	OB	OB+	27	<chem>N(=N\c1cc(c(cc1)O)C(=O)O)/c1cc(c(cc1)O)C(=O)[O-]</chem>
C2696	OB	OB+	27	<chem>c12c3c(n(c1CC[C@H](C2=O)Cn1cncc1)C)cccc3</chem>
C2697	OB	OB+	27	<chem>c1(cc(cc(c1)[C@H](C[NH2+]C(C)C)O)O</chem>
C2698	OB	OB+	27	<chem>O1[C@H]([C@H](CCCCC)C1=O)C[C@H](OC(=O)C(NC=O)CC(C)C)CCCCCCCC</chem>
C2699	OB	OB+	27	<chem>[C@@H](c1c(cccc1)C)(c1cccc1)OCC[NH+](C)C</chem>
C2700	OB	OB-	27	<chem>C1=C(CC(C)1OC(CC)CC)NC(=O)C[NH3+])C(=O)OCC</chem>
C2701	OB	OB+	27	<chem>[c@@]12([c@@][C][c@@H]([C@H]1O)O)[c@@H]1[C@@H]([C@H]([C@H]([C@H](O1)C)O)O)CC[C@H]1[C@@H]2[C@@H]([C@]2([C@@]1)CC[C@H]2C1=CC(=O)OC1)O)O)CO</chem>
C2702	OB	OB+	27	<chem>O[C@@]1([C@@]2([C@H]([C@H]3[C@@H]([C@@]4([C@@H](CC3)CC(=O)OC4)C)CC2)CC1)C)C</chem>
C2703	OB	OB-	27	<chem>c1(c(nc(o1)CCC(=O)[O-])c1cccc1)c1cccc1</chem>
C2704	OB	OB+	27	<chem>c12c(ccc(c1)Cl)NC(=O)[C@@H](N=C2c1cccc1)O</chem>
C2705	OB	OB+	27	<chem>c1cccc2c1C(=N)Cc1c(cccc1)N2C(=O)N</chem>
C2706	OB	OB+	27	<chem>[C@@H]12[C@@H]([C@@H]3CC[C@H]1[N+])3(C)CC)OC(=O)[C@@H](c1cccc1)CO)O2</chem>
C2707	OB	OB+	27	<chem>c1(c(cccc1)OCC=C)OC[C@@H](C[NH2+]C(C)C)O</chem>
C2708	OB	OB-	27	<chem>OCC[N+](C)C</chem>
C2709	OB	OB+	27	<chem>c1cccc(c1)[C@](C(=O)OCC#CC[NH+](CC)CC)(C1CCCCC1)O</chem>
C2710	OB	OB+	27	<chem>[C@]123[C@@]4([C@@H](Cc5c1c(c(cc5)OC)O)[C@H]2C(=O)CC4)[NH+](CC3)C)O</chem>
C2711	OB	OB-	27	
C2712	OB	OB+	27	

C2713	OB	OB+	27	c1(cc(ccc1)OC)C(=O)CC[NH2+][C@@H]([C@@H](c1ccccc1)O)C
C2714	OB	OB-	27	Oc1c(cc(c(c1C)CC1=NCCN1)C)C(C)C
C2715	OB	OB-	27	O1[C@@H]2[C@]34[C@](O)([C@H]([NH+](CC3)C)Cc3c4c1c(cc3)O)CCC2=O
C2716	OB	OB+	27	[C@]12[C@@H]([C@H]([C@H]3C(=C(c4c(ccc4O)[C@]3(O)C)O)C1=O)O)[C@@H](C(=C(C2=O)C(=O)N)O)[NH+](C)C)O
C2717	OB	OB-	27	[C@@H]12[C@](C(=O)[C@@H](C3=C([C@H](C[C@]3(C)C)([C@H]1OC(=O)c1ccccc1)O)OC(=O)[C@@H]([C@H](c1ccccc1)NC(=O)c1ccccc1)O)C)OC(=O)C([C@H](C[C@@H]1[C@]2(CO1)OC(=O)C)O)C
C2718	OB	OB+	27	Fe1cc2onc(c2cc1)C1CC[NH+](CC1)CCc1c(nc2n(c1=O)CCCC2)O
C2719	OB	OB+	27	c12c3cccc1CCC[C@@H]2CN(C3=O)[C@H]1C2CC[NH+](C1)CC2
C2720	OB	OB-	27	[C@]12[C@H]([C@H]3[C@H](CC1)[C@@]1([C@H](CC3)C[C@H]([C@H](C1)[N+]1(CCCCC1)C)OC(=O)C)C)[C@H]([C@@H]2OC(=O)C)[N+]1(CCCCC1)C)C
C2721	OB	OB+	27	c12c(nc([nH]1)S(=O)C)c1c(ccn1)OC)OC)cc(cc2)OC(F)F
C2722	OB	OB+	27	c12c(cc(c(c1)OC)OC)ccnc2Cc1cc(c(cc1)OC)OC
C2723	OB	OB+	27	OC([C@H]/C=C/[C@H]([C@@H]1[C@@]2([C@@H](CC1)/C(=C/C=C\1/[C@@H](O)C[C@H](O)C1)/CCC2)C)C)C(C)C
C2724	OB	OB-	27	[C@H]1([C@@H]([C@@H]([C@H]([C@@H]1O)N)O)[C@H]([C@@H]([C@@H]([C@@H]([C@@H]1O)CO)O)O)[NH3+])O)[C@H]1[C@@H]([C@@H]([C@@H]([C@@H]1O)CO)O)[C@H]1[C@@H]([C@@H]([C@@H]([C@@H]1O)CN)O)O)N)O
C2725	OB	OB+	27	[C@@H]1([C@H](COc2cc3c(cc2)OCO3)C[NH2+])CC1)c1ccc(cc1)F
C2726	OB	OB+	27	c1(c(cc2c(c1)n(cc(c2=O)C(=O)[O-])CC)F)N1CC[NH+](CC1)C
C2727	OB	OB+	27	c1(c(cccc1)OC[C@H](C[NH2+](C(C)C)O)C1CCCC1
C2728	OB	OB+	27	c12c(nen1CCC(CO)CO)c(=O)nc([nH]2)N
C2729	OB	OB+	27	c1(c(nc(c(c1OC)Cl)OC)C(Cl)Cl)Cl
C2730	OB	OB+	27	[C@H](C(S)(C)C)(C(=O)[O-])[NH3+]
C2731	OB	OB+	27	N12[C@@H]([C@@H](C1=O)NC(=O)Cc1ccccc1)SC([C@@H]2C(=O)[O-])(C)C
C2732	OB	OB+	27	N12[C@@H](C(S)[C@H]1[C@H](C2=O)NC(=O)COc1ccccc1)(C)C(=O)[O-]
C2733	OB	OB+	27	C(C(CO[N+](=O)[O-])(CO[N+](=O)[O-])CO[N+](=O)[O-])O[N+](=O)[O-]
C2734	OB	OB-	27	c1(ccc(cc1)OCCCCCOc1ccc(cc1)C(=N)N)C(=N)N
C2735	OB	OB-	27	[C@@]12(c3c(ccc(c3)O)C[C@H]([C@H]1C)[NH+](CC2)CC=C(C)C)C
C2736	OB	OB+	27	C1(C(=O)NC(=O)NC1=O)(C(CCC)C)CC
C2737	OB	OB+	27	N1(c2c(ccc2)C[C@H]1C(=O)[O-])C(=O)[C@@H](C[C@H](C(=O)OCC)C)C
C2738	OB	OB-	26	S(=O)(=O)O[C@H]1[C@H](O[C@@H]2OC[C@@H](O)[C@H](OS(=O)(=O)O)[C@H]2OS(=O)(=O)[O-])CO[C@@H](O)[C@@H]1OS(=O)(=O)O)O
C2739	OB	OB+	27	c12c(nen1C)n(c(=O)n(c2=O)CCCC(=O)C)C
C2740	OB	OB+	27	c12c3cccc1[nH]cc2C[C@@H]1[C@@H]3C[C@H](C[NH+]1CCC)CSC
C2741	OB	OB+	27	[NH2+]1C(CC(C2CCCC2)C2CCCC2)CCCC1
C2742	OB	OB+	27	N1([C@@H]2[C@H](C[C@H]1C(=O)[O-])CCCC2)C(=O)[C@@H]([NH2+][C@H](C(=O)OCC)CCC)C
C2743	OB	OB+	27	ClC(=CC1C(C1C(=O)OCc1cc(ccc1)Oc1ccccc1)(C)C)Cl
C2744	OB	OB+	27	N1(c2c(ccc(c2)Cl)Se2c1cccc2)CCC[NH+]1CCN(CC1)CCO
C2745	OB	OB+	27	c1(ccc(cc1)OCC)NC(=O)C
C2746	OB	OB+	27	c1ccc(cc1)C1([NH+]2CCCC2)CCCC1
C2747	OB	OB+	27	N(=C(\N=C(N)N)/N)/CCc1ccccc1
C2748	OB	OB+	27	C1(C(=O)c2c(cccc2)C1=O)c1ccccc1
C2749	OB	OB+	27	[C@@H](c1ncccc1)(c1ccccc1)CC[NH+](C)C
C2750	OB	OB+	27	C1(c2ccccc2)(C(=O)NC(=O)NC1=O)CC
C2751	OB	OB-	27	[C@]1(c2ccccc2)(C(=O)OCC)CC[N@@H+](CC1)CC[C@@H](c1ccccc1)O
C2752	OB	OB+	27	ClCC[NH+](C(COc1ccccc1)C)Cc1ccccc1
C2753	OB	OB+	27	N1(N(C(=O)C(=O)[C@@H]1CCCC)c1ccccc1)c1ccccc1
C2754	OB	OB+	27	c1ccc(c1)CCCC(=O)[O-]
C2755	OB	OB+	27	c1(cc(ccc1)O)[C@H](C[NH2+])C)O
C2756	OB	OB+	27	C1(c2ccccc2)(c2ccccc2)C(=O)NNC1=O
C2757	OB	OB-	27	c12c(ccc(c1)OC(=O)NC)N([C@@H]1[C@H]2CC[NH+]1)C)C
C2758	OB	OB+	27	c1ccc2c(c1)oc1c(ccc(c1C[NH+]1CCCC1)OC)c2=O

C2759	OB	OB+	27	n1(c2c(cccc2)[nH]c1=O)C1CC[NH+](CC1)CCC(c1ccc(cc1)F)c1ccc(cc1)F
C2760	OB	OB+	27	c1c(ccnc1)N/C(=N/C#N)/NC(C(C)(C)C)C
C2761	OB	OB+	27	c12c(cccc1[nH]cc2)OC[C@@H](C[NH2+])C(C)C)O
C2762	OB	OB+	27	[C@]1(Cc2ccc(cc2)OCCe2ncc(cc2)CC)(SC(=O)NC1)C=O
C2763	OB	OB+	27	c12c(cnc(n1)N1CC[NH2+])CC1)c(=O)c(en2CC)C(=O)[O-]
C2764	OB	OB-	27	N12[C@@@H]([C@@@H](C1=O)NC(=O)[C@@@H](c1ccccc1)NC(=O)N1C(=O)C(=O)N(CC1)CC)SC([C@@@H]2C(=O)[O-])(C)C
C2765	OB	OB+	27	c12c(ccc(c1)S(=O)(=O)N(C)C)Sc1c(cccc1)N2CCC[NH+]1CCC(CC1)CCO
C2766	OB	OB+	27	c1cc(ccc1F)n1nc(c(c1)c1ccc(cc1)Cl)CC(=O)[O-]
C2767	OB	OB-	27	n1(c2c(cccc2)c(=O)[nH]c2c1nccc2)C(=O)C[NH+]1CCN(CC1)C
C2768	OB	OB+	27	c1(c(cc(cc1S(=O)(=O)N)C(=O)[O-])N1CCCC1)Oe1ccccc1
C2769	OB	OB+	27	c12c(c(c(nc1N)N)C)ncc(n2)Cc1c(ccc(c1)OC)OC
C2770	OB	OB+	27	[C@@](c1ncccc1)(c1ccccc1)(CCC[NH+]1[C@@@H](CCC[C@@@H]1C)C)O
C2771	OB	OB+	27	S1(=O)(=O)c2c(cccc2)C(=C(N1C)C(=O)Nc1ncccc1)O
C2772	OB	OB+	27	c1(c([nH]c(=O)[nH]1)CC)C(=O)c1ccncc1
C2773	OB	OB+	27	S1[C@H]2N([C@H](C1(C)C)C(=O)OCOC(=O)C(C)C)C(=O)[C@H]2NC(=O)C([NH3+])c1ccccc1
C2774	OB	OB+	27	c1csc2c1/C(=C\1/CC[NH+](CC1)C)/c1c(cccc1)CC2
C2775	OB	OB-	27	O(C(c1c(e/2=C/C3=N/C(=C/C4=N/C(=C/e5[nH]c(e5C(O)C)C=C\1/[nH]2)C=C4CCC(=O)O)C)C(c1e/2=C/c3[nH]c(e3C(O)C)C=C/3/N=C(=C/C4=N=C(=C/e1/[nH]2)C=C4CCCC(=O)[O-])C)C(=C3)CCC(=O)O)C)C
C2776	OB	OB+	27	Fc1c(ccc(c1)F)C1(OCC(C1)COc1ccc(cc1)N1CCN(CC1)c1ccc(cc1)n1c(=O)n(nc1)C([C@@@H](O)C)CC)Cn1ncnc1
C2777	OB	OB+	27	c1(ccc(cc1)NC(=O)C)[C@H](C[NH2+])C(C)C)O
C2778	OB	OB+	27	[C@@@H]1(CCc2c(sc(n2)N)C1)[NH2+]CCC
C2779	OB	OB-	27	[C@H]12[C@H](C[C@@@H](C=C1C=C[C@@@H]([C@@@H]2CC[C@H](C[C@H](CC(=O)[O-])O)O)C)O)OC(=O)[C@H](CC)C
C2780	OB	OB-	27	[C@H]12N(C(=O)CN(C1)C(=O)C1CCCCC1)CCc1c2ccccc1
C2781	OB	OB+	27	c12c(c(nc(n1)N1CCN(CC1)C(=O)c1occc1)N)cc(c(c2)OC)OC
C2782	OB	OB+	27	[C@]12([C@@])(C(=O)CO)CC[C@H]1[C@H]1[C@H]([C@H](C2)O)[C@@]2(C(=CC(=O)C=C2)CC1)C)O)C
C2783	OB	OB+	27	[C@]12([C@@])(C(=O)CO)CC[C@H]1[C@H]1[C@H]([C@H](C(=O)C2)[C@@]2(C(=CC(=O)C=C2)CC1)C)O)C
C2784	OB	OB+	27	[O-]C(=O)C[C@H](CC(C)C)C[NH3+]
C2785	OB	OB+	27	c1(ccc(cc1)O)OC[C@H](C[NH2+])C(C)C)O
C2786	OB	OB-	27	C(=C1[C@H]([N+](CC1)(CC)CC)C)(c1ccccc1)c1ccccc1
C2787	OB	OB+	27	c1(c2c(cc(c1)OC)ccn2)N[C@@H](CCC[NH3+])C
C2788	OB	OB+	27	C1(c2ccccc2)(C(=O)NCNC1=O)CC
C2789	OB	OB+	27	S(=O)(=O)(c1ccc(cc1)C(=O)[O-])N(CCC)CCC
C2790	OB	OB-	27	c1(c(c(cc(c1)SC(Sc1cc(c(c1)C(C)C)O)C(C)(C)C)C(C)C)C(C)C)O)C(C)(C)C
C2791	OB	OB+	27	c1(ccc(cc1)N)C(=O)NCC[NH+](CC)CC
C2792	OB	OB-	27	O(CC[NH+](CC)CC)C(=O)c1ccc(cc1)N
C2793	OB	OB+	27	O[C@@@H]([C@@@H]([NH2+])C(C)C)CC)c1c2c(c(cc1)O)[nH]c(=O)cc2
C2794	OB	OB-	27	N1(c2c(ccc(c2)Cl)Sc2c1ccccc2)CCC[NH+]1CCN(CC1)C
C2795	OB	OB+	27	O[C@@](CC[NH+]1CCCC1)(c1ccccc1)C1CCCCC1
C2796	OB	OB+	27	[C@]12([C@@@H]([C@H]3[C@H](CC1)[C@@]1(C(=CC(=O)CC1)CC3)C)CC[C@H]2C(=O)C)C
C2797	OB	OB+	27	Clc1ccc(cc1)N/C(=N/C(=N/C(C)C)/N)/N
C2798	OB	OB-	27	S1c2c(cccc2)N(CCC[NH+](C)C)c2c1ccccc2
C2799	OB	OB+	27	N1(c2c(cccc2)Sc2c1ccccc2)C[C@H]([NH+](C)C)C
C2800	OB	OB-	27	c1(c(cccc1)OC[C@H](C[NH2+])CCC)O)C(=O)CCc1ccccc1
C2801	OB	OB+	27	c1ccc2c(c1)N(c1c(ccc(c1)C(=O)CC)S2)C[C@@@H](C)[NH+](C)C
C2802	OB	OB+	27	c1ccc(cc1)C[C@](c1ccccc1)(OC(=O)CC)[C@H](C)C[NH+](C)C
C2803	OB	OB+	27	c1(c2c(ccc1)ccccc2)[C@H]([C@@@H]([NH2+])C(C)C)C)O
C2804	OB	OB+	27	c1(cc(=O)[nH]c(=S)[nH]1)CCC







C2897	OB	OB+	27	c12c([nH]nc1C(=O)N)c(=O)n(nn2)C
C2898	OB	OB+	27	[C@@H]1(c2c(cc3c(e2)OCO3)[C@H]([C@H]2[C@H]1C(=O)OC2)O[C@H]1[C@@H]([C@H]([C@H]2[C@H](O1)CO[C@](O2)(c1sccc1)C)O)O)c1cc(c(c1)OC)O)OC
C2899	OB	OB+	27	S1(=O)(=O)c2c(scc2)C=C(N1C)C(=O)Nc1cccc1
C2900	OB	OB+	27	c1(c(cc2c(c1)nc(nc2N)N1CCN(CC1)C(=O)[C@@H]1CCCO1)OC)OC
C2901	OB	OB+	27	[NH+](Cc1c2c(ccc1)cccc2)(C/C=C/C#CC(C)(C)C)C
C2902	OB	OB-	27	c1(cc(cc(c1)O)O)[C@@H](C[NH2+](C(C)(C)C)O
C2903	OB	OB-	27	C([C@H]1CC[N@@H+](CC1)CCCC[C@@H](c1cccc1)C(C)(C)O)(c1cccc1)(c1cccc1)O
C2904	OB	OB+	27	c12c3cccc1[nH]cc2C[C@@H]1[C@@H]3C[C@@H](C[NH+](1)C)NC(=O)N(CC)CC
C2905	OB	OB+	27	C(c1cccc1)(c1cccc1)C[C@@H]([NH2+](C(C)(C)C)C
C2906	OB	OB+	27	c12c(cccc1CCCS2)OC[C@H](C[NH2+](C(C)(C)C)O c1(ccc(cc1)CCO)c1ccc(cc1)CC(C(=O)[O-
C2907	OB	OB+	27	)]OCC)OS(=O)(=O)C
C2908	OB	OB-	27	[C@]12([C@@H]3[C@H]([C@H]4[C@](CC3)([C@H](CC4)O)C)CCC1=CC(=O)CC2)C
C2909	OB	OB-	27	c12c(cc(c(c1)OC)OC)CC[NH+]1[C@H]2CC(=O)[C@H](C1)CC(C)C
C2910	OB	OB+	27	[C@@]12([C@H]([C@@H](C(=C(C1=O)C(=O)N)O)[NH+](C)C)C[C@@H]1C(=C(c3c(cccc3O)[C@]1(O)C)O)C2=O)O
C2911	OB	OB+	27	c12c([nH]cn1)c(=O)n(c(=O)n2)C
C2912	OB	OB-	27	s1c(c([n+](c1)Cc1c(nc(nc1)C)N)C)CCO
C2913	OB	OB+	27	c1ccc2c(c1)c(ccc2)N=C=S
C2914	OB	OB+	27	S=c1nc([nH]c2nc[nH]c12)N
C2915	OB	OB+	27	N1(c2c(ccc(c2)SC)Sc2c1cccc2)CC[C@H]1[NH+](CCCC1)C c1(c(cc(cc1)C[C@H](C(=O)[O-
C2916	OB	OB+	27	)]NH3+)]I)Oc1cc(c(c1)I)O)I
C2917	OB	OB+	27	c12c(ccc(c1)Cl)N(c1c(cccc1)N(S2(=O)=O)C)CCCCC(=O)[O-]
C2918	OB	OB+	27	C1(S(=O)(=O)CCCS1(=O)=O)(c1cc(c(cc1)OC)OC)CCCC[NH+](CCc1cc(c(cc1)OC)OC)C
C2919	OB	OB+	26	s1c(ccc1C(=O)c1cccc1)C(C)C(=O)[O-] [NH+]12[C@@H]([C@@H]([C@@H]1O)NC(=O)C(c1sccc1)C(=O)[O-])SC([C@@H]2C(=O)[O-
C2920	OB	OB-	27	)](C)C
C2921	OB	OB+	27	c12c(scc1)CC[NH+](C2)Cc1c(ccc1)Cl
C2922	OB	OB-	27	O[C@@]12[C@@H](C[C@H]3C(=C(O)c4c(c(cc(c4O)NC(=O)CNC(C)(C)C)N(C)C)C3)C1=O)[C@H]([NH+](C)C)C(=O)/C(=C(/O)N)/C2=O
C2923	OB	OB+	27	C1=CCCC(C1[NH+](C)C)(C(=O)CCC)c1cccc1
C2924	OB	OB+	27	c1(c(nsn1)OC[C@H](C[NH2+](C(C)(C)O)N1CCOCC1
C2925	OB	OB+	27	n1(c(nc1C)[N+](=O)[O-])CCS(=O)(=O)CC
C2926	OB	OB+	27	C(=O)([C@@H](S)C)NCC(=O)[O-]
C2927	OB	OB-	27	s1c(ccc1)C(O)(C(=O)OC1C[C@@H]2[N+](C@@H)([C@H]3O[C@@H]23)C1)(C)C)c1sccc1
C2928	OB	OB-	27	S(=O)(=O)(N[C@@H](Cc1ccc(cc1)O)CCCC1CC[NH2+](CC1)C(=O)[O-])CCCC
C2929	OB	OB+	27	c1(c2c(ccc1Cl)nsn2)NC1=NCCN1
C2930	OB	OB-	27	[C@H]1([C@@H]([C@@H]([C@@H]([C@@H]1N)N)O[C@H]1[C@@H](C[C@@H]([C@@H](O1)CN)O)N)O)[C@H]1[C@@H]([C@@H]([C@@H]([C@@H](O1)CO)O)[NH3+])O
C2931	OB	OB+	27	c1cc(c(c(c1)C)NC(=O)[C@H]([NH3+])C)C
C2932	OB	OB+	27	c1(ccc(cc1)C)S(=O)(=O)[N-]C(=O)NCCCC
C2933	OB	OB+	27	c1(cc(c(c(c1)O)O)[N+](=O)[O-])C(=O)c1ccc(cc1)C
C2934	OB	OB+	27	c1(c(cccc1)Nc1c(ccc1)Cl)C(=O)[O-]
C2935	OB	OB+	27	c1cc(cc(c1)OC[C@H](C[NH2+](C(C)O)C
C2936	OB	OB+	27	c1c(c(cc(c1S(=O)C)C)OC)OC
C2937	OB	OB+	27	c1(n(c(cc1)CC(=O)[O-])C)C(=O)c1ccc(cc1)C
C2938	OB	OB+	27	[C@H](c1c(ccc(c1)C)O)(c1cccc1)CC[NH+](C(C)C)C(C)C
C2939	OB	OB+	27	c12cc3c(c(=O)n1Cc1c2nc2c(c1)c(cc2)O)C[NH+](C)C)COC(=O)[C@@]3(CC)O c1(c(ccnc1)Nc1cc(ccc1)C)S(=O)(=O)[N-
C2940	OB	OB+	27	]C(=O)NC(C)C
C2941	OB	OB+	27	C(=C(c1cccc1)/CCCl)(\c1ccc(cc1)OCC[NH+](C)C)/c1cccc1
C2942	OB	OB+	27	[C@]1(c2cc(ccc2)OC)([C@@H](C[NH+](C)C)CCCC1)O





C3035	OB	OB+	26	Clc1cccc(cc1)OC(C(=O)OCC)(C)C
C3036	OB	OB+	26	Clc1cccc1C([NH+])1CCc2secc2C1)C(=O)OC
C3037	OB	OB+	27	[C@H]1([C@@H]2[NH+])([C@H](C)[C@H]1OC(=O)c1cccc1)CC2)C(=O)OC
C3038	OB	OB+	27	ClC1=CC2C(C3(C1=CC(=O)C1C3C1)C)CCC1(C2CCC1(O)C(=O)C)C
C3039	OB	OB-	27	O1CCc2cc(ccc12)CC[NH+]1CC(Cc1)C(C(=O)N)(c1cccc1)c1cccc1
C3040	OB	OB+	27	S(=O)(=O)(N(CC(C)C)CC(O)C(NC(=O)OC1C2CCOC2OC1)Cc1cccc1)c1ccc(cc1)N
C3041	OB	OB-	26	O=C(N(O)CCCCNC(=O)CCC(=O)N(O)CCCC[NH3+])CCC(=O)NCCCCCN(O)C(=O)C
C3042	OB	OB+	27	O1C2CC3C4C(C5(C(=CC(=O)C=C5)CC4)C)C(O)CC3(C)C2(N=C1C)C(=O)COC(=O)C
C3043	OB	OB+	27	FC(F)(F)c1cc(ccc1)CC([NH2+])CC(C)
C3044	OB	OB+	26	Clc1cc(ccc1Cl)C(=O)NC(CCC(=O)[O-])C(=O)N(CCCCC)CCCCO
C3045	OB	OB-	27	O(C)c1ccc2c(cc1)CC1C3C2(CC[NH+]1C)CCCC3
C3046	OB	OB-	26	Ic1c(c(c(c(c1NC(=O)C)I)NC(=O)C)I)C(=O)[O-]
C3047	OB	OB+	26	Fe1en(C2OC(C)C(O)C2O)c(=O)[nH]c1=O
C3048	OB	OB-	27	c12c(c(c3c(c1O)C)[C@]([C@H]3O[C@H]1O[C@H]([C@H]([C@H](C1)[NH3+])O)C)(C(=O)CO)O)O)C(=O)c1c(cccc1OC)C2=O
C3049	OB	OB+	27	O(C(C)(c1cccc1)c1ncccc1)CC[NH+](C)C
C3050	OB	OB+	27	O=C1CCC2(C3C(C4CCC(C(=O)C)C4(CC3)C)C=CC2=C1)C
C3051	OB	OB+	26	[O-]C(=O)C1=CC2=CCC3C(C2(CC1)C)CCC1(C3CCC1C(=O)NC(C)C)C
C3052	OB	OB-	27	S1CCCC(=O)NC(CCCNC(=N)N)C(=O)NCC(=O)NC(CC(=O)[O-])C(=O)NC(Cc2c3c([nH]c2)cccc3)C(=O)N2C(CCC2)C(=O)NC(C1)C(=O)N
C3053	OB	OB+	26	ClCCN(CCC1)C(=O)Oe1cc2c(cc1)C1C(CC2)C2CCC(OP(=O)(O)[O-])C2(CC1)C
C3054	OB	OB+	26	Clc1c(c(ccc1C(=O)C(=C)CC)OCC(=O)[O-])Cl
C3055	OB	OB-	27	O=C(Nc1c(ccc1C)C)C([NH+])(CCC)CC(C)
C3056	OB	OB+	26	Oe1cc(ccc1)C(O)C[NH2+](C)
C3057	OB	OB+	27	O(C)c1ccc(c(c(c1C)C)/C=C/C(=C/C(=O)OCC)/C)/C
C3058	OB	OB-	27	Clc1c2c(cc(c1O)C)C(C[NH2+])CC2)c1ccc(cc1)O
C3059	OB	OB+	26	OC(C1CC[NH+])(CC1)CCCC(O)c1ccc(cc1)C(C(=O)[O-])(C)C(c1cccc1)c1cccc1
C3060	OB	OB+	26	Fe1c2c(cc(c1N1CC[NH+])(CC1)C)F)c(=O)c(cn2CCF)C(=O)[O-]
C3061	OB	OB+	27	c1c(c(c(cc1)F)c1noc(c1C(=O)NC1C(=O)N2C1SC(C2(C(=O)[O-])C)(C)C)C)Cl
C3062	OB	OB+	27	O=c1[nH]c(nc2ncc(nc12)CNc1ccc(cc1)C(=O)NC(CCC(=O)O)C(=O)[O-])N
C3063	OB	OB+	27	C=C1/[C@H]2[C@@]([C@@]3([C@H]([C@@]4([C@@H](CC3)[C@@H]([C@@H](CC4)O)C)C)[C@@H](C2)O)C)C([C@@H]1OC(=O)C)C(\C(=O)[O-])/CCC=C(C)C
C3064	OB	OB+	26	O1C2CC34C56C(OC(=O)C5O)OC3(C2(O)C(C)C1=O)C(=O)OC4CC6C(C)C
C3065	OB	OB+	26	O1C2C(O)(C34OC5OC(=O)C(O)C65C3(C(OC4=O)CC6C(C)C)C2O)C(C)C1=O
C3066	OB	OB+	26	COe1c(cc(cc1)Cl)C(=O)NCCc1ccc(cc1)S(=O)(=O)[N-]C(=O)NC1CCCCC1
C3067	OB	OB+	26	O1c2c(cccc2)OCC1C1=NCCN1
C3068	OB	OB-	27	O=C1N(C(=O)C([NH2+])C(CCc2cccc2)C(=O)OCC)C(CN1C)C(=O)[O-]
C3069	OB	OB+	26	O1C2C(OCC2O)C(O[N+](=O)[O-])C1
C3070	OB	OB+	27	C1C(C2C(O1)C(CO2)O[N+](=O)[O-])O[N+](=O)[O-]
C3071	OB	OB+	26	S1(=O)(=O)N(C)/C=C(\O)/Nc2noc(c2)C)/C(=O)c2c1cccc2
C3072	OB	OB-	27	[C@@]1(c2c(cccc2)Cl)(CC(=O)CCC1)[NH2+](C)
C3073	OB	OB+	26	CC(=O)N1CCN(CC1)c1ccc(cc1)OCC1COC(Cn2ccnc2)(O1)c1ccc(cc1)Cl
C3074	OB	OB+	26	S1CC(N(C1)C(=O)C(O)C(NC(=O)C)C(NC(=O)COe1nccc2c1cccc2)CSC)Cc1cccc1C(=O)NC(C)C
C3075	OB	OB-	26	C[N+](C)C)CC(C(=O)[O-])O
C3076	OB	OB+	26	S1c2c(cc(cc2)OC)N(c2c1cccc2)CC(C[NH+](C)C)C
C3077	OB	OB+	27	[C@@H]1([C@H](NC(=O)[C@@H]2[NH+](C[C@@H](C2)CCC)C)[C@@H](O)C)[C@@H]([C@H]([C@H](O1)SC)O)O
C3078	OB	OB+	26	Clc1cc2c(cc1)Oe1c(ccc1)N=C2N1CC[NH+](CC1)C
C3079	OB	OB-	27	FC(F)(CCCC)C1(OC2C(CC1)C(CCCCCC(=O)[O-])C(=O)C2)O
C3080	OB	OB-	26	O1Ce2c(cc3n(Cc4c3nc3c(cc5c(c3)OCCO5)c4C[NH+])3CCN(CC3)C)c2=O)C(CC)C1=O

C3081	OB	OB+	27	CC1(C2CC3C(C(=O)C(=C(C3(C(=O)C2=C(c2c1cccc2O)O)O)C(=O)NC[NH2+])CCCC(C(=O)[O-])N)[NH+](C)C)O
C3082	OB	OB+	26	[NH2+](C)C1(C2CC(CCC2)C1(C)C)C
C3083	OB	OB+	26	O(C(=O)C)C1(CCC2C3C(CCC12C)C1(C(=CC(=O)CC1)C(=C3)C)C)C(=O)C
C3084	OB	OB-	27	OC1CCC2C3C(CCC12C)C1(C(CC(=O)CC1C)CC3)C
C3085	OB	OB+	26	OC1(CCC2C3C(CCC12C)C1(C(=CC(=O)CC1)CC3)C)C
C3086	OB	OB+	26	OC1C(O)C(O)C[NH+](CCO)C1CO
C3087	OB	OB-	27	O(C)c1c(ccc1OC)C[C@H]1[N@@+](CCc2c1cc(c2)OC)OC(CCCOC(=O)CC/C=C\CCC(=O)OCCC[N@+](CCc2c(ccc(c2)OC)OC)[C@@H]1Cc1cc(c(c1)OC)OC)OC)C)OC
C3088	OB	OB+	26	S(CC1=C(N2C(OC1)C(C2=O)(OC)NC(=O)C(C(=O)[O-])c1ccc(cc1)O)C(=O)[O-])c1[n+](nn[nH]1)C
C3089	OB	OB+	27	S1C2N(C(C(=O)[O-])C1(C)C)C(=O)C2NC(=O)c1c2c(ccc1OCC)cccc2
C3090	OB	OB+	26	O(C(=O)C1(CCC=CC1[NH2+])C)c1cccc1)CC
C3091	OB	OB-	27	c12c(c[nH]e1cccc2)C[C@H]1C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N1Cc1cccc1)NC(=O)[C@@H](Cc1cccc1)[NH3+])][C@@H](O)C)CCCCN
C3092	OB	OB+	26	O(C(CC)CC)C1C=C(CC([NH3+])C1NC(=O)C)C(=O)[O-]
C3093	OB	OB+	27	S1C2N(C(C(=O)[O-])C1(C)C)C(=O)C2NC(=O)c1c(noc1C)c1cccc1
C3094	OB	OB+	26	OC1CC(=O)N(C1)CC(=O)N
C3095	OB	OB-	26	C1C(C(C(C(O1)OC1COC(C(C1O)O)OC1COC(C(C1O)O)O)O)O)O
C3096	OB	OB+	27	[O-]C(=O)C1N(C2C(C1)CCCC2)C(=O)C([NH2+])C(CCC)C(=O)[O-])C
C3097	OB	OB+	27	OC(C([NH3+])C)c1cccc1
C3098	OB	OB-	27	ClC1CCC(CC1OC)/C=C(\C)/C1OC(=O)C2N(CCCC2)C(=O)C(=O)C2(OC(C(OC)CC2C)C(OC)CC(C/C(=C/C(CC)C(=O)CC(O)C1C)/C)C)O
C3099	OB	OB+	26	Clc1ccc(cc1)c1c(nc(nc1N)N)CC
C3100	OB	OB-	26	[n+]1(c2c(cc(cc2)N(C)C)ccc1/C=C\c1cc(n(c1C)c1cccc1)C)C
C3101	OB	OB+	27	S(=O)(=O)(NC1CC2C([NH+](C1)CCC)Cc1c(c(ccc1)O)C2)N(CC)CC
C3102	OB	OB+	26	O(C(=O)C([NH2+])C(C(=O)N1CCc2c(cccc2)C1C(=O)[O-])C)CCc1cccc1)CC
C3103	OB	OB+	27	[O-]C(=O)C1N(C2C(C1)CCCC2)C(=O)C([NH2+])C(CCc1cccc1)C(=O)[O-])C
C3104	OB	OB+	26	O=C(Nc1c(ccc1C)N)CCCC[NH2+])C(C)C
C3105	OB	OB+	27	Oc1cc(ccc1)O)C(O)C[NH2+])CCCN1c2c(nc1)n(C)c(=O)n(C)c2=O
C3106	OB	OB-	27	O1c2c3c4c(c(c2C)O)C(=O)C(=C2NC5(N=C42)CC[NH+](CC5)CC(C)C)NC(=O)/C(=C/C=C(C)C)C(O)C(C)C(O)C(C)C(OC(=O)C)C(C)C(OC)/C=C\OC1(C)C3=O)/C
C3107	OB	OB+	27	O1c2c3c4c(c(c2C)O)c(c(c4O)/C=N/N2CC[NH+](CC2)C2CCCC2)NC(=O)/C(=C/C=C\C(C)C)C(O)C(C)C(O)C(C)C(OC(=O)C)C(C)C(OC)/C=C\OC1(C)C3=O)/C)O
C3108	OB	OB+	26	Oc1c(c(=O)c2c(ccc2)n1C)C(=O)N(C)c1cccc1
C3109	OB	OB+	27	O1C(CC)C(O)C(C)C(C)/C(=N\OCOCOC)/C(CC(O)C)C(OC2OC(CC([NH+](C)C)C2O)C)C(C)C(OC2OC(C)C(O)C(OC)(C2)C)C(C)C1=O)C
C3110	OB	OB-	26	[NH+](C(Cc1cccc1)C)(CC#C)C
C3111	OB	OB+	26	S(=O)(=O)(Nc1ccc(cc1)C(=O)NCC[NH+](CC)CC)C
C3112	OB	OB-	26	s1cccc1CC[NH+]1CCC(N(C(=O)CC)c2cccc2)(CC1)COC
C3113	OB	OB+	26	S(=O)(CCC1C(=O)N(N(C1=O)c1cccc1)c1cccc1)c1cccc1
C3114	OB	OB-	26	O(C)c1cc2c([nH]cc2/C=N\NC(=N)N)CCCCc1
C3115	OB	OB+	27	O1C(CN(c2cc(ccc2)C)C1=O)CO
C3116	OB	OB+	27	[C@@]12([C@@]3([C@@H](C[C@H]1OC(O2)(C)C)[C@H]1[C@])([C@H](C3)O)([C@@H]2C(=CC(=O)C=C2)CC1)F)C)C(=O)CO
C3117	OB	OB-	26	C1CC[N+]2(C1)C1CCC2CC(C1)OC(=O)C(c1cccc1)(c1cccc1)O
C3118	OB	OB+	26	n1c2c(nc1)cc1c(c2)C2CC1C[NH2+])C2
C3119	OB	OB+	26	O1CC[NH2+])CC1COc1cccc1OCC
C3120	OB	OB-	27	O(C(=O)C)C1C2(C3[NH+](CCC43C(N(c3cc(c(cc43)C3)CC4CC(O)(CN(C4)CCc4c3[nH]c3c4cccc3)CC)C(=O)OC)OC)C)C1(O)C(=O)OC)CC=C2)CC
C3121	OB	OB+	27	Ce1cn(c(=O)[nH]c1=O)C1CC(C(O1)CO)N=[N+]=[N-]
C3122	OB	OB+	26	Brc1ccc(cc1)/C(=C\C[NH+](C)C)/c1cccn1
C3123	OB	OB+	25,28	Oc1c2cn[nH]c2nnc1
C3124	OB	OB+	25	c1ccc(cc1)C(c1cccc1)(C[C@@H]([NH+](C)C)C)[C@@H](OC(=O)C)CC
C3125	OB	OB+	25,28,29	NC(=N)NC(=O)c1nc(c(nc1N)N)Cl
C3126	OB	OB+	25	CC1(C)S[C@@H]2C(NC(=O)C([NH3+])c3ccc(cc3)O)C(=O)N2C1C(=O)[O-]

C3127	OB	OB-	25,28	[O-]C(=O)C[C@H](O)C[C@H](O)CCn1c(c(c1C(C)C)C(=O)Nc1cccc1)c1cccc1)c1ccc(cc1)F
C3128	OB	OB+	25	OC1=C(C(=O)C(=O)c2cccc12)C1CCC(c2ccc(cc2)Cl)CC1
C3129	OB	OB+	25	OCC(C(=O)OC1C[C@H]2[NH+](C)[C@H](CC2)C1)c1cccc1
C3130	OB	OB-	25	O[C@@]12O[C@@](NC(=O)[C@@H]3C=C4c5c6c([nH]c(c6C[C@H]4[NH+](C)C3)Br)ccc5)(C(=O)N1[C@H](C(=O)N1CCC[C@@H]21)CC(C)C(C)C
C3131	OB	OB+	25	CCOc1nc2c(n1Cc1ccc(cc1)c1c(cccc1)c1nnn[nH]1)c(ccc2)C(=O)[O-]
C3132	OB	OB+	25	C[C@H](CS)C(=O)N1CCC[C@H]1C(=O)[O-]
C3133	OB	OB+	25	COc1c(cccc1)OCC[NH2+]CC(O)COc1c2c([nH]c3c2cccc3)ccc1
C3134	OB	OB+	25	[O-]C(=O)C1=C(C=C)CS[C@H]2N1C(=O)[C@H]2NC(=O)/C(=N/OCC(=O)O)/c1csc(n1)N
C3135	OB	OB+	25	CC1=C(N2[C@H](SC1)[C@H](NC(=O)C([NH3+])c1cccc1)C2=O)C(=O)[O-]
C3136	OB	OB+	25	[O-]C(=O)C1=C(C)CS[C@H]2N1C(=O)[C@H]2NC(=O)C([NH3+])C1=CCC=CC1
C3137	OB	OB+	25	OC[C@@H](NC(=O)C(Cl)Cl)[C@H](O)c1ccc(cc1)[N+](=O)[O-]
C3138	OB	OB+	25	CC[NH+](CC)CCCC(C)Nc1c2ccc(cc2ncc1)Cl
C3139	OB	OB+	25	C[NH+](C)CCC(c1ccc(cc1)Cl)c1cccn1
C3140	OB	OB+	25	NS(=O)(=O)c1c(ccc(c1)C1(O)NC(=O)c2cccc12)Cl
C3141	OB	OB+	25,29	CN/C(=N\CCSCc1c([nH]cn1)C)/NC#N
C3142	OB	OB+	25	C[NH+](C)CCCC1(OCc2cc(ccc12)C#N)c1ccc(cc1)F
C3143	OB	OB+	25	o[C@H]1C@H[OC2]C@H[C@H](O)c1c@H3O[C@H]3O[C@H](O)[C@@](OC)C3)[C@H](C(=O)O[C@H](CC)[C@](O)C)[C@H](O)[C@H](C(=O)[C@H](OC)C)O[C@H](OC[C@@H]1NH+)(C)C
C3144	OB	OB+	25	[O-]C(=O)[C@H]1N2C(=O)C[C@H]2O/C1=C\CO
C3145	OB	OB+	25	O[C@H]1[C@H](O[C@H](C(NC(=O)[C@H]2[NH+](C)C[C@H](CCC)C2)C(Cl)C)[C@H](O)[C@@H]1O)SC [O-
C3146	OB	OB+	25	]C(=O)[C@@H]1N2C(=O)[C@@H](NC(=O)c3c(onc3c3cccc3Cl)C)[C@H]2SC1(C)C
C3147	OB	OB+	25,31	[C@@H]12C[C@@H](C)[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]1(F)[C@H]2CCC2=CC(=O)C=C[C@]12C
C3148	OB	OB+	25	CC1=NS(=O)(=O)c2cc(ccc2N1)Cl
C3149	OB	OB+	25	[O-]C(=O)Cc1cccc1Nc1c(ccc1Cl)Cl
C3150	OB	OB+	25	[O-]C(=O)[C@@H]1N2C(=O)[C@@H](NC(=O)c3c(onc3c3c(ccc3Cl)Cl)C)[C@H]2SC1(C)C
C3151	OB	OB+	25	C1C[C@@H](O[C@@H]1CO)n1cnc2c1ncnc2O
C3152	OB	OB+	25	o[C@H]1c[C@H](O[C@H]2[C@@H](O)C1C@H[OC2]C@H[C@H](O)c1c@H3[C@@H](O)C1C@H[OC2]C@H[C@H](O)[C@@](OC)C7=CC(=O)OC7)CC[C@]165O)C4O[C@@H]3C[C@@H]2C[C@H](O)C[C@H]1O
C3153	OB	OB-	25	[nH]1cc(c2cccc12)C(=O)OC1CC2[NH+] <sup>3</sup> CC(=O)C(C2)C[C@@H]3C1
C3154	OB	OB+	25	C[NH+](C)CC/C=C/1\c2c(cccc2)COc2c1cccc2
C3155	OB	OB-	25	COc1cccc2c1C(=O)c1c(c3c(c1O)[C@H](C[C@](C3)(O)C(=O)CO)O[C@H]1C[C@H]([NH3+])[C@H](O)[C@H](C)O1)O)C2=O
C3156	OB	OB+	25	O/C(=C\1/C(=O)[C@@H]([NH+](C)C)[C@@H]2[C@@H](O)[C@H]3C(=C(O)c4c(cccc4O)[C@@H]3C)C(=O)[C@]2(O)C1=O)/N
C3157	OB	OB+	25	N(C(=O)[C@H]1CC[C@H]2[C@@H]3CC[C@H]4NC(=O)C=C[C@]4(C)[C@H]3CC[C@]12C)C(C)C
C3158	OB	OB+	25,30,31	NS(=O)(=O)c1cc(c(cc1Cl)NCc1ccc1)C(=O)[O-]
C3159	OB	OB+	25	OC1(CC[NH+](CCCC(=O)c2ccc(cc2)F)CC1)c1ccc(cc1)Cl
C3160	OB	OB+	25	O[C@@H]1CO[C@@H]2[C@@H](O)[N+](=O)[O-]CO[C@H]12
C3161	OB	OB+	25	c1nn(cn1)C[C@]1(OC[C@@H](O1)COc1ccc(cc1)N1CCN(c2ccc(cc2)n2cnn(c2=O)[C@@H](C)CC)CC1)c1c(cc(cc1)Cl)Cl
C3162	OB	OB+	25	OC[C@@H]1O[C@H](n2ccc(nc2=O)N)CS1
C3163	OB	OB+	25	Cc1c(ccnc1CS(=O)c1nc2c([nH]1)cccc2)OCC(F)(F)F [O-
C3164	OB	OB+	25,30	]C(=O)[C@@H]([NH3+])Cc1cc(c(cc1)O)O
C3165	OB	OB+	25	OCc1c(nc(n1Cc1ccc(cc1)c1cccc1c1n[n-]nn1)CCCC)Cl
C3166	OB	OB-	25	O[C@H]1CC(=O)O[C@H](CC[C@H]2[C@H](C=CC3=C[C@H](C)C[C@H](OC(=O)[C@@H](C)CC)[C@H]23)C)C1 [O-
C3167	OB	OB+	25	]C(=O)[C@@H]([NH3+])Cc1ccc(cc1)N(CCC)CC1
C3168	OB	OB-	25	S=c1[nH]cnc2c1[nH]cn2
C3169	OB	OB+	25	O/C(=C\1/C(=O)[C@@H]([NH+](C)C)[C@@H]2[C@H]3C(=C(O)c4c(ccc(c4C3)N(C)C)O)C(=O)[C@]2(O)C1=O)/N
C3170	OB	OB+	25	O[C@@H]1CC(=O)[C@H](CCCCC(=O)OC)[C@H]1/C=C/CC(O)(C)CCCC
C3171	OB	OB+	25	[O-]C(=O)C1=C(CSc2nnnn2)CO[C@H]2N1C(=O)[C@@]2(OC)NC(=O)C(C(=O)O)c1ccc(cc1)O [O-
C3172	OB	OB+	25	]C(=O)c1cn(c2c(c(cc2c1=O)F)N1C[C@H]2[NH2+]CCC[C@H]2C1)OC)C1CC1

C3173	OB	OB+	25,31	CC(C)(C)[NH2+]CC(O)COc1c2c(ccc1)C[C@H]([C@H](C2)O)O
C3174	OB	OB+	25	Oc1c2e3c(cc1)C[C@H]1[C@@]4(CCC(=O)[C@H](O2)[C@]34CC[NH+]1CC1CC1)O
C3175	OB	OB+	25	CNS(=O)(=O)CCc1cc2c([nH]cc2C2CC[NH+](C)CC2)cc1
C3176	OB	OB+	25	Oc1cc2c(cc1)C[C@H]1[NH+](CC=C(C)C)CC[C@]2(C)[C@H]1C
C3177	OB	OB+	25	CCCCC1C(=O)N(N(C1=O)c1ccccc1)c1ccccc1
C3178	OB	OB+	25,31	O=C1NC(=O)C(N1)(c1ccccc1)c1ccccc1
C3179	OB	OB+	25	O[C@H](c1c2cc(ccc2ncc1)OC)[C@H]1[NH+]2CCC(C1)[C@@H](C=C)C2
C3180	OB	OB+	25,28	OC[C@H]1O[C@@H](n2nc(nc2)C(=O)N)[C@H](O)[C@@H]1O
C3181	OB	OB-	25	CO[C@H]1C=C(O)[C@]2(C)Oe3c(c4c(c3C)O)C(=O)C=C3NC5(CC[NH+](CC(C)O)CC5)N=C43NC(=O)C=C/C[C@H](C)[C@H](O)[C@@H](C)[C@H](O)[C@@H](C)[C@H](OC(=O)C)[C@H]1C)/C/C2=O
C3182	OB	OB-	25	CC(C)(C)NC(=O)[C@H]1C[C@H]2CCCC[C@@H]2C[N@@H+]1C[C@H](O)[C@@H](Cc1ccccc1)NC(=O)[C@@H](CC(=O)N)NC(=O)c1nc2c(cccc2)cc1
C3183	OB	OB+	25	OCC(C(=O)OC1C[C@@H]2[NH+](C)[C@@H](C1)[C@@H]1O[C@H]2)1c1ccccc1
C3184	OB	OB+	25,28,29	[nH]1c2c(n(nc2CC)C)c(=O)nc1c1c(ccc(c1)S(=O)(=O)N1CC[NH+](C)CC1)OCC
C3185	OB	OB+	25	Cc1cn([C@@H]2O[C@H](CO)C=C2)c(=O)[nH]c1=O
C3186	OB	OB-	25,29,30,31	[O-]C(=O)C1=C/C(=N/Nc2ccc(cc2)S(=O)(=O)Nc2ccccc2)/C=CC1=O
C3187	OB	OB+	25	COC1CC(CCC1O)/C=C(\C)/C1OC(=O)C2CCCCN2C(=O)C(=O)C2(O)OC(C(CC2)OC)C(CC(C)C/C(=C/C(CC=C)C(=O)CC(O)C1C)/C)OC
C3188	OB	OB+	25,28	NS(=O)(=O)c1c(ccc(c1)C[C@H]([NH2+]CCOe1ccccc1OCC)C)OC
C3189	OB	OB+	25	O/C(=C1/C(=O)[C@@H]([NH+](C)C)[C@@H]2C[C@H]3C(=C(O)c4c(cccc4O)C3(O)C)C(=O)[C@]2(O)C1=O)/N
C3190	OB	OB-	25	CCCCC1cc(c2c(c1)OC(C1C2C=C(C)CC1)(C)C)O
C3191	OB	OB+	25	Cc1c(ccc1)C(=CCC[NH+]1CCC[C@H](C1)C(=O)[O-])c1c(ccs1)C
C3192	OB	OB+	25,28	Oc1c(cc(cc1)C)[C@H](c1ccccc1)CC[NH+](C(C)C)C(C)C
C3193	OB	OB+	25	NS(=O)(=O)OC[C@]12OC(O[C@H]1[C@@H]1OC(O[C@H]1CO2)(C)C)(C)C
C3194	OB	OB+	25,28	Cc1nnc2n1c1c(cc(cc1)Cl)C(=NC2)c1ccccc1Cl
C3195	OB	OB+	25	[O-]C(=O)[C@@H](N(C(=O)CCCC)Cc1ccc(cc1)c1ccccc1c1n[nH]nn1)C(C)C
C3196	OB	OB+	25	CC(=O)CC(c1ccccc1)c1c(O)oc2ccccc2c1=O
C3197	OB	OB-	25	CC(=O)N[C@@H]1[C@H](NC(=N)N)C=C(OC1[C@H](O)[C@H](O)CO)C(=O)[O-]
C3198	PS	Nonsubstrate	172	c1ccccc1CCc2ccccc2OCc2ccccc2OC)c1
C3199	PS	Nonsubstrate	172	OC(=O)c1cc(C(=O)O)ccc1c1c2c(cc(c2)CCC(=O)O)O)oc2c1cc(c(=O)c2)CCC(=O)O
C3200	PS	Nonsubstrate	172	O=C(O[C@H]1[C@H](Oe2c(C1)c(cc(c2)O)O)c1cc(c(c1)O)OC)O)c1cc(c(c1)O)OC)O
C3201	PS	Nonsubstrate	172	O=c1c(cn(c(=O)[nH]1)C1C(C(C(O1)CO)O)O)F
C3202	PS	Nonsubstrate	172	O=c1c2c(cc(c2oc(c1)c1ccccc1)C/C=C(/CCC=C(C)C)/C)O)O
C3203	PS	Nonsubstrate	172	OC[C@H]1Oe2c(O[C@@H]1c1ccc(c1)OC)O)cc(cc2)c1oc2c(c(cc(c2C/C=C(/CCC=C(C)C)/C)O)O)c(=O)c1O
C3204	PS	Nonsubstrate	172	OC[C@H]1Oe2c(O[C@@H]1c1ccc(c1)OC)O)cc(cc2)c1oc2c(c(cc(c2CC=C(C)C)O)O)c(=O)c1O
C3205	PS	Nonsubstrate	172	O=c1c2c(cc3n1Cc1cc4c(nc31)cccc4N)[C@@](C(=O)OC2)(O)CC
C3206	PS	Nonsubstrate	172	O=C(Nc1c(cccc1C(C)C)C(C)C)CN(CC(=O)O)CC(=O)O
C3207	PS	Nonsubstrate	172	O=C(Oc1c(cccc1)C(=O)O)C
C3208	PS	Nonsubstrate	172	O=S(c1ccc2c(c1)nc([nH]2)NC(=O)OC)CCC
C3209	PS	Nonsubstrate	172	O=C(ON=CC(SC)(C)C)NC
C3210	PS	Nonsubstrate	172	NC12CC3CC(CC(C1)C3)C2
C3211	PS	Nonsubstrate	172	O=C(Oc1ccc(c1)C)N(C)C)NC
C3212	PS	Nonsubstrate	172	O=c1cc(oc2c1c(cc(c2)O)O)c1ccc(cc1)O
C3213	PS	Nonsubstrate	172	O=C(N)Cc1ccc(cc1)OCC(O)CNC(C)C
C3214	PS	Nonsubstrate	172	OC1=C(C(=O)e2ccccc2C1=O)[C@@H]1CC[C@H](CC1)c1ccc(cc1)Cl
C3215	PS	Nonsubstrate	172	Clc1nc(nc(n1)NCC)NC(C)C
C3216	PS	Nonsubstrate	172	CC(=O)OCOC(=O)c1cc(C(=O)OCOC(=O)C)ccc1c1c2c(cc(c2)CCCC(=O)OCOC(=O)C)O)oc2c1cc(c(=O)c2)CCCC(=O)OCOC(=O)C
C3217	PS	Nonsubstrate	172	c1ccc2cc3c4c5c(cccc5ccc4c2c1)cc3
C3218	PS	Nonsubstrate	172	n1c(c2nc(c(nc2nc1N1C[C@@H](O[C@@H](C1)C)C)N1C[C@H](O[C@H](C1)C)C)c1ccccc1)N(CC(O)(C)C)CCO





C3265	PS	Nonsubstrate	172	n1c2c(ccc1)c(ccc2)OCC(O)CN1CCN(CC1)C1c2ccccc2CCc2c1cccc2
C3266	PS	Nonsubstrate	172	O=C1OCC2C(c3c(C(C12)c1cc(c(c1)OC)OC)OC)cc1OCCc1c3)N(C)C
C3267	PS	Nonsubstrate	172	O=C1OCC2C(c3c(C(C12)c1cc(c(c1)OC)OC)OC)cc1OCCc1c3)NC
C3268	PS	Nonsubstrate	172	O=C(Oc1cc2c(cc1)cc(cc2)C(=N)N)c1ccc(cc1)N=C(N)N
C3269	PS	Nonsubstrate	172	O=C1CC[C@]2([C@@]34CCN([C@@H]2C2c3c(O[C@@H]14)c(cc2)O)CC=C)O
C3270	PS	Nonsubstrate	172	Clc1cc(ccc1)N1CCN(CC1)CCc1c(=O)n(c(n1)CC)CCOc1cccc1
C3271	PS	Nonsubstrate	172	O=C(OCC)C1=C(NC(=C(C1c1cc(ccc1)[N+](=O)[O-])C(=O)OC)C)C
C3272	PS	Nonsubstrate	172	ClC1C(C(C(C1Cl)Cl)Cl)ClCl
C3273	PS	Nonsubstrate	172	O=NN(Cc1c2ccccc2ccc1)C(=O)C(C)NC(=O)C(C)C
C3274	PS	Nonsubstrate	172	S(=O)(=O)(Nc1nc(cc(n1)C)C)c1ccc(cc1)NC(=O)COC(=O)c1c2[nH]c3ccccc3c(=O)c2ccc1
C3275	PS	Nonsubstrate	172	S(=O)(=O)(Nc1nc(cc(n1)C)C)c1ccc(cc1)Nc1c2ccccc2nc2c(cccc12)C(=O)NNCCO
C3276	PS	Nonsubstrate	172	O=C1c2c(c(ccc2[C@H](O1)C1c2c(CCN1C)cc1OCCc1c2OC)OC)OC
C3277	PS	Nonsubstrate	172	COc1ccc(cc1)c1cc(c2ccccc2n1)C(O)C1NCCCC1
C3278	PS	Nonsubstrate	172	O=C(NCC(=O)NC1C(C(C(OC1C)NC1=NC=NC2=NC=NC12)O)O)CCCCCCCCCCCC(C)C
C3279	PS	Nonsubstrate	172	O=c1n(cccn1)[C@H]1[C@@H]([C@@H]([C@H](O1)CO)O)O
C3280	PS	Nonsubstrate	172	O=c1n(c2c3cc4OCCc4cc3C(=O)c2c2cc(cc12)OC)OC)C
C3281	PS	Nonsubstrate	172	O=C1C(C(N(C1C(=O)OCC)c1cccc1)C)c1cccc1C(=O)OCC [O-
C3282	PS	Nonsubstrate	172	][N+](=O)c1c(cc(c1)OC)N][N+](=O)[O-] O=C(C1=C(OCCS1)C)Nc1ccc(c(c1)C(=O)OC(C)C)Cl
C3283	PS	Nonsubstrate	172	O=S(=O)(Nc1cccc1OC)c1cc(C(C)C)ccc1OCCOc1ccc(C(C)C)cc1S(=O)(=O)Nc1cccc1OC
C3284	PS	Nonsubstrate	172	O=C(c1c2ccccc2ccc1O)N/N=C(/CCC(=O)Nc1cc(C)ccc1C)\C(C)C(=O)c1ccc(cc1)O
C3285	PS	Nonsubstrate	172	O=c1cc2c(nn1Cc1cccc1Cl)cccc2
C3286	PS	Nonsubstrate	172	CS(=O)(=O)c1c2c(nc3ccccc3n2)n2cc(nc2c1N)Cl
C3287	PS	Nonsubstrate	172	O=C(c1ccc(cc1)OC)C(c1n(c2ccccc2c1C(=O)c1ccc(cc1)OC)C(=O)c1ccc(cc1)OC)C(=O)c1ccc(cc1)OC
C3288	PS	Nonsubstrate	172	Fe1ccc(cc1)[C@@](CN1CC[C@]2(CC1)N(CN(C2=O)CC(C)C)c1cccc1)(C1OCCO1)C
C3289	PS	Nonsubstrate	172	S=c1c(c(ccn1C1C(C(O)C(C(O1)CO)O)C)c1cccc1)C#N
C3290	PS	Nonsubstrate	172	CC(=O)c1c(c2occc2)c(c(=S)n(c1C)C1C(C(O)C(C(O1)CO)O)O)C#N
C3291	PS	Nonsubstrate	172	S=C1C(=Nc2ccccc2)N(C(=Nc2ccc[n+](c2)Cc2ccccc2)N1c1cccc1)c1cccc1
C3292	PS	Nonsubstrate	172	O=c1c2ccccc2nc(n1c1ccc(cc1)c1ccc(cc1)N1C(=O)CSC1c1cccc1NC)c1cccc1
C3293	PS	Nonsubstrate	172	Clc1ccc(cc1)c1c2C(=O)CC(C)C)Cc2n(c(=S)c1C#N)[C@H]1[C@@H]([C@@H]([C@@H]([C@@H]([C@@H](O1)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C
C3294	PS	Nonsubstrate	172	N#CC1=C(N(C(=CC1c1cccc1)c1cccc1)C1C(C(C(C(O1)CO)O)O)O)S
C3295	PS	Nonsubstrate	172	N#CC1=C(N(C(=CC1c1cccc1)c1cccc1)C1C(C(C(C(O1)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)S
C3296	PS	Nonsubstrate	172	CC(=O)OC1C(C(C(OC1n1c(=S)c(cc2c1CCCC2)C#N)COC(=O)C)OC(=O)C)OC(=O)C
C3297	PS	Nonsubstrate	172	S=c1c(cc2c(n1C1C(C(O)C(C(O1)CO)O)O)CCCCC2)C#N
C3298	PS	Nonsubstrate	172	S=c1c(cc2c(n1C1C(C(O)C(C(O1)CO)O)O)CCCC2)C#N
C3299	PS	Nonsubstrate	172	OC(=O)c1n(c(nc1C(O)C)C)CCC)Cc1ccc(cc1)c1c(cccc1)c1nn[nH]n1
C3300	PS	Nonsubstrate	172	O(c1c(cccc1)OCC=C)CC(O)CNC(C)C
C3301	PS	Nonsubstrate	172	c1c(cccc1)CCN=C=S
C3302	PS	Nonsubstrate	172	n1c(cccc1)C(c1cccc1)CCN(C)C
C3303	PS	Nonsubstrate	172	OC1=C(N(S(=O)(=O)c2ccccc12)C)C(=O)Nc1cccc1
C3304	PS	Nonsubstrate	172	O=C1[C@@H]2[C@@H](c3cc4OCCc4cc3[C@@H]([C@H]2CO1)O)c1cc(c(c1)OC)OC)OC
C3305	PS	Nonsubstrate	172	OC(c1cccc1)(CCN1CCCC1)C1CCCCC1
C3306	PS	Nonsubstrate	172	O=C(c1c(cccc1)OCC(O)CNCCC)CCc1cccc1
C3307	PS	Nonsubstrate	172	Clc1cc(c(cc1)C1(OC(CO1)CCC)Cn1cnc1)Cl
C3308	PS	Nonsubstrate	172	Oc1cc2c(c[nH]c2cc1)CCCCN1CC=C(CC1)c1cccc1
C3309	PS	Nonsubstrate	172	O=C(O)[C@@H](N)CSCC=C(CCC=C(C)CCC=C(C)C)C
C3310	PS	Nonsubstrate	172	

C3311	PS	Nonsubstrate	172	OC[C@H](c1cccc1)C(=O)O[C@H]1CC2N(C(C1)[C@H]1O[C@@H]21)C
C3312	PS	Nonsubstrate	172	O=C(O[C@@H]1[C@H]2C(=C[C@H](C)C1)C=C[C@@H]([C@@H]2CC[C@H]1OC(=O)C[C@H](O)C1)C)C(C)CC
C3313	PS	Nonsubstrate	172	O=C(N(c1cccc1)C1(CCN(CC1)CCc1cccc1)COC)CC
C3314	PS	Nonsubstrate	172	O=S(=O)(Nc1cccc1)c1ccc(cc1)N=Nc1ccc(c(e1)C(=O)O)O
C3315	PS	Nonsubstrate	172	O=S(=O)(NC)Cc1ccc2c(e1)e(e[nH]2)CCN(C)C
C3316	PS	Nonsubstrate	172	O=S(=O)(O)CCNC(=O)CC[C@@H](C)[C@@H]1[C@@]2([C@H](C[C@H]3[C@H]([C@@H]2CC1)[C@@H](C[C@H]1[C@]3(CC[C@H](C1)O)C)O)O)C
C3317	PS	Nonsubstrate	172	O(c1e2e3c(cc1OC)CCN([C@H]3Cc1cc(Oc3ccc(C[C@@H]4N(CCc5c4cc(O2)c(e5)OC)C)cc3)c(cc1)OC)C)C
C3318	PS	Nonsubstrate	172	ClC(Cl)(Cl)C(N1CCN(CC1)C(NC=O)C(Cl)(Cl)Cl)NC=O
C3319	PS	Nonsubstrate	172	c1ccc2c(e1)N(c1c(CC2)cccc1)CC(C)CN(C)C
C3320	PS	Nonsubstrate	172	S(=O)(=O)(O)c1cc2cc(c(c2c(e1)N)O)N=Nc1c(cc(cc1)c1cc(c(cc1)N=Nc1c(c2c(cc2cc1S(=O)(=O)O)S(=O)(=O)N)O)C)S(=O)(=O)O
C3321	PS	Nonsubstrate	172	O=C(O)[C@@H](N(C(=O)CCCC)Cc1ccc(cc1)c1c(ccc1)c1nn[nH]n1)C(C)C
C3322	PS	Nonsubstrate	172	COe1c(ccc(e1)CCN(C)CCCC(C)C)(C#N)c1cc(c(cc1)OC)OC
C3323	PS	Nonsubstrate	172	O=C1N(C(=O)C(O1)(C=C)C)c1cc(cc1)ClCl
C3324	PS	Nonsubstrate	172	BrC1ccc(cc1)/C(=C)CN(C)C/c1cccc1
C3325	PS	Nonsubstrate	171	COC1C(O)C2CN3CCc4c([nH]e5e4ccc(OC)e5)C3CC2C1C(=O)O
C3326	PS	Nonsubstrate	171	COe1ccc(Cc2c(c3c([nH]n(e3=O)c3cccc3)c3cccc3)c(=O)[nH]nc2c2ccc(C)cc2)cc1
C3327	PS	Nonsubstrate	163	COe1cc(cc(OC)c1OC)C1C2C(COC2=O)C(OC2OC3COC(OC3C(O)C2O)c2cccc2)c2cc3c(OCO3)cc12
C3328	PS	Nonsubstrate	157	CSCCC(NC(=O)C(CC(C)C)NC(=O)C(CC(C)C)NC(=O)C)C=O
C3329	PS	Nonsubstrate	157	COC(=O)C(C)NC(=O)C(C)NC(=O)C(C)NC(=O)C
C3330	PS	Nonsubstrate	149	OC(=O)Cc1c(O)ccc(e1)/N=N\c1ccc(cc1)S(=O)(=O)Nc1cccc1
C3331	PS	Nonsubstrate	149	Oe1ccc(cc1)/N=N\c1ccc(cc1)S(=O)(=O)Nc1cccc1
C3332	PS	Nonsubstrate	96,41	COe1ccc(Cc2c(C3C(=O)N(N=C3c3cccc3)c3cccc3)c(=O)[nH]nc2c2ccc(C)cc2)cc1
C3333	PS	Nonsubstrate	75	COe1cccc2c1C(=O)c1c(c(O)c3CC(O)(CC(OC4CC(N)C(I)C(C)O4)c3e1O)C(=O)CO)C2=O
C3334	PS	Nonsubstrate	75	CC1OC(CC(N)C1O)OC1CC(O)(Cc2c(O)c3c(cc12)C(=O)e1cccc1C3=O)C(=O)C
C3335	PS	Nonsubstrate	53	CCCCC(O)CC(O)CC(=O)CCCC(=O)CC(O)CC(=O)CCCCC(O)CC(O)CC(=O)CCCC(=O)CC(O)CC(=O)CCCC(=O)C
C3336	PS	Nonsubstrate	41	COC(=O)C(=C)C
C3337	PS	Nonsubstrate	132	NCCC(Oc1ccc(cc1)C(F)(F)F)c1cccc1
C3338	PS	Nonsubstrate	74	Nc1nc(S)c2nc[nH]c2n1
C3339	PS	Nonsubstrate	133,68,93,39	CCOC(=O)C1(CCN(C)CC1)c1cccc1
C3340	PS	Nonsubstrate	53	CN1CCN(CC1)c1c(F)cc2c(=O)c(cn(CCF)c2c1F)C(=O)O
C3341	PS	Nonsubstrate	68	Cc1cn(C2OC(CO)C=C2)c(=O)[nH]c1=O
C3342	PS	Nonsubstrate	76	CCCCC(C)C(OC(=O)C)CC(C)C(=O)C(=O)C(C)CC(O)CCCC(O)CC(O)C(C)N)OC(=O)CC(CC(=O)O)C(=O)O
C3343	PS	Nonsubstrate	157	CCCCC(C)C(OC(=O)C)CC(C)C(=O)C(=O)C(C)CC(O)CCCC(O)CC(O)CC(=O)CCCCC(O)CC(O)CC(=O)CCCC(=O)CC(O)CC(=O)CCCC(=O)C
C3344	PS	Nonsubstrate	125	CC(C)(C#N)c1cc(cc(Cn2cnc2)c1)C(C)C#N
C3345	PS	Nonsubstrate	106	NC(=O)c1cc[n+](CC2=C(N3C(SC2)C(NC(=O)C(c2cccc2)S(=O)(=O)O)C3=O)C(=O)[O-])cc1
C3346	PS	Nonsubstrate	71,53,71,96,4	OCC(=O)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
C3347	PS	Nonsubstrate	74	CN1CCC(C(O)C1)c1c(O)cc(O)c2c1oc(cc2=O)c1cccc1Cl
C3348	PS	Nonsubstrate	168,68,130	Cc1ccc(cc1)/C(=C)CN1CCCC1/c1cccc1
C3349	PS	Nonsubstrate	44	COe1ccc(cc1)c1coc2cc(O)cc(O)c2c1=O
C3350	PS	Nonsubstrate	53,96	COC(=O)Cl
C3351	PS	Nonsubstrate	114,149	Nc1cc(C(=O)O)c(O)cc1
C3352	PS	Nonsubstrate	126	NC(=N)NCc1cccc1)c1
C3353	PS	Nonsubstrate	170,53,96	Oe1c2OC3C(=O)CCC4(O)C5N(CC6CC6)CCC34c2c(cc1)C5
C3354	PS	Nonsubstrate	121	CC(O)C1C2C(C)C(=C(N2C1=O)C(=O)O)SC1CNC(C1)C(=O)Nc1ccc(cc1)C(=O)[O-]
C3355	PS	Nonsubstrate	125	NC1C(=O)NOC1
C3356	PS	Nonsubstrate	155	OC(CNCc1cccc1)COe1cccc1C(=O)CCc1cccc1





C3449	PS	Substrate	172	Clc1ccc(cc1)[C@H]1CN2CCN=C2c2c1cccc2
C3450	PS	Substrate	172	O=C(c1cn(c2cccc12)C)[C@@H]1CCc2[nH]cnc2C1
C3451	PS	Substrate	172	CC(C)c1scc(n1)CN(C)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1cccc1)C[C@@H](O)[C@@H](Cc1cccc1)NC(=O)OCc1scnc1
C3452	PS	Substrate	172	O=C(OC)[C@@H](N)CSCC=C(CCC=C(C)CCC=C(C)C)C
C3453	PS	Substrate	172	Fe1ccc(cc1)C(c1ccc(cc1)F)CNC1CCN(CC1)c1nc(nc(n1)NCC=C)NCC=C
C3454	PS	Substrate	172	O=C(O[C@H]1C[C@H](C=C2[C@H]1[C@H]([C@H](C=C2)C)CC[C@H](C[C@H](CC(=O)O)O)O)C(C)C(C)C
C3455	PS	Substrate	172	O[C@H](CCCCCCCCCCCC)[C@@H](N)CO
C3456	PS	Substrate	172	Fe1ccc(cc1)C(=O)CCCN1CCC2(CC1)N(CNC2=O)c1cccc1
C3457	PS	Substrate	172	O=C(OC1CC2CN3CCc4c(C3CC2C(C1OC)C(=O)OC)[nH]c1cc(OC)ccc41)C=Cc1cc(c(c1)OC)OC)OC
C3458	PS	Substrate	172	O(C)c1ccc2nc3cccc3c(NC(C)CCN(CC)CC)c2c1
C3459	PS	Substrate	172	S1C2N(C=C(C1)CS1n(nnn1)C)C(=O)O)C(=O)C2NC(=O)C1S/C(=C\C(=O)N)/C(=O)O)/S1
C3460	PS	Substrate	172	O=C1C2C(CO1)C(c1cc3OCOe3cc1C2c1cc(c(c1)OC)OC)OC)NC(=O)C
C3461	PS	Substrate	172	Fe1ccc(cc1)Cn1c(nc2cccc12)NC1CCN(CC1)CCc1ccc(cc1)OC
C3462	PS	Substrate	172	C1CCCC1=CCCN1CCc2c(C1)cc(OC)c(OC)c2
C3463	PS	Substrate	172	c12cccc(OC)c1CCCC2=CCCN1CCCC1
C3464	PS	Substrate	172	c12ccc(OC)cc1CCC=C2CCCN1CCc2c(C1)cc(OC)c(OC)c2
C3465	PS	Substrate	172	O=C(O)C[C@H](O)C[C@H](O)CCn1c(c(c1C(C)C)C(=O)Nc1cccc1)c1cccc1)c1ccc(cc1)F
C3466	PS	Substrate	172	c12cccc(OC)c1CCCC2CCCN1CCc2c(C1)cc(OC)c(OC)c2
C3467	PS	Substrate	172	c12cc(OC)c(OC)cc1CCCC2CCCN1CCc2c(C1)cc(OC)c(OC)c2
C3468	PS	Substrate	172	c1c(ccc1)[P+](c1cccc1)(c1cccc1)c1cccc1
C3469	PS	Substrate	172	O[C@H](COc1c(nsn1)N1CCOCC1)CNC(C)C
C3470	PS	Substrate	172	Oc1c(c2cc3Cn4c(=O)c5c(cc4c3nc2cc1)C(C(=O)OC5)(O)CC)CN(C)C
C3471	PS	Substrate	172	Clc1ccc2c(c1)[C@@H]1CN(C[C@H]1c1c(O2)cccc1)C
C3472	PS	Substrate	172	C[N+](CCCC)(CCCC)CCCC
C3473	PS	Substrate	172	FC(F)Fc1ccc2Sc3c(N(c2c1)CCCN1CCN(CC1)C)cccc3
C3474	PS	Substrate	172	N[C@@H](Cc1ccc(cc1)O)C(=O)N[C@H](C)C(=O)NCC(=O)N(C)[C@@H](Cc1cccc1)C(=O)NCCO
C3475	PS	Substrate	172	CC(=O)OC1C2(C=CCN3CCC4(c5cc(c(cc5N(C4C1(O)C(=O)OC)C)OC)C1(c4c(CCN5CC(C1)CC(C5)(O)CC)c1cccc1[nH]4)C(=O)OC)C23)CC
C3476	PS	Substrate	172	O=C(c1ccc(cc1)N=[N+]=[N-])NCC[N+](CC)(CC)C
C3477	PS	Substrate	172	O=C(OC)[C@]1(C[C@H]2[C@](CN(CC3c1[nH]c1cccc31)C2)(O)CC)c1cc2c(cc1OC)N([C@@H]1[C@@]32[C@H]2N(CC=C[C@@]2([C@H]([C@@]1(O)C(=O)N)O)CC)CC3)C
C3478	PS	Substrate	172	O=C(OC)[C@]1(C[C@H]2C=C(CN(CC3c4cccc4[nH]c13)C2)CC)c1cc2c(cc1OC)N([C@@H]1[C@@]32[C@H]2N(CC=C[C@@]2([C@H]([C@@]1(O)C(=O)OC)OC(=O)C)CC)CC3)C
C3479	PS	Substrate	172	O(CC(C)C)CC(N1CCCC1)CN(c1cccc1)Cc1cccc1
C3480	PS	Substrate	172	O1COe2c1cc1c(c2)CC[n+]2cc3c(c(ccc3cc12)OC)OC
C3481	PS	Substrate	172	O=C(Nc1ccc(c1)C(F)(F)F)C#N)C(O)(C)CS(=O)(=O)c1ccc(cc1)F
C3482	PS	Substrate	172	N#C/N=C\N[C@H]1CC[C@@H](CC1)C)/NS(=O)(=O)c1ccc(cc1)CCNC(=O)c1c(ccc(c1)Cl)OC
C3483	PS	Substrate	172	O=C1N(CCN1)CCN1CCC(CC1)c1c2c(nc1)c1ccc(cc1)F)ccc(c2)c1nnn(n1)C
C3484	PS	Substrate	172	CC(C)C)c1oc(nc1)CSc1sc(nc1)NC(=O)C1CCNCC1
C3485	PS	Substrate	172	N#Cc1c(ccc1)OCC(O)CNC(C)C
C3486	PS	Substrate	172	Cc1ccc(/C(=C/CN2CCCC2)/c2nc(/C=C\C(=O)N3CCCC3)ccc2)cc1
C3487	PS	Substrate	172	Cc1ccc(/C(=C/CN2CCCC2)/c2nc(/C=C\C(=O)N3CCOCC3)ccc2)cc1
C3488	PS	Substrate	172	O=C(O[C@H](COP(=O)(O)OC[C@H](N)C(=O)O)COC(=O)CCCCNc1c2nonc2c(cc1)[N+](=O)[O-])CCCCCCCCCCCC
C3489	PS	Substrate	172	FC(F)(c1ccc(ncc1)N1CCN(CC1)CCCC1CCCC1=O)F
C3490	PS	Substrate	172	CC(=O)OCOC(=O)CN(CC(=O)OCOC(=O)C)Cc1c(cc2c(c1)C1(c3cc(c(cc3O2)OC(=O)C)CN(CC(=O)OCOC(=O)C)CC(=O)OCOC(=O)C)c2cccc2C(=O)O1)OC(=O)C
C3491	PS	Substrate	172	O=C(N(CC)CC)Nc1cc(c(cc1)OCC(O)CNC(C)C)C(=O)C
C3492	PS	Substrate	172	O1c2c3[C@H](Cc4ccc(Oc5c(ccc[C[C@@H]6c7c(cc(c1c7)OC)CCN6C)c5)OC)cc4)N(Cc3cc1OCOe21)C
C3493	PS	Substrate	172	O=C(O)C[C@H](O)C[C@H](O)C=C/c1c(c(nc1C(C)C)C(C)C)COC)c1ccc(cc1)F
C3494	PS	Substrate	172	COCOc1cccc2OCC3=C(C)CC[C@]4(OC(=O)O[C@H]4c12)C3(C)C





C3587	PS	Substrate	110155	CC(=O)c1cccc1OCC(O)CN1CCN(CC1)c1ccc(F)cc1
C3588	PS	Substrate	141	COC(CCc1cccc1)c1cccc1OCC(O)CN(C(C)C)C(C)C
C3589	PS	Substrate	141	OC(COe1cccc(c1)C(=O)CCe1cccc1)CN1CCN(CC1)c1ccc(F)cc1
C3590	PS	Substrate	141	CC(C)N(CC(O)COe1ccc(cc1)C(=O)CCe1cccc1)C(C)C
C3591	PS	Substrate	145,95	CCC(N1CCCC1=O)C(=O)N
C3592	PS	Substrate	71	C12CCC(=O)C1(C)CCC1C2CC=C2CC(O)CCC12C
C3593	PS	Substrate	109	O/C(=C/1\C(=O)C(N(C)C)C2C(O)C3C(=O)c4c(ccc40)C3(O)C)C(=O)C2(O)C1=O)/N
C3594	PS	Substrate	171	CCC1(CCC(O1)C1(C)CCC2(CC(O)C(C)C(O2)C(C)C(OC)C(C)C(=O)O)1)C1OC(CC1C)C1OC(O)(CO)C(C)CC1C
C3595	PS	Substrate	145,89	C12CC(O)C(O)(C(=O)CO)C1(C)CC(O)C1(F)C2CCC2=CC(=O)C=CC12C
C3596	PS	Substrate	93	CCCN1CCC(CC1)(C(=O)OCC)c1cccc1
C3597	PS	Substrate	141	CC(=O)c1cccc1OCC(O)CN1CCCC1
C3598	PS	Substrate	155	CCCNCC(O)c1c(Cc2ccccc2)c2ccccc2o1
C3599	PS	Substrate	110155	OC(COe1cccc1C(=O)CCe1cccc1)CN1CCOCC1
C3600	PS	Substrate	127	C1CCN(N=O)C(=O)NC1CCCC1
C3601	PS	Substrate	110155	OC(COe1cccc1C(=O)CCe1cccc1)CN1CCCC1
C3602	PS	Substrate	171	O=C(NC(CCc1cccc1)/C=C\S(=O)(=O)c1cccc1)C(Cc1cccc1)NC(=O)N1CCOCC1
C3603	PS	Substrate	,163,171,49,53	OC1CC(=O)OC(/C(=C/c2esc(n2)C)/C)CC2OC2CCCC(C)C(O)C(C(=O)C1(C)C)C
C3604	PS	Substrate	0,52,69,89,96,	CN/C(=N/CCSc1c(C)[nH]cn1)/NC#N
C3605	PS	Substrate	80	COc1c(OC)c(OC)c2c(CC(C)(O)C(C)Cc3c2c(OC)c2OCOe2c3)c1
C3606	PS	Substrate	9,52,53,54,57,	COC1CC(CCC1O)/C=C(\C)/C1OC(=O)C2CCCCN2C(=O)C(=O)C2(O)OC(C(CC2C)OC)C(CC(C)C/C(=C/C(CC=C)C(=O)CC(O)C1C)/C)OC
C3607	PS	Substrate	2,53,61,69,86,	COe1cc(cc(OC)c1O)C1C2C(COC2=O)C(OC2OC3COC(OC3C(O)C2O)c2cccs2)c2c1cc1OCOe1c2
C3608	PS	Substrate	140,49,61,74	CC(Cc1cccc1)NCCC(c1cccc1)c1cccc1
C3609	PS	Substrate	68	CC(C)CC(NC(=O)C(Cc1cccc1)NC(=O)CNC(=O)C(C)NC(=O)C(N)Cc1ccc(O)cc1)C(=O)O
C3610	PS	Substrate	141	O[C@@@H](COe1cccc1C(=O)CCe1cccc1)CN1CC[C@@](O)(CC1)c1cccc1
C3611	PS	Substrate	71,49,52,53,5	CCCCc1oc2ccccc2c1C(=O)c1cc(I)c(OCCN(CC)CC)c(I)c1
C3612	PS	Substrate	141	OC(COe1cccc1C(O)CCe1cccc1)CN1CCCC1
C3613	PS	Substrate	127	CN(C)CCOe1cc2c(c3ccccc3C2=O)c2c1cccc2
C3614	PS	Substrate	171	COC1/C=C\OC2(C)Oe3c(C)c(O)c4c(O)c(NC(=O)/C=C\C=C\C(C)C(O)C(C)C(O)C(C)C(OC(=O)C)C1C)/C)c/C=N/N1CCN(C)CC1)c(O)c4c3C2=O
C3615	PS	Substrate	0,163,49,53,96	CCOC(=O)Oe1c(OC)cc(cc1OC)C(=O)OC1CC2CN3CCc4c([nH]c5e4ccc(OC)c5)C3CC2C(C1OC)C(=O)OC
C3616	PS	Substrate	100	N(C(=O)N(CC)CC)C1CN(C)C2Cc3c[nH]c4cccc(c34)C2C1
C3617	PS	Substrate	99	COe1ccc2CCCC(CCCN3CCc4c(C3)cc(OC)c(OC)c4)c2c1
C3618	PS	Substrate	135,140,49,52	OCCOe1ccc(cc1)C(C)(C)CC(C)(C)C
C3619	PS	Substrate	68	CCC1CN2CCc3cc(OC)c(OC)cc3C2CC1CC1NCCc2cc(O)c(OC)cc12
C3620	PS	Substrate	145,68,89	OC(CC(NC(=O)C(N1C(=O)NCCCC1)C(C)C)Cc1cccc1)C(NC(=O)COe1c(ccc1C)C)Cc1cccc1
C3621	PS	Substrate	100	CC1CC2C3CCC4=CC(=O)C=CC4(C)C3C(=O)CC2(C)C1(O)C(=O)CO
C3622	PS	Substrate	52	CN(C)CCC=C1c2c(CCc3c1cccc3)cccc2
C3623	PS	Substrate	171	CCC1(O)CC2CN(C1)CCc1c([nH]c3ccccc13)C(C2)(C(=O)OC)c1c(OC)cc2N(C=O)C3C4(CCN5CC=CC(CC)(C45)C(OC(=O)C)C3(O)C(=O)OC)c2c1
C3624	PS	Substrate	51,68	CCCOe1c(cc(en1)S(=O)(=O)N1CCN(CC)CC1)c1nc2c(CC)n(Cc3cccn3)nc2c(=O)[nH]1
C3625	PS	Substrate	74	Fe1c(Cc2n[nH]c(=O)cc2)ccc(Cl)c1Oe1cccc1
C3626	PS	Substrate	55	COC(=O)C12OCC34C1C(OC(=O)/C=C(\C)/C(C)C)C(=O)OC3CC1C(=C(O)C(=O)CC1(C)C4C(O)C2O)C
C3627	PS	Substrate	68	NS(=O)(=O)N1CCN(CC1)C1CN(CCC2(CCC(=O)N(CC3CC3)C2)c2cc(Cl)c(Cl)cc2)C1
C3628	PS	Substrate	8,61,69,103,11	ccc1nc(=O)c(C(O)c(C)C/C=C/C)N(C)C(=O)c(C(C)C)N(C)C(=O)c(C(C)C)N(C)C(=O)c(C)N(C)C(=O)c(C)N(C)C(=O)c(C(C)C)N(C)C(=O)c(NC(=O)C)C(C)C(=O)c(NC(=O)C)C(C)C(=O)CN(C)C1=O)C(C)C
C3629	PS	Substrate	122	Ce1nc(Nc2nce(s2)C(=O)Ne2c(C)cccc2Cl)cc(n1)N1CCN(CCO)CC1
C3630	PS	Substrate	50	cc(C)[C@@H](NC(=O)[C@@H](CCCN=C(N)N)NC(=O)[C@@H](N)CC(=O)N)C(=O)N[C@@H](Cc1ccc(O)cc1)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1cnc[nH]1)C(=O)N1CCC[C@@H]1C(=O)N[C@@H](Cc1cccc1)C(=O)O
C3631	PS	Substrate	4,145,146,69,1	C12CCC3(CCC(=O)O3)C1(C)CCC1C2C(CC2=CC(=O)CCC12C)SC(=O)C
C3632	PS	Substrate	55	CN(C(=O)C)c1ccc(Nc2cc(C)nc3c2c2c([nH]cn2)cc3)cc1



C3633	PS	Substrate	67,99	<chem>COc1cc2c(CN(CC/C=C\3/CCCc4c3cccc4OC)CC2)cc1OC</chem>
C3634	PS	Substrate	9,53,61,69,86,	<chem>CCC12C=CCN3CCC4(C13)C(N(C)c1c4ccc(OC)c1)C(O)(C2OC(=O)C)C(=O)OC</chem>
C3635	PS	Substrate	69	<chem>[O-][N+](=O)c1ccc(C[P+](c2ccccc2)(c2ccccc2)c2ccccc2)cc1</chem>
C3636	PS	Substrate	145,69,100,128	<chem>CN1CCCC(CC1)n1nc(Cc2ccc(Cl)cc2)c2ccccc2e1=O</chem>
C3637	PS	Substrate	52	<chem>CCN1CCCC1CNC(=O)c1cc(c(N)cc1OC)S(=O)(=O)CC</chem>
C3638	PS	Substrate	69	<chem>CNCC(O)c1cc(OC(=O)C(C)(C)C)c(OC(=O)C(C)(C)C)cc1</chem>
C3639	PS	Substrate	45,52,69,128,3	<chem>COc1c(OCCNCC(O)COc2c3c([nH]c4c3cccc4)ccc2)cccc1</chem>
C3640	PS	Substrate	81	<chem>OC(=O)C(O/N=C\(\C(=O)NC1C(=O)N2C(=C(C[n+]3ccccc3)CSC12)C(=O)[O-])/c1csc(n1)N(C)C</chem>
C3641	PS	Substrate	69,171,52,53,6	<chem>CCOe1ccc(cc1)c1nc2ccc(cc2[nH]1)c1nc2c([nH]1)ccc(c2)N1CCN(C)CC1</chem>
C3642	PS	Substrate	52,90,95	<chem>Nc1nc(N)c(nn1)c1c(Cl)c(Cl)ccc1</chem>
C3643	PS	Substrate	63,169,49,52,5	<chem>COC(=O)c1ccccc1c1c2ccc(=NH2+)cc2oc2c1ccc(N)c2</chem>
C3644	PS	Substrate	171,52,53,68,6	<chem>CC(C)(C)NC(=O)C1CC2CCCC2CN1CC(O)C(Cc1ccccc1)NC(=O)C(CC(=O)N)NC(=O)c1ccc2cccc2n1</chem>
C3645	PS	Substrate	125	<chem>O=C1CCc2c(N1)ccc(OCCCCe1nnnn1C1CCCCC1)c2</chem>
C3646	PS	Nonsubstrate	68,74,86,89,1	<chem>COc1cc(NC(=O)c2cc3cccc3nc2)c(cc1OC)C(=O)Nc1ccc(CCN2CCc3cc(OC)c(OC)cc3C2)cc1</chem>
C3647	PS	Nonsubstrate	172	<chem>Fe1cc(c(cc1)C(O)(Cn1cncn1)Cn1cncn1)F</chem>
C3648	PS	Nonsubstrate	68	<chem>CC(OCc1ccccc1)C1NC(=O)C(CCCCN)NC(=O)C(Cc2c[nH]c3ccccc23)NC(=O)C(Cc2ccccc2)NC(=O)CCCCCN1=O</chem>
C3649	PS	Nonsubstrate	125	<chem>OC(COe1nsnc1N1CCOCC1)CNC(C)(C)C</chem>
C3650	PS	Nonsubstrate	172	<chem>O=C(OC)[C@@]1([C@@@H])([C@@]2(C=CCN3CC[C@@]4(c5c(N([C@@@H]14)C)cc(cc5)OC)[C@H]23)CC)OC(=O)C)O</chem>
C3651	PS	Nonsubstrate	172	<chem>O=S(=O)(C(C=NOC(=O)NC(C)C)C)C</chem>
C3652	PS	Nonsubstrate	172	<chem>O=C(O)c1c(cccc1)O</chem>
C3653	PS	Nonsubstrate	164,68	<chem>CCCC/C=C\C/C=C\C=C/C=C/C/[C@@@H](SC[C@@@H](NC(=O)CC[C@@@H](N)C(=O)O)C(=O)NCC(=O)O)[C@@@H](O)CCCC(=O)O</chem>
C3654	PS	Nonsubstrate	172	<chem>O=C(O)[C@@@H]1CCCN1C(=O)[C@H](C)CS</chem>
C3655	PS	Nonsubstrate	68	<chem>CC1(C)SC2C(NC(=O)C(N)c3ccccc3)C(=O)N2C1C(=O)O</chem>
C3656	PS	Nonsubstrate	172	<chem>Fe1cc2c(cc1)NC(=O)[C@@@H](N2C(=O)OC(C)C)CC</chem>
C3657	PS	Nonsubstrate	172	<chem>O=C(c1ccc2c(c1)nc([nH]2)NC(=O)OC)c1ccccc1</chem>
C3658	PS	Nonsubstrate	0,163,49,53,96	<chem>Cc1c(N/N=C\2/C(=O)c3c(cc(cc3N)S(=O)(=O)[O-])C=C2S(=O)(=O)[O-])ccc(c1)c1cc(C)c(N/N=C\2/C(=O)c3c(cc(cc3N)S(=O)(=O)[O-])C=C2S(=O)(=O)[O-])cc1</chem>
C3659	PS	Nonsubstrate	68	<chem>NC(CCC(=O)O)C=C</chem>
C3660	PS	Nonsubstrate	172	<chem>O[C@H](/C=C/CCCCCCCCCCCC)[C@@@H](N)CO</chem>
C3661	PS	Nonsubstrate	172	<chem>oc(=O)[C@H](C)[C@H]1[C@H]([C@H]([C@H]([C@H]1)C)C)[C@@@H](C)C(C)C1</chem>
C3662	PS	Nonsubstrate	172	<chem>O=C(NC1CCCCC1)NS(=O)(=O)c1ccc(cc1)CCNC(=O)c1c(ccc(c1)Cl)OC</chem>
C3663	PS	Nonsubstrate	172	<chem>O[C@H]([C@H](O)CO)[C@H](O)[C@H](O)CO</chem>
C3664	PS	Nonsubstrate	172	<chem>O=C1C(C(=O)N(N1c1ccccc1)c1ccccc1)CCS(=O)c1ccccc1</chem>
C3665	PS	Nonsubstrate	172	<chem>O=C1N(C(=O)c2ccccc12)CSP(=S)(OC)OC</chem>
C3666	PS	Nonsubstrate	125	<chem>NS(=O)(=O)c1c(OC)ccc(c1)CC(NCCOe1ccccc1OCC)C</chem>
C3667	PS	Nonsubstrate	172	<chem>O=C(Nc1ccc(cc1)O)C</chem>
C3668	PS	Nonsubstrate	68,70,74	<chem>Nc1nc(=O)n(cc1)C1OC(CO)C(O)C1(F)F</chem>
C3669	PS	Nonsubstrate	70	<chem>Cc1ncc(CNC(=O)N(CCC1)N=O)c(N)n1</chem>
C3670	PS	Nonsubstrate	172	<chem>O=c1n(nnn1CCN1CCC(CC1)(N(c1ccccc1)C(=O)CC)COC)CC</chem>
C3671	PS	Nonsubstrate	172	<chem>n1c(c(nc2c1c(nc(n2)N)N)N)c1ccccc1</chem>
C3672	PS	Nonsubstrate	172	<chem>O[C@H]1CC[C@@]2([C@@@H]3[C@@@H](CC=C2C1)[C@H]1[C@@](CC3)([C@H](CC1)[C@H](C)CC[C@@@H](CC)C(C)C)C)C</chem>
C3673	PS	Nonsubstrate	172	<chem>O=C(OC1c[n+](ccc1)C)N(C)C</chem>
C3674	PS	Nonsubstrate	172	<chem>O(c1c(cc2c(c1)CCN([C@H]2Cc1c(cc(c1)OC)OC)Oc1cc2c(cc1OC)c1c(cc3c1[C@H](C2)N(CCC3)C)OC)OC)OC)C</chem>
C3675	PS	Nonsubstrate	172	<chem>O=C(N(C)C)Cc1n2cc(ccc2nc1c1ccc(cc1)C)C</chem>
C3676	PS	Nonsubstrate	172	<chem>Clc1c(c(ccc1)Cl)CC(=O)N=C(N)N</chem>
C3677	PS	Nonsubstrate	172	<chem>O=C1CC[C@H]2C(=C1)CC[C@H]1[C@H]3[C@@]([C@H]21)([C@](CC3)(C#C)O)C</chem>
C3678	PS	Nonsubstrate	172	<chem>O=c1c2ccccc2n(c2ccccc12)CCCN1c2c(c(=O)c3ccccc13)cccc2</chem>

C3679	PS	Nonsubstrate	172	O=C(N1CCN(CC1)c1ccc(cc1)OC[C@H]1CO[C@](O1)(c1c(cc(cc1)Cl)Cl)Cn1ence1)C
C3680	PS	Nonsubstrate	172	C#CCN([C@@H](Cc1ccccc1)C)C
C3681	PS	Nonsubstrate	145	CC(C)(Oc1ccc(CCNC(=O)c2ccc(Cl)cc2)cc1)C(=O)O
C3682	PS	Nonsubstrate	172	S=c1c(c2c(c(n1C1C(C(O)C(C(O1)CO)O)O)c1secc1)CCc1c2ccccc1)C#N
C3683	PS	Nonsubstrate	145	Cc1ccc(C)c(OCCCC(C)(C)C(=O)O)c1
C3684	PS	Nonsubstrate	172	O=C(O)[C@@H](N)Cc1ccc(cc1)N(CCC1)CCCl
C3685	PS	Nonsubstrate	155	COc1c(cccc1)N1CCN(CC(O)c2c(Cc3ccccc3)c3ccccc3o2)CC1
C3686	PS	Nonsubstrate	172	CCC(=C(c1ccccc1)c1ccc(cc1)OCCN(C)C)c1ccccc1
C3687	PS	Nonsubstrate	172	O=C(O)[C@@H]1[C@H]([C@@H]([C@@H]([C@@H]2CN3CCc4c5ccc(cc5[nH]c4[C@H]3C[C@H]12)OC)O)OC
C3688	PS	Nonsubstrate	172	O=S(=O)(Nc1ccc(on1)C)c1ccc(cc1)N
C3689	PS	Nonsubstrate	172	CC(=O)OC1C(C(C(OC1n1c(=S)c(C#N)c(c(c1C)C(=O)OCC)c1ccc(cc1)Cl)COC(=O)C)OC(=O)C)OC(=O)C
C3690	PS	Nonsubstrate	172	O=C(N)N1c2c(C=Cc3ccccc13)ccccc2
C3691	PS	Nonsubstrate	172	Cn1c2ccccc2c2c1C(=O)N(CC2)CCCCN(C)C
C3692	PS	Nonsubstrate	172	O=C1[C@H](C2SCC(=C(N12)C(=O)O)C[n+])1ccc(cc1)C(=O)N)NC(=O)C(c1ccccc1)S(=O)(=O)O
C3693	PS	Nonsubstrate	172	Clc1cc(ccc1)N1CCN(CC1)CCCN1c(=O)n2ccccc2n1
C3694	PS	Nonsubstrate	172	c12cc(OC)c(OC)cc1CCC=C2CCCN1CCc2c(C1)cc(OC)c(OC)c2
C3695	PS	Nonsubstrate	167,68,69,128	CCOC(=O)C1=C(C)NC(=C(C1c1ccc(Cl)c1Cl)C(=O)OC)C
C3696	PS	Nonsubstrate	172	O=C/C=C/c1ccc(cc1)O)CC(=O)/C=C/c1ccc(cc1)O
C3697	PS	Nonsubstrate	172	Clc1c(n(c(n1)CCCC)Cc1ccc(cc1)c1c(cccc1)c1nn[nH]n1)C(=O)O
C3698	PS	Nonsubstrate	172	O=c1c(cc2CCCCCc2n1C1C(C(C(O1)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)C#N
C3699	PS	Nonsubstrate	172	O=C(Nc1ccc(cc1)OCC(O)CNC(C)C)C
C3700	PS	Nonsubstrate	172	O=C(OC)[C@@H](N)CS
C3701	PS	Nonsubstrate	172	FC(F)(F)c1cc(ncc1)Oc1ccc(cc1)OC(C)C(=O)OCCCC
C3702	PS	Nonsubstrate	125	CN1CCC(CN2c3ccccc3Sc3c2ccccc3)C1
C3703	PS	Nonsubstrate	172	S=c1c(c(c(n1C1C(C(C(O1)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)c1ccccc1)C(=O)C)c1ccc(cc1)OC)C#N
C3704	PS	Nonsubstrate	36	COc1c2Oc3ccc(CC4N(C)CCc5cc(OC)c(O)c6c(OC)c(OC)c(Br)c7c6C(Cc(cc1)c2)N(C)CC7)cc45)cc3
C3705	PS	Nonsubstrate	93	CCOC(=O)C1(CCN(CCCc2ccccc2)CC1)c1ccccc1
C3706	PS	Nonsubstrate	172	OC(=O)c1cc(C(=O)O)ccc1c1c2c(cc(c2)CCCC(=O)O)O)oc2c1cc(c(=O)c2)CCCC(=O)O
C3707	PS	Nonsubstrate	172	O=c1cc(oc2c1ccccc2)c1ccccc1
C3708	PS	Nonsubstrate	172	O=C1CC[C@@]2(C=C1)CC[C@H]1[C@@H]3CC[C@@]([C@@]3(CC[C@H]21)C)(O)C(=O)CO)C
C3709	PS	Nonsubstrate	163	CC1OC(C(O)C(O)C1O)n1c(C)c(C(=O)C)c(c2ccco2)c(C#N)c1=S
C3710	PS	Nonsubstrate	172	O=C1OCC2C(c3c(C12)c1cc(c(c1)OC)OC)OC)cc1OCOc1c3)N(C)C(=O)C
C3711	PS	Nonsubstrate	146	CC(C)NCC(O)COc1c2ccccc2ccc1
C3712	PS	Nonsubstrate	172	CC(=O)OCOC(=O)c1cc(C(=O)OCOC(=O)C)ccc1c1c2c(cc(c2)CCC(=O)OCOC(=O)C)O)oc2c1cc(c(=O)c2)CCC(=O)OCOC(=O)C
C3713	PS	Nonsubstrate	172	OC[C@H]1Oe2c(O[C@@H]1c1ccc(c(c1)OC)O)cc(cc2)c1oe2c(c(cc(c2)O)O)c(=O)c1O
C3714	PS	Nonsubstrate	172	[O-][N+](=O)c1c2cc3c(nc2ccc1)c1cc2c(c(=O)n1C3)COC(=O)[C@]2(O)CC
C3715	PS	Nonsubstrate	172	N#CC1=C(N(C=CC1c1ccccc1)c1ccccc1)C1C(C(C(C(O1)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)S
C3716	PS	Nonsubstrate	171	CC(CCC(=O)NCCC[N+](C)(C)CCCS(=O)(=O)[O-])C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CC(O)C12C
C3717	PS	Nonsubstrate	172	Clc1ccc2c(c1)C(=NCC(=O)N2)c1ccccc1
C3718	PS	Nonsubstrate	172	c1ccc2c(c1)/C=C\CCN(C)C/c1c(C=C2)ccccc1
C3719	PS	Nonsubstrate	172	Clc1ccc(cc1)C(c1ccccc1)CCN(C)C
C3720	PS	Nonsubstrate	172	S=C1N(C(=Nc2[n+](ccccc2)Cc2ccccc2)N(C1=Nc1ccccc1)c1ccccc1)c1ccccc1
C3721	PS	Nonsubstrate	172	COc1cccc(COc2ccccc2CCc2ccccc2)c1OC
C3722	PS	Nonsubstrate	155	CCCN(C)CC(O)COc1ccccc1C(=O)CCc1ccccc1
C3723	PS	Nonsubstrate	172	O=C1[C@H]2[C@H](CO1)Cc1cc3OCOc3cc1[C@H]2c1cc(c(c(c1)OC)OC)OC
C3724	PS	Nonsubstrate	172	S=c1c(c(cc(n1C1C(C(C(O1)CO)O)O)O)C)C)C#N



C3771	PS	Substrate	172	O=S(=O)(c1cccc1)CCc1cc2c(cc1)[nH]cc2C[C@H]1CCCN1C
C3772	PS	Substrate	102	CCCC1nc2c(cc(cc2C)e2nc3c(ccc3)n2C)n1Cc1ccc(cc1)c1ccccc1C(=O)O
C3773	PS	Substrate	70	cc1c@1(O)C1C@H1O1C@H2[C@@H]1(C@H1O1C@H3C1C@H1O1C@H4C(=O)C@H1(C)O4[C@@H]1(C)O3[C@@H]1(C)O2N(C)C)e2c(O)c3c(cc2[C@H]1C(=O)OC)C(=O)c1c(c(O)ccc1)C3=O
C3774	PS	Substrate	102	OC(=O)C1N2C(=O)C(NC(=O)c3c(OCC)ccc4cccc34)C2SC1(C)C
C3775	PS	Substrate	166	Fe1ccc(cc1)C(=O)CCCN1CCC2(CC1)N(CNC2=O)c1ccc(Br)cc1
C3776	PS	Substrate	172	O=C(O)Cc1cc2C(=CCCN(C)C)c3c(COe2cc1)cccc3
C3777	PS	Substrate	47	CCCCCCCCCCCC[N+](C)(C)Cc1ccccc1
C3778	PS	Substrate	100	CCCCOc1cc(cc1N)C(=O)OCCN(CC)CC
C3779	PS	Substrate	172	Fe1ccc(cc1)C(=C1CCN(CC1)CCCC(=O)N1CCCC1)c1ccc(cc1)F
C3780	PS	Substrate	140,49,96,41	Ne1ccc(cc1)C(=C1C=C/C(=N)/C=C1)c1ccc(N)cc1
C3781	PS	Substrate	171	CCC12C=CCN3CCC4(C13)C(N(C)c1cc(OC)ccc41)C(O)(C2CC(=O)C)C(=O)OC
C3782	PS	Substrate	172	O=C(c1cc(nc2cccc12)OCCCC)NCCN(CC)CC
C3783	PS	Substrate	172	O=c1[nH]e2ccenc2n(e2cccc12)C(=O)CN1CCN(CC1)C
C3784	PS	Substrate	131	C[N+](C)(C)c1ccc(/C=C\C=C/C=C\C2ccccc2)cc1
C3785	PS	Substrate	172	O=C(NC1CCCC1)Nc1ccc(cc1)OCC(O)CNC(C)(C)C
C3786	PS	Substrate	42	C[P+](C)(c1ccccc1)c1ccccc1
C3787	PS	Substrate	134	CC(C)CC(NC(=O)C(Ce1ccccc1)NC(=O)CNC(=O)C(C)NC(=O)C(N)C)Cc1ccc(O)cc1)C(=O)Oe1ccccc1/C=C\C(=O)C
C3788	PS	Substrate	145,81	o1c@H1[C@@H]1O1C@H2[C@@H]1C@H1O1C@H3O1C@H4[C@@H]1C@H1O1C@H5OC3[C@@H]1C@H1O1C@H6OC3[C@@H]1C(=O)O1C@H7CC1C@H1O1C@H8OC1C@H9O1C@H10N(C)C1C@H11C1C@H12(O)C)C)O1C@H13C1C@H14N(C)C
C3789	PS	Substrate	145,52	COe1ccc(cc1)C(CN(C)C)C1(O)CCCCC1
C3790	PS	Substrate	100	CN(C)CCOC(C)(e1ccccc1)c1ccc(Cl)cc1
C3791	PS	Substrate	68	CCC1CN2CCc3cc(OC)c(OC)cc3C2CC1CC1NCCe2c1[nH]c1c2cc(O)cc1
C3792	PS	Substrate	172	Oe1ccc2c(c1)CC[C@H]1[C@H]3[C@@H]1(CC[C@H]21)[C@H](CC3)(C#C)O
C3793	PS	Substrate	172	O=C1c2cccc2C(=O)e2c(c3c(c(c12)O)[C@H](C[C@@H]1)(C3)O)C(=O)O[C@H]1C[C@@H]([C@@H]([C@@H](O1)C)O)N)O
C3794	PS	Substrate	172	[N-]=[N+]=Nc1cc(ccc1)CCN(C)CCCC(C#N)(c1cc(c(c(c1)OC)OC)OC)C(C)C
C3795	PS	Substrate	155	CCNCC(O)c1c(CC)c2ccccc2o1
C3796	PS	Substrate	172	O=C(Nc1cc(c(cc1)OCC(O)CNC(C)C)C(=O)C)CCC
C3797	PS	Substrate	100	COe1cc2c(cc1)nc2c2C(=O)C1CC2CCN1CC2C=C
C3798	PS	Substrate	172	O=C1C(O)C(C)C(C)CC(=O)N1CCCN1CCN(CC1)c1ncccc1
C3799	PS	Substrate	172	O=C1[C@H](C2SCC(=C(N12)C(=O)O)CSc1n(mnn1)C)(OC)NC(=O)C1S/C(=C\C(=O)N)/C(=O)O)/S1
C3800	PS	Substrate	145,69,81,128	o1c@H11c@H21C@H3[C@@H]1O1C@H42C@H5(C)O1C@H6OC(=O)C(=O)O1C@H7C)CC=C=C1C@H8O1C@H9C1C@H10C1C@H11C1C@H12CC=O)O1C@H13C1C@H14O1C@H15O1C@H16O1C@H17O1C@H18O1C@H19O1C@H20C@H21C@H22C@H23C@H24C@H25C@H26C@H27C@H28C@H29C@H30C@H31N(C)C
C3801	PS	Substrate	172	O=C[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)C)CC(C)C)CC(C)C)CCCN=C(N)N
C3802	PS	Substrate	52,53,54,69,85	OC(CN1CCN(Ce2cnc2)CC1C(=O)NC(C)(C)C)C(C(=O)NC1c2cccc2CC1O)Cc1ccccc1
C3803	PS	Substrate	172	O=C(/C=C/c1cccc(n1)/C(=C\CN1CCCC1)/c1ccc(cc1)C)O
C3804	PS	Substrate	172	Clc1ccc2c(ccnc2c1)NC(C)CCN(CC)CC
C3805	PS	Substrate	172	O=c1c2c(cc3n1Cc1c(c4c(nc31)cccc4)CCNC(C)C)[C@@H](C(=O)OC2)(O)CC
C3806	PS	Substrate	172	CN(C)c1ccc2c(c3ccc(=[N+](C)C)cc3se2c1)c1ccccc1
C3807	PS	Substrate	100	CCSc1cc2c(Sc3cccc3N2CCN2CCN(C)CC2)cc1
C3808	PS	Substrate	172	N#C/N=C(\NC1CCCC1)/NS(=O)(=O)c1ccc(cc1)CCNC(=O)c1c(ccc(c1)Cl)OC
C3809	PS	Substrate	45	CCCNCC(O)COe1ccc(O)cc1C(=O)CCc1ccccc1
C3810	PS	Substrate	172	Clc1ccc2c(c1)CCc1ccnc1C2=C1CCNCC1
C3811	PS	Substrate	172	CN1CCN(CC1)C1=Nc2c(Nc3c1cccc3)ccc(c2)Cl
C3812	PS	Substrate	99	COe1cccc2c1CCCC2CCCN1CCN(CC1)C1CCCCC1
C3813	PS	Substrate	172	O=C(O)[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)O)c1cc2c(cc1)[C@H]1CC[C@H]3[C@@H](CC[C@H]3[C@H]1CC2)O)C)O)O
C3814	PS	Substrate	71	OC1CC2=CCC3C4CCC(C(=O)C)C4(C)CCC3C2(C)CC1
C3815	PS	Substrate	172	O=C(O)c1ccc(cc1)O)OC(C)Cc1c(c(c2C(=O)C=C(c3c2c1c1c2c(C(=O)C=C(c32)OC)c(c(c1CC(OC(=O)c1ccccc1)C)OC)O)OC)O)OC
C3816	PS	Substrate	172	O=C1CC[C@H]2([C@@H]3[C@@H]1CC[C@H]2C1)[C@@H]1CC[C@@H]([C@@H]1(C3)C)O)C



C3863	PS	Substrate	172	c12ccc(OC)cc1CCCC2CCCN1CCc2c(C1)cc(OC)c(OC)c2
C3864	PS	Substrate	172	OCC(=O)C1(Cc2c(c3C(=O)c4cccc(e4C(=O)c3c(c2C(C1)OC1OC(C(C(C1)N)O)C)O)OC)O)O
C3865	PS	Substrate	172	O=C(C=CO)C@H]C@]2[C@@]CC1)[C@H][C@H]C@H20]C@]2[C@H]CC1)C@H]CC2)O[C@H]C[C@@H]([C@H]([C@H]O1)C)O[C@H]C[C@@H]([C@H]([C@H]O1)C)O)O)O)O)O)O)C
C3866	PS	Substrate	52,65,68,89	Cc[C@@H]C)C@H]O[C@]2[C@H]3[C@H]C=C(C)[C@H]O[C@H]4[C@H]OC)C@H]O[C@H]5[C@H]OC)C@H]O)C@H]([C@]O5)C@H]O4)C@H]C)C=C=C4CO)C@H]5[C@H]O)C=C(C@H]C(=O)O3)C@H]45O)CO2)C=C@H]1C
C3867	PS	Substrate	172	Oc1ccc(cc1)c1[nH]c(e2n(c1)c(=O)c(n2)Cclcccc1)Cc1cccc1
C3868	PS	Substrate	172	O=C(C=CO)C@H]C@]2[C@@]CC1)[C@H][C@H]C@H20]C@]2[C@H]CC1)C@H]CC2)O[C@H]C[C@@H]([C@H]([C@H]O1)C)O[C@H]C[C@@H]([C@H]([C@H]O1)C)O)O)O)O)O)O)C
C3869	PS	Substrate	172	c12cc(OC)ccc1CCC=C2CCCN1CCc2c(C1)cc(OC)c(OC)c2
C3870	PS	Nonsubstrate	172	O=C1C(C(CN1CC)CCN1CCOCC1)(c1cccc1)c1cccc1
C3871	PS	Nonsubstrate	172	CC(=O)CC(c1c(=O)oc2ccccc2c1O)c1cccc1
C3872	PS	Nonsubstrate	172	S1c2c(N(c3cccc13)CC(N(C)C)C)cccc2
C3873	PS	Nonsubstrate	75	COC1CN(CCO1)C1CC(OC2CC(O)(Cc3c(O)c4c(c(O)c23)C(=O)c2c(cccc2OC)C4=O)C(=O)CO)OC(C)C1O
C3874	PS	Nonsubstrate	172	O=C(OCC(COC(=O)N)(C)CCC)N
C3875	PS	Nonsubstrate	172	Fe1ccc(cc1)C1(c2ccc(cc2CO1)C#N)CCCN(C)C
C3876	PS	Nonsubstrate	149,170,53,96	OC(=O)C1=C/C(=N)Nc2ccc(cc2)S(=O)(=O)Nc2cccn2)/C=CC1=O
C3877	PS	Nonsubstrate	172	Oc1ccc(cc1)c1[nH]c(e2n(c1)c(=O)c(n2)Cclcccc2cc1)Cc1cccc1
C3878	PS	Nonsubstrate	163	COc1cccc1NS(=O)(=O)c1c(OCCOe2ccc(cc2)C(C)(C)C)ccc(c1)C(C)C
C3879	PS	Nonsubstrate	172	O=C(OOC(=O)OCc1cccc1)OCc1cccc1
C3880	PS	Nonsubstrate	172	OC(=O)c1cccc(c1)NC(=O)[C@@H]1C[C@]@H](CN1)SC1=C(N2C([C@H]1C)[C@H](C2=O)[C@H](O)C)C(=O)O
C3881	PS	Nonsubstrate	172	COc1c(cc2c(c1)sc(e2)C1=NNC(=O)CC1C)OC
C3882	PS	Nonsubstrate	172	[n+]1(ccc(cc1)c1cc[n+](cc1)C)C
C3883	PS	Nonsubstrate	125	Cc1nnc2CN=C(c3cccc3Cl)c3cc(Cl)ccc3n12
C3884	PS	Nonsubstrate	3,171,49,53,68	CC(=CCC/C(=C\CC/C(=C\CSCC(N(C(=O)O)/C)/C)C
C3885	PS	Nonsubstrate	172	Clc1c(cc(c1)OP(=S)(OC)c1cccc1)Cl)Br
C3886	PS	Nonsubstrate	172	O=C(O)CN(CC(=O)O)Cc1c(cc2c(c1)C1(c3ccc(c(c3O2)O)CN(CC(=O)O)CC(=O)O)c2c(C(=O)O1)cccc2)O
C3887	PS	Nonsubstrate	172	O=C1CC2(CC(=O)N1CCCCN1CCN(CC1)c1nccn1)CCCC2
C3888	PS	Nonsubstrate	5,68,69,86,128	CC#CC1(O)CCC2C3CCC4=CC(=O)CCC4=C3C(CC12C)c1ccc(cc1)N(C)C
C3889	PS	Nonsubstrate	172	Fe1ccc2n3cnc(c3CN(C(=O)c2c1)C)C(=O)OCC
C3890	PS	Nonsubstrate	172	c1nc2ccccc2n1Cc1cccc(c1)c1n[nH]nn1
C3891	PS	Nonsubstrate	172	FC(F)(F)c1ccc(cc1)OC(c1cccc1)CCNC
C3892	PS	Nonsubstrate	172	ClC(Cl)(Cl)C(c1ccc(cc1)OC)c1ccc(cc1)OC
C3893	PS	Nonsubstrate	172	O=c1n(c(c1)C)C)c1cccc1
C3894	PS	Nonsubstrate	68,86	ClC(Cl)C(c1ccc(Cl)cc1)c1cccc1Cl
C3895	PS	Nonsubstrate	171,96,41	Cc1cc(C)nc(NS(=O)(=O)c2ccc(NC(=O)COC(=O)c3c4nc5ccccc5c(O)c4ccc3)cc2)n1
C3896	PS	Nonsubstrate	171,96,41	CC(C)C(=O)NC(C)C(=O)N(Cc1cc2c(ccc2)cc1)N=O
C3897	PS	Nonsubstrate	172	O=C(O[C@H]1[C@H](Oe2c(C1)c(cc(c2)O)O)c1cc(c(c1)O)O)O)c1cc(c(c1)O)OC)O
C3898	PS	Nonsubstrate	172	O=C1CC[C@]2([C@@]34CCN([C@]@H]2Cc2c3c(O[C@@H]14)c(cc2)O)CC1CC1)O
C3899	PS	Nonsubstrate	172	O=C(Nc1c(ccc1C)C)CN(CC)CC
C3900	PS	Nonsubstrate	172	O=C(c1[nH]c2ccccc2c1)N[C@]@H]1C(=O)N(c2ccccc2C(=N1)c1cccc1)C
C3901	PS	Nonsubstrate	170,53,96	NC(=N)N/N=C/c1c(Cl)cccc1Cl
C3902	PS	Nonsubstrate	163	COc1cc(cc(OC)c1O)C1C2C(COC2=O)C(OC2OC3COC4(CCN(C)CC4)OC3C(O)C2O)c2cc3c(OCO3)cc12
C3903	PS	Nonsubstrate	172	OC(c1cccc1)(CCN1CCCC1)C1CC2=CC1C2
C3904	PS	Nonsubstrate	172	O=C(OCCN(Cc1cccc1)C)C1=C(NC(=C(C1c1ccc(cc1)[N+](=O)[O-])C(=O)OC)C)C
C3905	PS	Nonsubstrate	172	Fe1cc2c(nc1N1CCNCC1)n(cc(c2=O)C(=O)O)CC
C3906	PS	Nonsubstrate	157,68	Cc1c(c(N)nc(N)n1)c1cc(Cl)c(Cl)cc1
C3907	PS	Nonsubstrate	159,68	CCCCN1C(=O)C(=C/C=C/C=C2/oc3ccccc3n2CCCS(=O)(=O)O)C(=O)N(CCCC)C1=S
C3908	PS	Nonsubstrate	172	Clc1ccc(cc1)N(C(=O)Cc1cccc1)C1CCN(CC1)C(C)C

C3909	PS	Nonsubstrate	172	Cn1c2c(cccc2)c(e1)C=CC(=O)c1c(OC)cc(OC)cc1OC
C3910	PS	Nonsubstrate	149	NC(=O)Cc1c(O)ccc(c1)/N=N\c1ccc(cc1)S(=O)(=O)Nc1ccccn1
C3911	PS	Nonsubstrate	172	O=C1C(C(N(C(C1C)e1cccc1)C)e1cccc1)C
C3912	PS	Nonsubstrate	145	CC(C)OC(=O)C(C)(C)Oe1ccc(cc1)C(=O)c1ccc(Cl)cc1
C3913	PS	Nonsubstrate	172	O=C1c2cc(ccc2C2(O1)c1ccc(cc1Oe1cc(ccc21)O)O)C(=O)O
C3914	PS	Nonsubstrate	172	O=C(/C=C/C/C=C/C=C/C=C/C1=C(CCCC1(C)C)C)\C)\C)O
C3915	PS	Nonsubstrate	155	Ce1c(cccc1)N1CCN(CC(O)COc2ccccc2C(=O)CCc2ccccc2)CC1
C3916	PS	Nonsubstrate	125	COe1cc(C(O)C(C)N)c(OC)cc1
C3917	PS	Nonsubstrate	172	Clc1ccc(cc1)C(=NCCCC(=O)N)c1c(ccc(c1)F)O
C3918	PS	Nonsubstrate	145	CC(NC(C)(C)C)C(=O)c1cccc(Cl)c1
C3919	PS	Nonsubstrate	172	N#Cc1c(=O)nc([nH]c1c1ccc(cc1)C)SC
C3920	PS	Nonsubstrate	162,68	Ne1nc(=O)n(cc1)C1COC(CO)O1
C3921	PS	Nonsubstrate	172	Clc1ccc(cc1)[C@@](OCC[C@H]1CCCN1C)(c1cccc1)C
C3922	PS	Nonsubstrate	172	O=C(OC)C1=C(NC(=C(C1c1c(cccc1)[N+](=O)[O-])C(=O)OC)C)C
C3923	PS	Nonsubstrate	172	N1=C(NCC1)CN1c2cccc2C(=CC(C1C)C)C
C3924	PS	Nonsubstrate	163	COe1cc(cc(OC)c1OC)C1CC(C)(Oe2cc3c(OCO3)cc12)N1CCCC1
C3925	PS	Nonsubstrate	172	O=C(/C=C/C1cc(c(cc1)O)OC)CC(=O)/C=C/c1ccc(c(c1)OC)O
C3926	PS	Nonsubstrate	172	OCC=C(CCC=C(CCC=C(C)C)C)C
C3927	PS	Nonsubstrate	172	O=C(OC)Nc1[nH]c2cc(ccc2n1)SCCC
C3928	PS	Nonsubstrate	172	OC(c1cccc1)(c1cccc1)C1CCNCC1
C3929	PS	Nonsubstrate	172	O=C(c1cc(c(c1)OC)OC)OC)c1c2ccc(cc2[nH]c1)OC
C3930	PS	Nonsubstrate	172	N#CC1=C(N(C(=CC1c1cccc1)c1cccc1)C1C(C(C(O1)CO)O)O)O)S
C3931	PS	Nonsubstrate	172	O=C(Oc1c2ccccc2ccc1)NC
C3932	PS	Nonsubstrate	172	O=C1CC[C@@]2(C=C1)CC[C@H]1[C@@@H]3CC[C@@@H]([C@@@]3(CC[C@H]21)C)O)C
C3933	PS	Nonsubstrate	68	Clc1ccc(Cn2cc(C(=O)C(=O)Nc3ccccc3)c3ccccc23)cc1
C3934	PS	Nonsubstrate	172	n1c2c(c(c3c1CCCC3)N)cccc2
C3935	PS	Nonsubstrate	172	Ce1ccc(/C(=C/CN2CCCC2)/c2nc(/C=C\C(=O)OC(C)C)ccc2)cc1
C3936	PS	Nonsubstrate	172	O=C(O)c1c(=O)c2cc(c(cc2n(c1)CC)N1CCN(CC1)C)F
C3937	PS	Nonsubstrate	63,171,53,96,4	CSc1nc(c2ccc(C)cc2)c(C#N)c(=O)[nH]1
C3938	PS	Nonsubstrate	172	O=c1n(ccc(n1)N)[C@H]1[C@H]([C@@H]([C@H](O1)CO)O)O
C3939	PS	Nonsubstrate	45	NCC(O)COc1cccc1C(=O)CCc1cccc1
C3940	PS	Nonsubstrate	172	O=C1c2c(c3ccc(cc3)OC)c(C#N)c(=S)n(c2CC(C)(C)C1)C1C(C(C(O1)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C
C3941	PS	Nonsubstrate	172	O1Cc2c(C(=CCN(C)C)c3ccccc13)cccc2
C3942	PS	Nonsubstrate	172	O=S(c1ccc2c(c1)nc([nH]2)NC(=O)OC)c1cccc1
C3943	PS	Nonsubstrate	172	[O-][N+](=O)c1ccc2c(c1)C(=NCC(=O)N2)c1cccc1
C3944	PS	Nonsubstrate	172	O=C(/C=C/c1ccc(c(c1)O)O)c1c(cc(c(c1)CC=C(C)C)O)O
C3945	PS	Nonsubstrate	172	O=C(O)c1c(=O)c2cc(c(cc2n(c1)C1CC1)N1CCNCC1)F
C3946	PS	Nonsubstrate	172	O=C1OCC2C(c3c(C(C12)c1cc(c(c1)OC)OC)OC)cc1OCCc1e3)N
C3947	PS	Nonsubstrate	172	O(c1c(ccc1)CC=C)CC(O)CNC(C)C
C3948	PS	Nonsubstrate	70	CCc1c2cc(O)ccc2nc2e1Cn1c2cc2c(COC(=O)C2(O)CC)c1=O
C3949	PS	Nonsubstrate	172	CC(=O)OC1C(C(C(OC1n1c(=S)c(C#N)c(c(c1C)C(=O)C)c1cccc1)COC(=O)C)OC(=O)C)OC(=O)C
C3950	PS	Nonsubstrate	172	Oc1cc2oc(cc(=O)c2c(c1)O)c1cccc1
C3951	PS	Nonsubstrate	172	c1ccc2c(c1)N(c1c(CC2)cccc1)CCNC
C3952	PS	Nonsubstrate	172	S=c1c(cc2c(n1C1C(C(O)C(C(O1)CO)O)O)CCC2)C#N
C3953	PS	Nonsubstrate	172	CCC1(c2cc3c4nc5ccccc5cc4Cn3c(=O)c2COC1=O)O
C3954	PS	Nonsubstrate	172	CC(=O)OC1C(C(C(OC1n1c(=S)c(cc2c1CCCCC2)C#N)COC(=O)C)OC(=O)C)OC(=O)C

C3955	PS	Substrate	55	CC(N)C(=O)NC1C2C(O)C(O)CC(=O)C2=C(O)OC1(C)C(C)C1
C3956	PS	Substrate	172	C1=CCCN(C)C
C3957	PS	Substrate	172	FC(F)(F)COc1ccnc(c1C)CS(=O)c1[nH]e2ccccc2n1
C3958	PS	Substrate	63,69	COe1ccc(cc1)C1C(=C(S)N(C2OC(COC(=O)C)C(OC(=O)C)C(OC(=O)C)C2OC(=O)C)C(=C1C(=O)C)c1ccccc1)C#N
C3959	PS	Substrate	68,88	CC1(C)SSC(C)(C)C(NC(=O)C(N)Ce2ccc(O)cc2)C(=O)NCC(=O)NC(Cc2ccccc2)C(=O)NC1C(=O)O
C3960	PS	Substrate	172	O=C(OCOC(=O)C)CN(c1ccc(cc1)OCCOc1c(N(CC(=O)OCOC(=O)C)CC(=O)OCOC(=O)C)ccc(c2c3c(cc4c2cc(Cl)c(=O)c4)cc(O)c(Cl)c3)c1)C)CC(=O)OCOC(=O)C
C3961	PS	Substrate	5,52,77,104,1	NS(=O)(=O)OCC12OC(OC1C1OC(OC1CO2)(C)C)(C)C
C3962	PS	Substrate	172	O=C(OCCNC(=O)c1ccc(cc1)N=[N+]=[N-])C1=C(NC(=C(C1c1c(cccc1)C(F)(F)F)C(=O)OCC)C)C
C3963	PS	Substrate	172	N(=Cc1c2ccccc2c(c2ccccc12)C=NCC1=NCCN1)NC1=NCCN1
C3964	PS	Substrate	145	O/C(=C/1\C(=O)C(N(C)C)C2C(O)C3C(=C(O)c4c(cccc4O)C3C)C(=O)C2(O)C1=O)/N
C3965	PS	Substrate	41	OC1CC2C(NC(=O)c3c(O)c4c(OCO4)cc23)C(O)C1O
C3966	PS	Substrate	59	CC(C)CC1N2C(=O)C(NC(=O)C3CC4C(Ce5c[nH]e6cccc4c56)N(C)C3)(OC2(O)C2CCCN2C1=O)C(C)C
C3967	PS	Substrate	39	CC1=C(C=C)/C=C\c2c(C)c(CCC(=O)O)c(C[C@H]3N=C(/C=C\4/NC(=O)C(=C4C)C=C)C(=C3CCC(=O)O)C)[nH]2)/NC1=O
C3968	PS	Substrate	172	O=C(Oc1cc(ccc1)[N+](C)(C)N(C)C
C3969	PS	Substrate	172	n1c(ncc(c1N)Cc1cc(c(c1)OC)OC)OC)N
C3970	PS	Substrate	63	N1c2ccccc2P2(=c3ccccc3=Ne3ccccc23)c2ccccc12
C3971	PS	Substrate	145	N(/C(=C/[N+](=O)[O-])/NCCSCc1csc(n1)CN(C)C)C
C3972	PS	Substrate	172	CS(=O)(=O)N1CCN(CC1)[C@H]1CN(C1)CC[C@]1(CN(C(=O)CC1)CC1CC1)c1ccc(c(cc1)Cl)Cl
C3973	PS	Substrate	68	COe1ccc(CC2N(C)C(=O)C(C)NC(=O)C(C)NC(=O)C3Cc4cc(Oc5ccc(cc5)C(O)C(N(C)C(=O)C(C)NC2=O)C(=O)N3C)c(O)cc4)cc1
C3974	PS	Substrate	172	O=C(O[C@@H]1COCC1)N[C@@H](Cc1ccccc1)[C@H](O)CN(CC(C)C)S(=O)(=O)c1ccc(cc1)N
C3975	PS	Substrate	172	ClCc1ccc(cc1)Cn1c(=CC=CC2=N(c3c(O2)cccc3)C)n(c2cc(c(cc12)Cl)Cl)Cc1ccc(cc1)CC1
C3976	PS	Substrate	172	O[C@@H]1[C@@H]2Oc3c4[C@@@]52CCN([C@@H]([C@@H]5C=C1)Cc4ccc3O)C
C3977	PS	Substrate	172	O=C1c2c3c4n(C5O[C@@](n6c4e(c2CN1)c1ccccc61)[C@@H]([C@@H](C5)NC)OC)C)C1ccccc31
C3978	PS	Substrate	50	OC1CC(O)CC(OC(=O)/C=C/c2cc(O)c(O)cc2)C1O)C(=O)O
C3979	PS	Substrate	172	O=C1N[C@H]2CS[C@H]([C@H]2N1)CCCCC(=O)O
C3980	PS	Substrate	172	C[N+](=c1ccc2c(c3ccc(s3)C(=S)N3CCCC3)c3cc4CCCN5CCCc(c3sc2e1)c45)C
C3981	PS	Substrate	172	S1C2N(C(=C(C1)CSc1n(nnn1)C)C(=O)O)C(=O)C2NC(=O)C(NC(=O)N1C(=O)C(=O)N(CC1)CC)c1ccc(cc1)O
C3982	PS	Substrate	172	O=S(=O)(N(c1nc(c(n1)C(C)C)/C=C/[C@@H](O)C[C@@H](O)CC(=O)O)c1ccc(cc1)F)C)C
C3983	PS	Substrate	34	ccc(C)C1N(C)C(=O)C(C)CC(N)C(=O)C(C)C(=O)O)C(O)C(N(C)C(=O)C(NC(=O)C(C)C)N(C)C(=O)C2CCCN2C(=O)C(C)OC(=O)C(Cc2ccc(OC)cc2)NC(=O)C(C)C)N(C)C(=O)CNC1=O)C(C)C
C3984	PS	Substrate	172	O(c1ccc(cc1)C(C)(C)CC(C)(C)C)CCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO
C3985	PS	Substrate	172	N#Cc1ccc(cc1)Cn1ene1CN1CCN(C(=O)C1)c1cc(ccc1)Cl
C3986	PS	Substrate	171,52,53,69,	CCC(=O)C(C)C(C)N(C)C)(c1ccccc1)c1ccccc1
C3987	PS	Substrate	172	S1C2N(C(=C(C1)CSc1nnc(s1)C)C(=O)O)C(=O)C2NC(=O)Cn1cnnn1
C3988	PS	Substrate	172	Ne1c2c(c(c(cc2nc(c1)N1CCCN(CC1)C(=O)N1CCOCC1)OC)OC)c1ccc(cc1)F
C3989	PS	Substrate	172	Fe1ccc(cc1)C(=O)NCCN1CCN(CC1)c1c2OC[C@@H](Oe2ccc1)CO
C3990	PS	Substrate	68,101	CC(C)CC1NC(=O)C(C)N(C)C(=O)CNC(=O)/C(=C/c2ccccc2)/N(C)C1=O
C3991	PS	Substrate	172	CCC(=C(CC)c1ccc(cc1)O)c1ccc(cc1)O
C3992	PS	Substrate	55	COe1cccc2c1C(=O)c1c(O)c3c(CC(O)(CC3OC3CC(N)C(O)C(C)O3)/C(=N/NC(=O)c3ccccc3)/C)c(O)c1C2=O
C3993	PS	Substrate	145,52,69	N1CCC(c2ccc(F)cc2)C(COe2cc3c(OCO3)cc2)C1
C3994	PS	Substrate	172	C1N(CCOCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CCc1ccccc1)/C=C/S(=O)(=O)c1ccccc1
C3995	PS	Substrate	145,68,81,39	O/C(=C/1\C(=O)C(N(C)C)C2CC3C(=C(O)c4c(cccc4O)C3(O)C)C(=O)C2(O)C1=O)/N
C3996	PS	Substrate	69,128	CC(C)C1NC(=O)C(NC(=O)c2c3Nc4e(Oc3c(C)cc2)c(O)c2oc(=O)c(nc2c4C(=O)NC2(C)OC(=O)C(C)C)N(C)C(=O)C(N(C)C(=O)C3CCN3C(=O)C(NC2=O)C(C)C)c2ccccc2)C(C)OC(=O)C(C)C)N(C)C(=O)C2CCCN2C1=O
C3997	PS	Substrate	172	NC(CC=C)c1c(cccc1)c1c2c(on1)cccc2
C3998	PS	Substrate	172	OC1=C(N(S(=O)(=O)c2ccsc12)C)C(=O)Nc1ncccc1
C3999	PS	Substrate	172	O=C(O)[C@H]1C(SC2[C@@H](C(=O)N12)NC(=O)[C@@H](c1ccc(cc1)O)N)(C)C
C4000	PS	Substrate	135,52	CCCCCCCC/C=C/CCCCCCCC(=O)OCCOCC(OCCO)C1OCC(OCCO)C1OCCO









C4139	PI	Noninhibitor	173	c12c(oc(c(c1=O)OC)c1ccc(c(c1)OC)OC)cc(cc2O)OC
C4140	PI	Noninhibitor	173	N1([C@@H](C[C@H]2[C@H](C1)CCCC2)C(=O)NC(C)(C)C)[C@@H]([C@@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)c1nc2c(cc1)cccc2)CC(=O)N)O
C4141	PI	Inhibitor	173	c12N3CCCC1cc1c(c2CCC3)[se]c2c(c1c1sc(cc1)C(=S)N1CCCCC1)ccc(=[N+](C)C)c2
C4142	PI	Noninhibitor	173	COc1cc2oc(cc(=O)c2c(OC)c1C)c1ccc1
C4143	PI	Noninhibitor	173	c1(c(c(c2c(c1)OC(c1ccccc1)CC2=O)O)C)OC
C4144	PI	Noninhibitor	173	COc1ccc(cc1)c1cc(=O)c2c(OC)c(OC)c(OC)c(OC)c2o1
C4145	PI	Noninhibitor	173	[C@@]12([C@@H]([C@@]3([C@@H]([C@@H]2O)C3)OC(=O)C)[C@@H]([C@@]2(C(=C([C@@H](C2)OC(=O)[C@@H]([C@@H](NC(=O)c2ccccc2)c2ccccc2)O)[C@@H](C1=O)OC(=O)C(C)O)OC(=O)c1ccccc1)C
C4146	PI	Noninhibitor	173	c1(ccccc1)[P+](c1ccccc1)(c1ccccc1)c1ccc1
C4147	PI	Noninhibitor	173	O1[C@@]2(C[C@@H]([C@@H]O[C@@H]3O[C@@H]([C@@H]N(C)C)[C@@H]3OC(=O)C)[C@@H]([C@@H]O[C@@H]3O[C@@H]([C@@H]OC(=O)C)[C@@H]OC3)C)[C@@H](C(=O)O)[C@@H]([C@@H]OC(=O)C)[C@@H](C2=O)C)C)C)C)C1
C4148	PI	Noninhibitor	173	C(=O)(c1c(n(nc1C)C)OCC(CN(C(C)C)C(C)O)c1ccccc1
C4149	PI	Noninhibitor	173	C(=O)(c1c(n(nc1C)c1ccccc1)OCC(CN(C(C)C)C(C)O)c1ccccc1
C4150	PI	Inhibitor	173	c12C=C3C4C(c1sc1c(c2c2ccccc2)ccc(=[N+](C)C)c1)CCCN4CCCC3
C4151	PI	Inhibitor	173	c12C=C3C4C(c1[se]c1c(c2c2ccccc2)ccc(=[N+](C)C)c1)CCCN4CCCC3
C4152	PI	Inhibitor	173	c1cc2c(c3c([se]c2cc1N(C)C)ccc(=[N+](C)C)cc3)c1sc(cc1)C(=S)N1CCCCC1
C4153	PI	Inhibitor	173	n1ccc(cc1)COc1c(cccc1)CCc1cccc(c1)OC
C4154	PI	Inhibitor	173	n1ccc(cc1)COc1c(cccc1)CCc1cccc1
C4155	PI	Inhibitor	173	COc1c2c(=O)cc(oc2cc(c1)OC)c1cc(c(c1)OC)OC)OC
C4156	PI	Inhibitor	173	N1(Cc2c(CC1)cc(c(c2)OC)OC)CCCC1=CCC(c2c1ccccc2)OC
C4157	PI	Inhibitor	173	c1cc(c2c(c1)/C(=C/CCN1Cc3c(CC1)cc(c(c3)OC)OC)/CCC2)OC
C4158	PI	Inhibitor	173	c1(OC)ccc2c(c1)/C(=C/CCN1Cc3c(CC1)cc(c(c3)OC)OC)/CCC2
C4159	PI	Inhibitor	173	[C@@H]1(CN(CC1)Cc1ccccc1)OC(=O)C1=C(NC(=C([C@@H]1c1cc([N+](=O)[O-])ccc1)C(=O)OC)C)C
C4160	PI	Inhibitor	173	[C@@H]1(C(=C(NC(=C1C(=O)OC)C)C(=O)OC1CN(Cc2ccccc2)CCC1)c1cc(ccc1)[N+](=O)[O-]
C4161	PI	Inhibitor	173	c12ccc(N(C)C)cc1sc1c(c2c2ccccc2)ccc(=[N+](C)C)c1
C4162	PI	Inhibitor	173	[C@@H]1(C[C@@H](OC)C2=C([C@@]3([C@@]([C@@H](C2=O)OC)(O)c2c3c(c(c3c2[C@@H](C[C@H](O3)c2ccccc2)O)OC)OC)O1)c1ccccc1
C4163	PI	Inhibitor	173	c12n(c3c(nc1cc/c(=N/C(C)C)/e2)Nc1ccc(Cl)cc1)ccccc3)c1ccc(cc1)Cl
C4164	PI	Inhibitor	173	O1CCN(CCCNC(=O)c2c(OCC)cccc2)CC1
C4165	PI	Inhibitor	173	C1(C(=O)N(c2c(S[C@@H]1c1ccc(cc1)OC)cccc2)CCN(C)C)OC(=O)C
C4166	PI	Inhibitor	173	C1(C(=C(NC(=C1C(=O)OCCN(c1ccccc1)Cc1ccccc1)C)C)P1(=O)OCC(CO1)(C)C)c1cc(ccc1)[N+](=O)[O-]
C4167	PI	Inhibitor	173	c12c(c(ccc1)OC)[nH]c1c(c2=O)cccc1C(=O)Nc1ccc(cc1)CCN1CCc2c(C1)cc(c(c2)OC)OC
C4168	PI	Inhibitor	173	c1(C(C#N)(C(C)C)CCN(CCc2cc(c(cc2)OC)OC)C)cc(c(c(c1)OC)OC)OC
C4169	PI	Inhibitor	173	n1(c(=O)n(nc1)C(CC)C)c1ccc(N2CCN(c3ccc(OC[C@@H]4O[C@@](c5c(cc(cc5)Cl)Cl)(Cn5nnc5)OC4)cc3)CC2)cc1
C4170	PI	Inhibitor	173	c12ccc(N(C)C)cc1[se]c1c(c2c2ccccc2)ccc(=[N+](C)C)c1
C4171	PI	Inhibitor	173	C1=C([C@@H]([C@@H](C=C=C2[C@@]3([C@@H](C(=O)O)[C@@H]4[C@@H](C1)O[C@@]1(C4)CC[C@@H]([C@@H]O1)[C@@H](CC)C)C=C([C@@H]([C@@H]3OC2)O)O)C)[C@@H]O1C)[C@@H]([C@@H](C1)OC)O[C@@H]([C@@H]([C@@H](O1)O)O)C)C
C4172	PI	Inhibitor	173	C1([C@H]2c3c(cccc3)[C@@H](c3c([C@@H]12)cccc3)N1CCN(CC1)C[C@H](COc1c2c(nc2)ccc1)O)(F)F
C4173	PI	Inhibitor	173	C1(C(=C(NC(=C1C(=O)OC)C)C(=O)OCCN1CCN(CC1)C(c1ccccc1)c1ccccc1)c1cc(ccc1)[N+](=O)[O-]
C4174	PI	Inhibitor	173	N(c1c(cccc1)CCc1cccc(c1)OC)Cc1cc(ccc1)OC
C4175	PI	Inhibitor	173	N(c1c(cccc1)CCc1cccc(c1)OC)Cc1c(c(ccc1)OC)OC
C4176	PI	Inhibitor	173	N(c1c(cccc1)CCc1cccc(c1)OC)Cc1cc(c(cc1)OC)OC
C4177	PI	Inhibitor	173	N(c1c(cccc1)CCc1cccc(c1)OC)Cc1cc(cc(c1)OC)OC
C4178	PI	Inhibitor	173	c1(ccccc1CCc1cccc1)OCc1c(c(ccc1)OC)OC
C4179	PI	Inhibitor	173	C1(=O)C2=CC[C@H](c3ccccc3)O[C@@]32[C@](C(=C1OC)OC)(c1c(c2c(c(c1OC)OC)O[C@H](C[C@@H]2O)c1ccccc1)O3)OC
C4180	PI	Inhibitor	173	C1(=O)C2=CC[C@H](c3ccccc3)O[C@@]32[C@](C(=C1OC)OC)(c1c(c2c(c(c1OC)OC)O[C@H](C[C@@H]2OC)c1ccccc1)O3)OC
C4181	PI	Inhibitor	173	C1(=C(NC(=C([C@@H]1c1ccccc1)[N+](=O)[O-])C(=O)OC)C)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1
C4182	PI	Inhibitor	173	C1(=C(NC(=C(C1c1cc([N+](=O)[O-])ccc1)C(=O)OC)C#N)C)C(=O)OC(C)C
C4183	PI	Inhibitor	173	C1(=C(NC(=C(C1c1c([N+](=O)[O-])ccc1)C(=O)OC)C)C(=O)OCC(C)C
C4184	PI	Inhibitor	173	O(c1cc(C(C)C)C)CCCNCc2cc(OC)c(OC)cc2)C#N)ccc1OC)C



C4231	PI	Noninhibitor	175	<chem>c12c(cccc1)nc(cc2C(=O)NCCCNCNC(=O)c1cccc(c1)OCc1cccc1)OCc1cccc1)c1cccc1</chem>
C4232	PI	Noninhibitor	175	<chem>c1cc(c(cc1CN1CCCN(Cc2ccc(c(e2)OC)OC)C1c1ccc(cc1)N(CCCI)CC1)OC)OC</chem>
C4233	PI	Noninhibitor	175	<chem>c1cc(c(cc1CN1CCCN(Cc2ccc(c(e2)OC)OC)C1c1ccc(cc1)N(CCCI)CC1)OC)OC</chem>
C4234	PI	Inhibitor	175	<chem>c1ccc(cc1)CN(c1cccc1)C[C@H](COCC(C)C)N1CCCC1</chem>
C4235	PI	Noninhibitor	175	<chem>c1cc(c(cc1CN1CCCN(Cc2ccc(c(e2)OC)OC)C1c1ccc(cc1)N(CCCI)CC1)OC)OC</chem>
C4236	PI	Noninhibitor	175	<chem>c12c(cccc2)c(ccc1)CN(C/C=C/c1cccc1)C</chem>
C4237	PI	Noninhibitor	175	<chem>c1cc(c2c3c1C[C@@H]1[C@@]4(CC[C@@H]([C@@H]([C@]34CCN1CC1CCC1)O2)O)O)O</chem>
C4238	PI	Noninhibitor	175	<chem>c1cc(c2c3c1C[C@@H]1[C@@]4(CCC(=O)[C@@H]([C@]34CCN1CC=C)O2)O)O</chem>
C4239	PI	Noninhibitor	175	<chem>c1cc(c2c3c1C[C@@H]1[C@@]4(CCC(=O)[C@@H]([C@]34CCN1CC1CC1)O2)O)O</chem>
C4240	PI	Noninhibitor	175	<chem>c12c(cccc1)[nH]c1c2C[C@@]2([C@@]34c5c(ccc(c5O[C@@H]14)O)C[C@@H]2N(CC3)CC1CC1)O</chem>
C4241	PI	Noninhibitor	175	<chem>c1ccc(cc1)[C@@H]1c2cccc(c2)CN(C1)C)N</chem>
C4242	PI	Noninhibitor	175	<chem>c1ccc(cc1)C1=NCC(=O)Nc2ccc(cc12)Cl</chem>
C4243	PI	Inhibitor	175	<chem>c1cc(cc1)OC[C@@H](CNCCc1ccc(c(c1)OC)OC)O)C</chem>
C4244	PI	Noninhibitor	175	<chem>c1ccc2c(c1)/C(=C/[C@@H]1C3CCN(CC3)C1)/c1ccc(cc1S2)Cl</chem>
C4245	PI	Noninhibitor	175	<chem>c12c(ccc2)c(c(c1)OC)OC[C@@H](C)NCCC(=O)c1cccc(c1)OC)O)C</chem>
C4246	PI	Noninhibitor	175	<chem>c1cc(cc1)/C(=C(/C)N1ccnc1)/OCCOc1ccc(cc1)Cl)Cl)Cl</chem>
C4247	PI	Noninhibitor	175	<chem>c1c2c(cc(c1)OCCN(CC)CC)OCCN(CC)CC)oc(=O)cc2C</chem>
C4248	PI	Noninhibitor	175	<chem>c1cc(cc1)/C(=N/OCc1ccc(cc1)Cl)Cl)/Cn1ccnc1)Cl)Cl</chem>
C4249	PI	Noninhibitor	175	<chem>c1c2c(cc3c1OCO3)n(cc(c2=O)C(=O)O)CC</chem>
C4250	PI	Noninhibitor	175	<chem>c1ccc(c(c1)OCC=C)OC[C@@H](CNC(C)C)O</chem>
C4251	PI	Noninhibitor	175	<chem>c1ccc(cc1)[C@H]([C@H](C)NCCC(=O)c1cccc(c1)OC)O</chem>
C4252	PI	Noninhibitor	175	<chem>c1ccc(cc1)OCCN1CCC(CC1)n1c2cccc2[nH]c1=O</chem>
C4253	PI	Noninhibitor	175	<chem>C(=O)(C[C@@H](C[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCO</chem>
C4254	PI	Noninhibitor	175	<chem>c12c(cc(c(c1)OC)OC)c(Cc1ccc(c(c1)OC)OC)ncc2</chem>
C4255	PI	Noninhibitor	175	<chem>C#CCOC[C@H]1CO[C@@](c2ccc(cc2)Cl)(Cn2ccnc2)O1</chem>
C4256	PI	Noninhibitor	175	<chem>c1c2c(cc(c1F)N1CCN(CC1)C)n(cc(c2=O)C(=O)O)CC</chem>
C4257	PI	Noninhibitor	175	<chem>c1(c(c(c(c1)Cl)Cl)Cl)Cl)O</chem>
C4258	PI	Noninhibitor	175	<chem>C1CCC(CC1)C(C[C@H]1CCCCN1)C1CCCC1</chem>
C4259	PI	Noninhibitor	175	<chem>c1ccc(cc1)CCN</chem>
C4260	PI	Noninhibitor	175	<chem>c1ccc2c(c1)N(c1cccc1O2)C(=O)CC1</chem>
C4261	PI	Noninhibitor	175	<chem>c1ccc(cc1)Cc1cccc1OCCN(C)C</chem>
C4262	PI	Noninhibitor	175	<chem>c1cc(ccc1N1CCN(CCCN(C)C)CC1)NC(=O)C</chem>
C4263	PI	Inhibitor	175	<chem>c12c3cccc1C1=C[C@@H](C(=O)N[C@@]4(C(=O)N5[C@H](C(=O)N6[C@@H](CCC6)[C@]5(O)O4)CC(C)C(C)C)CN([C@@H]1Cc2c([nH]3)Br)C</chem>
C4264	PI	Noninhibitor	175	<chem>c1ccc(cc1)C1(c2cccc2)C(=O)O[C@H](CCN2CCCC2)O1</chem>
C4265	PI	Noninhibitor	175	<chem>c1cc(c(cc1[C@H](C(=O)O)C)Cl)N1CC=CC1</chem>
C4266	PI	Noninhibitor	175	<chem>c1ccc(cc1)C1(c2cccc2)CCC(CC1)NC(C)C</chem>
C4267	PI	Noninhibitor	175	<chem>c1ccc(cc1)C(c1cccc1)OCCN([C@H](C)COc1cccc1)C</chem>
C4268	PI	Noninhibitor	175	<chem>c12c(c(cc2)OC)N[C@@H](C)CCN)nccc1</chem>
C4269	PI	Noninhibitor	175	<chem>c1ccc(c(c1)C)OC[C@H](CNCCn1cc(c(=O)[nH]c1=O)C)O</chem>
C4270	PI	Noninhibitor	175	<chem>c1cc(c(c(c1)Nc1cc(nc1)SCC(=O)O)Cl)C)C</chem>
C4271	PI	Noninhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1cccc1OC[C@H](C[N+](CC)(CC)C)O</chem>
C4272	PI	Noninhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1cccc1OC[C@H](C[N+](CCC)(C)C)O</chem>
C4273	PI	Inhibitor	175	<chem>c1ccc(cc1)/C(=N\CC(C)C)/N1CCN(CCCCC)CC1</chem>
C4274	PI	Noninhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1cccc1OC[C@@H](C[N+](C(C)C)(C(C)C)C)O</chem>
C4275	PI	Noninhibitor	175	<chem>c1ccc(c(c1)C(=O)C)OC[C@H](CN1CCCC1)O</chem>
C4276	PI	Noninhibitor	175	<chem>c1cc(ccc1C(=O)C)OC[C@H](CN1CCCC1)O</chem>

C4277	PI	Noninhibitor	175	c1ccc(c(c1)C(=O)CC)OC[C@@H](CN1CCOCC1)O
C4278	PI	Noninhibitor	175	c1cc(cc(c1[C@@]1(Cn2cncn2)OC[C@@H](CCC)O1)C1)C1
C4279	PI	Noninhibitor	175	c1ccc(c(c1)OC(=O)NC)OC(C)C
C4280	PI	Noninhibitor	175	c1cc2c(cc1C[C@H](C)NC[C@H](c1ccc(c(c1)O)O)O)OCO2
C4281	PI	Noninhibitor	175	c12c(ncnc1N(C)C)n(en2)[C@H]1[C@@H]([C@@H]([C@@H](CO)O1)NC(=O)[C@H](Cc1ccc(cc1)OC)N)O
C4282	PI	Noninhibitor	175	c1ccnc(c1)N(Cc1ccc(cc1)OC)CCN(C)C
C4283	PI	Inhibitor	175	c1ccc(cc1)[C@H](c1ccc(cc1)Cl)N1CCN(Cc2ccc(cc2)C(C)(C)C)CC1
C4284	PI	Noninhibitor	175	c12c(cc(c(c1)OC)OC)nc(nc2N)N1CCN(CC=C)CC1
C4285	PI	Noninhibitor	175	c12c([C@H](N[C@@H](N(CCO)CCO)O2)N(CC)CC)nc(nc1N(CC)CC)N(CCO)CCO
C4286	PI	Noninhibitor	175	c12c(c(nc(n2)N(CCO)CCO)N2CCOCC2)nc(nc1N1CCOCC1)N(CCO)CCO
C4287	PI	Noninhibitor	175	c12c(c(nen2)N2CCOCC2)ncnc1N1CCOCC1
C4288	PI	Noninhibitor	175	c1ccc(cc1)[C@@H]1C(Nc2c(c(nc(n2)N2CCOCC2)N(CCO)CCO)O1)N1CCOCC1
C4289	PI	Noninhibitor	175	c12c(nc(en2)N2CCOCC2)nc(nc1N1CCOCC1)N1CCOCC1
C4290	PI	Noninhibitor	175	c12c(nc(c(n2)Cl)N(C)C)nc(nc1N(C)C)N1CCNCC1
C4291	PI	Noninhibitor	175	c12c(nc(c(n2)Cl)N2CCOCC2)nc(nc1N1CCOCC1)N1CCNCC1
C4292	PI	Noninhibitor	175	c1cc(cc2c1C[C@@H]1[C@H]3CCCC[C@]23CCN1C)OC
C4293	PI	Noninhibitor	175	c12c(cc(c(c1)OC)[nH]c1c2CCN2[C@@H]1C[C@@H]1[C@H](C(=O)O)C([C@@H](C[C@@H]1C2)O)OC
C4294	PI	Inhibitor	175	c12c(cccc2)c(ccc1)C(=O)N(CCCC)CCN(CC)CC
C4295	PI	Noninhibitor	175	c1ccc(cc1)c1cc(=O)e2c(cc(c2o1)OC1[C@@H](C([C@@H](C(CO)O1)O)O)O)O
C4296	PI	Noninhibitor	175	c12c3c4c(c(c1O)C)O[C@@](C4=O)(C)O/C=C/[C@@H]([C@@H](C)[C@H](C)[C@H](C)[C@H](C)[C@H](C)[C@H](C)/C=C/C(C(=O)Nc(cc3OCC(=O)O)e2O)/C)O)OC(=O)C)OC
C4297	PI	Noninhibitor	175	c12c3c4c(c(c1O)C)O[C@@](C4=O)(C)O/C=C/[C@@H]([C@@H](C)[C@H](C)[C@H](C)[C@H](C)[C@H](C)/C=C/C(C(=O)Nc(cc3O)e2O)/C)O)OC(=O)C)OC
C4298	PI	Noninhibitor	175	c1cc(cc(c1)OC)[C@@H](c1ccc(cc1)C(=O)N(CC)CC)N1[C@@H](C)CN([C@H](C)C1)CCC
C4299	PI	Noninhibitor	175	c1ccc(cc1)[C@@H](C(=O)OCCN1CCN(CCC(=O)e2ccc(cc2)OC)CC1)CC
C4300	PI	Noninhibitor	175	c1ccc(cc1)CC(=O)OCCN1CCN(CC1)CCOC(=O)Cc1ccccc1
C4301	PI	Noninhibitor	175	c1ccc(cc1)CCC(=O)OCCN1CCN(CC1)CCOC(=O)CCc1ccccc1
C4302	PI	Noninhibitor	175	c1ccc(cc1)[C@H](C(=O)OCCN(CCCN(CCOCC(=O)[C@H](c1ccccc1)CC)C)C)CC
C4303	PI	Noninhibitor	175	c1ccc(cc1)[C@@H](C(=O)OCCN1CCN(CCCOC(=O)[C@@H](c2ccccc2)CC)CC1)CC
C4304	PI	Noninhibitor	175	c1ccc(cc1)NC(=O)c1ccccc1OCCN(CC)CC
C4305	PI	Inhibitor	175	c1cnc(nc1)N1CCN(CCCCN2C(=O)CC3(CC2=O)CCCC3)CC1
C4306	PI	Noninhibitor	175	c1ccc(cc1)[C@H](C(=O)OC1C[C@@H]2[C@@H]3[C@H]([C@H](C1)N2C)O3)CO
C4307	PI	Noninhibitor	175	C#CCN([C@H](C)Cc1ccccc1)C
C4308	PI	Noninhibitor	175	C1=C[C@H](C)C(CC[C@H](C[C@H](CC(=O)O)O)[C@@H]2C1=CC(C)CC2OC(=O)C(C)(C)CC
C4309	PI	Noninhibitor	175	c1c(c(cc(c1F)F)F)[C@H](CC(=O)N1Cc2n(c(C(F)(F)F)nn2)CC1)N
C4310	PI	Noninhibitor	175	c1ccc(cc1)C[C@@H](c1ccccc1)C(=O)OCCN(CC)CC
C4311	PI	Noninhibitor	175	C1=C([C@H]2CC[C@@]3([C@H]4CC[C@]5(C[C@H](CC[C@@]5(C=O)[C@H]4CC[C@]23C)O)O)COC1=O
C4312	PI	Noninhibitor	175	c1cc(ccc1CS[C@@H](c1ccc(cc1)Cl)Cl)Cn1ccnc1Cl
C4313	PI	Noninhibitor	175	c1cc(cc(c1)Cl)Nc1c2c(c(C)nc2nc[nH]1)C
C4314	PI	Noninhibitor	175	c1cc(ccc1NC(=O)NC1CCCC1)OC[C@@H](CNC(C)(C)C)O
C4315	PI	Noninhibitor	175	C(#CC(C)(C)C)/C=C/CN(Cc1c2c(ccc1)cccc2)C
C4316	PI	Inhibitor	175	C1=C2CC[C@H]3[C@@H]4C[C@H](C)[C@H](C(=O)C)[C@]4(C)CC[C@H]3[C@]2(C)CCC1=O
C4317	PI	Noninhibitor	175	c1c2c(cc(c1OC)OC)[C@H]1CC(=O)[C@@H](CC(C)C)CN1CC2
C4318	PI	Noninhibitor	175	c1cc(ccc1CN(c1ncccn1)CCN(C)C)OC
C4319	PI	Noninhibitor	175	c1c2c(ccc1Cl)sc(=O)n2CC(=O)N1CCN(CC1)CCO
C4320	PI	Noninhibitor	175	c1cc(cc2c1c1ccc(cc1C2=O)OCCN(CC)CC)OCCN(CC)CC
C4321	PI	Noninhibitor	175	c1cc(cc(c1[C@@H](Cn1ccnc1)OCc1ccsc1Cl)Cl)Cl
C4322	PI	Noninhibitor	175	c1ccc(c(c1)C)OC[C@@H](CNCCO)c1ccc(cc1)C(=O)N)O

C4323	PI	Noninhibitor	175	c1c2e(cc(c1O)O)[C@@H](Cc1cc(c(c(c1)OC)OC)OC)NCCC2
C4324	PI	Noninhibitor	175	c1ccc(c(c1)C1=NCc2n(c3ccc(cc13)Cl)c(C)nn2)Cl
C4325	PI	Noninhibitor	175	C(=O)N[C@@H](C(Cl)(Cl)Cl)N1CCN(CC1)[C@H](C(Cl)(Cl)Cl)NC=O
C4326	PI	Noninhibitor	175	c12e(c(c(c(c1)OC)OC)OC)ne(nc2N)N1CCN(C(=O)OCC(C)(C)O)CC1
C4327	PI	Noninhibitor	175	c1c(cc(c(c1OC)OC)OC)C(=O)N1CCOCC1
C4328	PI	Noninhibitor	175	c1cc(c(c(c1C(=O)OCC[N+](CC)(CC)CC)OC)OC)OC
C4329	PI	Noninhibitor	175	c1cc(cc(c1[C@@@]1(Cn2ccnc2)OC[C@H](CS2ccc(cc2)NC(=O)OCC)O1)Cl)Cl
C4330	PI	Noninhibitor	175	c1ccc(cc1)CC(=O)N([C@H]1CC[C@]2(CCCO2)C[C@@H]1N1CCCC1)C
C4331	PI	Noninhibitor	175	c1ccc(cc1)C1=C(c2ccc(cc2)OCCN(CC)CC)c2ccc(cc2C1)OC
C4332	PI	Noninhibitor	175	c1ccc(cc1)C(=C1CCN(CC1)CCOCCOCC(=O)O)c1ccccc1
C4333	PI	Noninhibitor	175	c1ccc(c(c1)N1CCN(CCCNc2cc(=O)n(c(=O)n2C)C)CC1)OC
C4334	PI	Noninhibitor	175	c1ccc2cc1[C@H](C(=O)N)C@@H(C(C(=O)N)C@@H(C3ccc(cc23)O)C(=O)O)[C@H](c2ccc(cc12)C)O)c2ccc(cc2)C[C@@H](C@@H)(C@@H)(C@@H)C(=O)N[C@@H](C(=O)N)C(=O)O
C4335	PI	Noninhibitor	175	c1c(cc(cc1Cl)Cl)N1C(=O)[C@](C=C)(C)OC1=O
C4336	PI	Noninhibitor	175	c12c(cccc1)[nH]c1e2CCN2C[C@H](C[C@]1(c1cc3c(cc1OC)N(C=O)[C@@H]1[C@@@]43CCN3[C@H]4[C@](C=CC3)(CC)[C@H]([C@@]1(C(=O)OC)OC(=O)C)C(=O)OC)C[C@@](CC)(C2)O
C4337	PI	Noninhibitor	175	C(=C\C=C\COC(=O)CCCCCCCCCCCCC)C)/C=C/C=C/C1=C(C)CCCC1(C)C)\C
C4338	PI	Noninhibitor	175	c12c(ccc(c2)S(=O)(=O)NCCCCN)c(ccc1)Cl
C4339	PI	Noninhibitor	175	c12c(cccc2S(=O)(=O)NCCCCCN)c(ccc1)Cl
C4340	PI	Noninhibitor	175	c1ccc(cc1)c1ccc(cc1)CC[C@H](C)CC(=O)OCCN(C)C
C4341	PI	Noninhibitor	175	c1ccc(cc1)[C@@H](c1c(c2ccccc2oc1=O)O)CC(=O)C
C4342	PI	Noninhibitor	175	c1cc(cnc1)/C(=C\CN(C)C)/c1ccc(cc1)Br
C4343	PI	Noninhibitor	175	c12c(ccc(c1)C[C@H]1COC(=O)N1)[nH]cc2CCN(C)C
C4344	PI	Noninhibitor	175	c1ccc(c(c1)N1CCN(Cc2c(c3ccc(cc3)F)[nH]c(=O)O)CC1)OC
C4345	PI	Noninhibitor	175	c1cc(ccc1[N+](=O)[O-])OC(=O)N(C)C
C4346	PI	Noninhibitor	175	c12e3c(ccc1)c(=O)n(c(=O)c3cc(c2)[N+](=O)[O-])CCN1CCCC1
C4347	PI	Noninhibitor	175	c1ccc(cc1)n1c(=O)cc(C)n1C
C4348	PI	Noninhibitor	175	c1ccc(cc1)Cl(c2ccccc2)C(=O)NC(=O)N1
C4349	PI	Noninhibitor	175	c1ccc(cc1)C1=NCC(=O)Nc2ccc(cc12)[N+](=O)[O-]
C4350	PI	Noninhibitor	175	c1ccc2e(c1)c(=O)[nH]c1cccnc1n2C(=O)CN1CCN(CC1)C
C4351	PI	Noninhibitor	175	c12cnc(nc1n(cc(c2=O)C(=O)O)CC)N1CCCC1
C4352	PI	Noninhibitor	175	c12cnc(nc1n(cc(c2=O)C(=O)O)CC)N1CCNCC1
C4353	PI	Noninhibitor	175	c12c(cccc1)[nH]cc2C[C@@H](C(=O)O)N
C4354	PI	Inhibitor	175	c12c(cccc2OC[C@@H](CN2CCN(C3c4ccccc4CCc4cccc34)CC2)O)ncccc1
C4355	PI	Noninhibitor	175	c1cc(/C=C/C(=O)O)nc(c1)/C(=C/CN1CCCC1)/c1ccc(cc1)C
C4356	PI	Noninhibitor	175	CCCCCCCCCCCCCCC[C@@H]([C@H](CO)N)O
C4357	PI	Noninhibitor	175	[C@H]([C@@H]([C@@H](CO)O)O)O([C@H](CO)O)O
C4358	PI	Noninhibitor	175	c1ccc(cc1)C(c1ccccc1)(C1CCN(CCC[C@H](c2ccc(cc2)C(C(=O)O)(C)C)O)CC1)O
C4359	PI	Noninhibitor	175	C(=O)(C[C@@H](C[N+](C)(C)O)O
C4360	PI	Noninhibitor	175	c1ccc(cc1)N1CCN(C[C@@H](CO)O)CC1
C4361	PI	Noninhibitor	175	c1ccc(cc1)CCc1ccc(cc1)[C@H](Cn1ccnc1)O
C4362	PI	Noninhibitor	175	c1cc(ccc1[C@H](C1(CCCCC1)O)CN(C)C)O
C4363	PI	Noninhibitor	175	c1cc2c(c(c1)O)C(=O)C1=C([C@@]3(C(=O)C(=C([C@H]([C@@H]3C[C@H]1[C@@]2(C)O)N(C)C)O)C(=O)NCN1CCCC1)O)O
C4364	PI	Noninhibitor	175	C1=C2C[C@H](CC[C@]2(C)[C@@H]2CC[C@]3(C)[C@@H](CC[C@@]3(C(=O)C)O)[C@@H]2C1)O
C4365	PI	Inhibitor	175	c1ccc2e(c1)C(=CCCN[C@@H](C)Cc1ccc(c(c1)OC)OC)c1ccccc1CC2
C4366	PI	Noninhibitor	175	c12c(c(nc(n2)N(CCO)CCO)N2CCCC[C@H](C2)O)nc(nc1N1CCC[C@H](C1)O)N(CCO)CCO
C4367	PI	Noninhibitor	175	c1cc(cc2c1[C@@@]1CC[C@@]3(C)[C@@H](CC[C@@H]3O)[C@H]1CC2)O
C4368	PI	Noninhibitor	175	C1=C2[C@@H]3CC(C)(C)CC[C@]3(C(=O)O)CC[C@@]2(C)[C@]2(C)CC[C@H]3[C@](C)(CC[C@@H](C3(C)C)O)[C@H]2C1



C4369	PI	Noninhibitor	175	c1ccc(cc1)C[C@H]1[C@H]2[C@@H](C(=C)[C@H]([C@H]3/C=C/C[C@H](C)C[C@@@]/C=C/[C@H]([C@]23C(=O)N1)O)(C)O)O)C
C4370	PI	Noninhibitor	175	c1cc(cc2c1[C@@H]1CC[C@@]3(C)[C@@H](C[C@H](C3O)O)[C@H]1CC2)O
C4371	PI	Noninhibitor	175	C1=C(C(=O)[C@@]2(CC(=C[C@@H]3[C@@H]4C(C)(C)[C@@]4([C@@H]([C@@H](C)[C@]3([C@H]12)O)O)O)CO)O)C
C4372	PI	Noninhibitor	175	C1=C(C(=O)[C@@]2(CC(=C[C@@H]3[C@@H]4C(C)(C)[C@@]4([C@@H]([C@@H](C)[C@]3([C@H]12)O)O)O)OC(=O)C)CO)O)C
C4373	PI	Noninhibitor	175	C1=C(C(=O)[C@@]2(CC(=C[C@@H]3[C@@H]4C(C)(C)[C@@]4([C@@H]([C@@H](C)[C@]3([C@H]12)O)O)O)OC(=O)CCC)CO)O)C
C4374	PI	Inhibitor	175	c12c(cccc2O[C@H](CN2CCN(C(=O)C(Cc3ccccc3)Cc3ccccc3)CC2)O)nc1
C4375	PI	Noninhibitor	175	c1ccc2c(c1)C(=C1CCN(CC1)C)c1ccccc1C2O
C4376	PI	Noninhibitor	175	C(=C(C)C)CC1=C([C@]2(C(=O)[C@](C1=O)(CC=C(C)C)C[C@H](CC=C(C)C)[C@@]2(C)CCC=C(C)C)CC(C)C)O
C4377	PI	Noninhibitor	175	c12c3ccccc1C1=C[C@@H](C(=O)N[C@@H](C)CO)CN([C@H]1Cc2c[nH]3)C
C4378	PI	Noninhibitor	175	c12c3ccccc1C1=C[C@@H](C(=O)N[C@@H](CC)CO)CN([C@@H]1Cc2cn3C)C
C4379	PI	Noninhibitor	175	c12c(c(nc(n2)N(CCO)C)N2CCCC2)nc(nc1N1CCCC1)N(CCO)C
C4380	PI	Noninhibitor	175	c12c(c(nc(n2)N(CCO)CCO)N)nc(nc1N)N(CCO)CCO
C4381	PI	Noninhibitor	175	c12c(c(nc(n2)N(CCO)CCO)N2CC=CCC2)nc(nc1N1CC=CCC1)N(CCO)CCO
C4382	PI	Noninhibitor	175	c12c(c(nc(n2)N2CC[N+](CC2)(C)C)N2CCCC2)nc(nc1N1CCCC1)N(CCO)CCO
C4383	PI	Noninhibitor	175	c12c(c(nc(n2)N(CCO)CCO)N2CCCC2)nc(nc1N)N(CCO)CCO
C4384	PI	Noninhibitor	175	c12c(c(nc(n2)N(CCO)CCO)N(CCO)CCO)nc(nc1N(CCO)CCO)N(CCO)CCO
C4385	PI	Noninhibitor	175	c1ccc2c(c1)C=Cc1ccccc1N2CCCN1CCN(CC1)CCO
C4386	PI	Noninhibitor	175	c12c(c(nc(n2)NCCO)N2CCCC2)nc(nc1N1CCCC1)NCCO
C4387	PI	Noninhibitor	175	C(=C(C)C)CC/C(=C/CC/C(=C/CC/C(=C/CC/C(=C/CC/C(=C/CC/C(=C/CC/C(=C/CC/C(=C/CO)/C)/C)/C)/C)/C)/C
C4388	PI	Noninhibitor	175	c1ccc(cc1)[C@](CCN1CCCC1)(C1CCCC1)O
C4389	PI	Noninhibitor	175	c1ccc(cc1)[C@@](CCN1CCCC1)([C@@H]1C[C@H]2C=C[C@@H]1C2)O
C4390	PI	Noninhibitor	175	c1ccc2c(c1)c(=O)n1c(/C(=C)c3ccc(c3)O)/OCC1)n2
C4391	PI	Noninhibitor	175	c1ccc(cc1)c1ccccc1O)C(=O)OCCN(CC)CC
C4392	PI	Noninhibitor	175	c1cc2c3e(c1)CCN([C@@H]3Cc1ccc(c21)O)O)C
C4393	PI	Noninhibitor	175	c1cc(c2c(c1NCCNCCO)C(=O)c1c(c(cc1O)O)C2=O)NCCNCCO
C4394	PI	Noninhibitor	175	c1cc(ccc1C[C@H](C)NC[C@@H](c1cc(cc1)O)O)O
C4395	PI	Inhibitor	175	c12c3c4c(c5c1c(c(cc2OC)O)C(=O)C(=C5C[C@@H](C)OC(=O)c1ccccc1)OC)C(=C(C(=O)c4c(cc3OC)O)OC)C[C@@H](C)OC(=O)Oe1ccc(cc1)O
C4396	PI	Noninhibitor	175	c1ccc(cc1)CN1[C@H](c2nc3ccccc3c(=O)n2[C@H]1c1ccccc1)O)C
C4397	PI	Noninhibitor	175	c1cc(c(cc1[C@H](CNC)O)O)O
C4398	PI	Noninhibitor	175	c1cc(c(cc1[C@H](CNCCCCCN[C@@H](c1ccc(c(c1)O)O)O)O)O)O
C4399	PI	Noninhibitor	175	c1cc(c(cc1C[C@@H]1c2cc(c(cc2CCN1C)O)O)O)O
C4400	PI	Noninhibitor	175	c1cc(c(cc1C[C@@H]1c2cc(c(cc2CCN1)O)O)O)O
C4401	PI	Noninhibitor	175	c1cc(ccc1CC[C@H](C)NCCc1ccc(c(c1)O)O)O
C4402	PI	Noninhibitor	175	c1cc(cc(c1)NC(=O)C(=O)N/N=C/c1ccc(c(c1)O)O)[N+](=O)[O-]
C4403	PI	Noninhibitor	175	c1cc(cc2c1[C@@H]1C(=CC2)[C@H]2CCC(=O)[C@]2(C)CC1)O
C4404	PI	Noninhibitor	175	c1cc(cc2c1[C@@H]1CC[C@@]3(C(=O)CC[C@H]3[C@@H]1CC2)C)O
C4405	PI	Inhibitor	175	c1ccnc(c1)[C@@H](c1ccc(cc1)Cl)OCCN(C)C
C4406	PI	Noninhibitor	175	c12c(ccc(c2)O)c2c(cc1)[C@H]1CCC(=O)[C@@]1(C)CC2
C4407	PI	Noninhibitor	175	c1c2c(cc(c1O)O)[C@@H](C)NCC2
C4408	PI	Noninhibitor	175	c1ccc(cc1)CC[C@H](C)N[C@@H](C)[C@H](c1ccc(cc1)O)O
C4409	PI	Noninhibitor	175	c1cc(ccc1CCN[C@@H](C)[C@@H](c1ccc(cc1)O)O)O
C4410	PI	Noninhibitor	175	c1ccc(cc1)C[C@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)NCC(=O)N)C(C)C)C)C)CCC(=O)O)NC(=O)[C@@H](C)NC(=O)[C@H](Cc1ccc(cc1)O)N
C4411	PI	Noninhibitor	175	c1cc(c(cc1[C@H](CNC(C)C)C)O)CO)O
C4412	PI	Noninhibitor	175	C(=C(C)/OP(=O)(OC)OC)C(=O)OC
C4413	PI	Noninhibitor	175	c1cc(cc(c1)[N+](=O)[O-])[C@@H]1C(=C(C)NC(=C1P1(=O)OCC(C)(C)CO1)C)C(=O)OCCCCCCCCC
C4414	PI	Inhibitor	175	C1=C2CC[C@H]3[C@@H]4CC[C@](C(=O)C)([C@@]4(C)CC[C@@H]3[C@@]2(C)CCC1=O)O



C4461	PI	Noninhibitor	175	c1ccc(c(c1)C)N1CCN(Cc2n3c(CCCC3)nn2)CC1
C4462	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)C(=O)CCN(CC)CC
C4463	PI	Noninhibitor	175	c12c(nc(c3ccccc3)n2)N)nc(nc1N)N
C4464	PI	Noninhibitor	175	c12e(c(nc(n2)N(C)C)N2CCCCC2)nc(nc1N1CCCCC1)N(C)C
C4465	PI	Noninhibitor	175	c12e(c(nc(n2)N2CCCCC2)N2CCCCC2)nc(nc1N1CCCCC1)N1CCCCC1
C4466	PI	Noninhibitor	175	c12c(cccc1)c(c1ccccc1)nc(c2)N1CCNCC1
C4467	PI	Noninhibitor	175	c12c(cccc1)nc1c(c2N)CCCC1
C4468	PI	Noninhibitor	175	c12e(cccc2)nc2c(c1)cccc2
C4469	PI	Noninhibitor	175	c12c(cccc1)nc(cc2)N1CCNCC1
C4470	PI	Noninhibitor	175	c12c(cccc1)nc1c(c2N)CCN1C1CCCC1
C4471	PI	Noninhibitor	175	c1ccc(cc1)[C@H](c1cccn1)CCN(C)C
C4472	PI	Noninhibitor	175	c1ccc(cc1)Cc1cccn1
C4473	PI	Inhibitor	175	c1ccc(cc1)[C@H](c1ccccc1Cl)OCCN1CCN(Cc2ccccc2C)CC1
C4474	PI	Noninhibitor	175	c1ccc(cc1)CN(c1cccn1)CCN(C)C
C4475	PI	Noninhibitor	175	c1ccc(cc1)Cn1ccn1
C4476	PI	Noninhibitor	175	c12c(cccc1)oc(c2)C(=O)N1CCN(Cc2ccccc2)CC1
C4477	PI	Noninhibitor	175	c12c(cccc1)oc(c2CC)[C@H](CNCCC)O
C4478	PI	Noninhibitor	175	c1ccc(cc1)[C@H](c1nc(CCN(CC)CC)on1)CC
C4479	PI	Noninhibitor	175	c1ccc(cc1)c1nc(NCCN(CCCC)CCCC)on1
C4480	PI	Noninhibitor	175	c12c(cc(cc1)O)sc(c2C(=O)c1ccc(cc1)OCCN1CCCCC1)c1ccc(cc1)O
C4481	PI	Noninhibitor	175	c1ccnc(c1)N(Cc1ccsc1)CCN(C)C
C4482	PI	Noninhibitor	175	c1cc[n+](cc1)CC1=C(C(=O)O)N2C(=O)[C@H]([C@@H]2SC1)NC(=O)/C(=N)OC(C(=O)O)(C)C/c1esc(n1)N
C4483	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCN(CC)CC
C4484	PI	Noninhibitor	175	c1cc(C2C(=C(C)NC(=C2C(=O)OCC(=O)O)C)C(=O)OCC(=O)O)sc1
C4485	PI	Noninhibitor	175	c1ccc(cc1)N(C1CCN(CC1)C)Cc1cccs1
C4486	PI	Noninhibitor	175	c1ccc(cc1)N(Cc1cccs1)CCN(C)C
C4487	PI	Noninhibitor	175	c1cc(ccc1CN(c1nccs1)CCN(C)C)OC
C4488	PI	Inhibitor	175	c1ccc2c(c1)/C(=C)CCN(C)C/c1cc(ccc1S2)Cl
C4489	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCN
C4490	PI	Inhibitor	175	c1cc(c2c(c1C(=O)C)OCCO2)OC[C@@H](CN1CCN(C(=O)/C=C/c2cc(c(c2)OC)OC)OC)CC1)O
C4491	PI	Inhibitor	175	c1ccc(cc1)/C=C/CN1CCN(C(c2ccccc2)c2ccccc2)CC1
C4492	PI	Inhibitor	175	c12c(cccc1)n(c(CN1CCN(C/C=C/c3ccccc3)CC1)n2)CCC(=O)c1ccccc1
C4493	PI	Inhibitor	175	c12c(cccc1)nc(c2)N1CCN(CCCC(=O)c2ccc(cc2)F)CC1
C4494	PI	Inhibitor	175	c1ccc(cc1)[C@@](c1ccc(cc1)Cl)(C)OCC[C@H]1CCCN1C
C4495	PI	Inhibitor	175	c12c(cccc1)n(c(CN1CCCC1)n2)Cc1ccc(cc1)Cl
C4496	PI	Inhibitor	175	c1ccc(cc1)/C=C/CN1CCN([C@@H](c2ccccc2)c2ccc(cc2)Cl)CC1
C4497	PI	Inhibitor	175	c1ccc2c(c1)CCc1ccc(cc1N2CCCN(C)C)Cl
C4498	PI	Inhibitor	175	c1ccc2c(c1)/C(=C)CCN1CCN(CC1)CCO/c1cc(ccc1S2)Cl
C4499	PI	Inhibitor	175	c1ccc(cc1)[C@H](c1ccc(cc1)Cl)OCCN1CCCCC1
C4500	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCN
C4501	PI	Inhibitor	175	c1cc(ccc1C(c1ccc(cc1)F)CCCN1CCC(CC1)n1c2ccc(cc2[nH]c1=O)Cl)F
C4502	PI	Inhibitor	175	c1ccc2c(c1)C(=C1CCN(CC1)C)c1cc(ccc1O2)Cl
C4503	PI	Inhibitor	175	c1ccc2c(c1)N=C(c1cc(ccc1S2)Cl)N1CCN(CC1)C
C4504	PI	Inhibitor	175	c1ccc2c(c1)/C(=C)CCN1CCN(CCC(=O)NC)CC1/c1cc(ccc1S2)Cl
C4505	PI	Inhibitor	175	C=C[C@@@]1(C)CC(=O)[C@]2([C@]3(C)[C@H](C(C)C)CC[C@@@H]3O)[C@@H]([C@@H]([C@]2(C)O1)OC(=O)C)O)O
C4506	PI	Inhibitor	175	c1cc(cc2c1c(c(=O)o2)Cl)C)OP(=S)(OCC)OCC







C4645	PI	Inhibitor	175	<chem>C=C1[C@@H]([C@H]2[C@@H](C(=O)[C@@H](/C=C/C(C)C)[C@@H]([C@H]([C@H]1OC(=O)C(C)C)OC(=O)C)OC(=O)C)C[C@](C)([C@@H]2OC(=O)C)OC(=O)C)OC(=O)C</chem>
C4646	PI	Inhibitor	175	<chem>C(#N)[C@@](c1ccc(c1)Cl)Cl)(CCCN(Cc1ccc(c1)OC)OC)C(C)C</chem>
C4647	PI	Inhibitor	175	<chem>C(#N)[C@@](c1ccc(c1)OC)OC)(CCCN(Cc1ccc(c1)Cl)Cl)C(C)C</chem>
C4648	PI	Inhibitor	175	<chem>c1ccc(cc1)c1cc(=O)c2ccc(c2[nH]1)C(=O)Nc1ccc(cc1)OCCN(Cc1ccc(c1)OC)OC)C</chem>
C4649	PI	Inhibitor	175	<chem>C(#N)[C@@](c1cc(c(c1)OC)OC)OC)(CCCN(Cc1cc(c(c1)OC)OC)OC)C(C)C</chem>
C4650	PI	Inhibitor	175	<chem>C(#N)[C@@](c1ccc(c1OC)OC)OC)(CCCN(Cc1ccc(c1)OC)OC)C(C)C</chem>
C4651	PI	Inhibitor	175	<chem>C(#N)[C@](c1ccc(c1OC)OC)OC)(CCCN(Cc1ccc(c1)OC)OC)C(C)C</chem>
C4652	PI	Inhibitor	175	<chem>C(#N)[C@@](c1ccc(c1OC)OC)OC)(CCCN(Cc1ccc(c1)OC)OC)C(C)C</chem>
C4653	PI	Inhibitor	175	<chem>C(#N)[C@@](c1ccc(c1OC)OC)OC)(CCCN(Cc1ccc(c1)OC)OC)C(C)C</chem>
C4654	PI	Inhibitor	175	<chem>c12c(ccc2OC[C@@H](CN2CCN(C3c4cccc4[C@H]4C[C@H]4c4cccc34)CC2)O)nccc1</chem>
C4655	PI	Inhibitor	175	<chem>c1cc(c1c1C[C@H]1c2cc(c2c2CCN1C)OC)OC)OC</chem>
C4656	PI	Inhibitor	175	<chem>c1cc(ccc1C(=O)CCCN1CCC(C(=O)c2ccc(cc2)F)CC1)F</chem>
C4657	PI	Inhibitor	175	<chem>c1cc(ccc1CN1C(=O)NC(=S)N(Cc2ccc(cc2)Cl)CC1)Cl</chem>
C4658	PI	Inhibitor	175	<chem>c12c(ccc1)nc1c(ccc1C(=O)Nc1ccc(cc1)OCCN(Cc1ccc(c1)OC)OC)C)n2</chem>
C4659	PI	Inhibitor	175	<chem>c1cc(c(c1)C)NC(=O)CN1CCN(Cc1ccc(cc2)F)c2ccc(cc2)F)CC1)C</chem>
C4660	PI	Inhibitor	175	<chem>c1ccc(cc1)[C@@H](c1ccc(cc1)Cl)OCCN1CCOCC1</chem>
C4661	PI	Inhibitor	175	<chem>c1ccc(cc1)CC(=O)N(c1ccc(cc1)Cl)C1CCN(C(C)C)CC1</chem>
C4662	PI	Inhibitor	175	<chem>c1ccc(cc1)C1(c2ccccc2)C(=O)N(CCCN2CCN(c3ccccc3)Cl)CC2)[C@H](C)N1</chem>
C4663	PI	Inhibitor	175	<chem>c1ccc(cc1)C1CCN(CC1)CCCN1C(=O)C(c2ccccc2)(c2ccccc2)N[C@H]1C</chem>
C4664	PI	Inhibitor	175	<chem>c1ccc2c(c1)c(=O)n1cccc(c1n2)C(=O)Nc1ccc(cc1)OCCN(Cc1ccc(c1)OC)OC)C</chem>
C4665	PI	Inhibitor	175	<chem>c1ccc(cc1)C1(c2ccccc2)C(=O)N(C(=O)N1)CCCN1CCOCC1</chem>
C4666	PI	Inhibitor	175	<chem>c1ccc(cc1)C1CCN(CC1)CCCN1C(=O)C(c2ccccc2)(c2ccccc2)NC1=O</chem>
C4667	PI	Inhibitor	175	<chem>c1ccc(cc1)C1(c2ccccc2)C(=O)N(C(=O)N1)CCC(=O)N</chem>
C4668	PI	Inhibitor	175	<chem>c1ccc(cc1)/C=C/c1ccc(cc1)C(C)(C)C/c1ccc(cc1)OCCN(CC)CC</chem>
C4669	PI	Inhibitor	175	<chem>c1ccc(cc1)[C@H](c1ccc(cc1)OCCN(CC)CC)Cc1ccc(cc1)OC</chem>
C4670	PI	Inhibitor	175	<chem>C(#N)[C@](c1ccc(c1)OC)OC)(CCCNc1c2c(cc3c1ccccc3)ccccc2)C(C)C</chem>
C4671	PI	Inhibitor	175	<chem>C1=C[C@@H](C)[C@@H](/C=C/[C@@H](C)[C@@H]([C@@H](C)[C@H](C)C(C2=CC(=O)C=C(C2=O)NC(=O)/C(=C1)/C)OC)OC)O)/C)OC(=O)N</chem>
C4672	PI	Inhibitor	175	<chem>c1ccc(cc1)C(c1ccccc1)N1CCN(CC1)CCOC(=O)C1=C(C)NC(=C(C(=O)OC)[C@@H]1c1ccccc1)[N+](=O)[O-]C</chem>
C4673	PI	Inhibitor	175	<chem>c1ccc2c(c1)C1c3ccccc3C2(CC1)CCCNc</chem>
C4674	PI	Inhibitor	175	<chem>c1ccc2c(c1)c(=O)c1ccc(c1[nH]2)C(=O)Nc1ccc(cc1)OCCN(Cc1ccc(cc1)C)C</chem>
C4675	PI	Inhibitor	175	<chem>c1cc(c1c1C(=O)OCCCN([C@@H](C)Cc1ccc(cc1)OC)CC)OC)OC</chem>
C4676	PI	Inhibitor	175	<chem>c1ccc(cc1)[C@@H](c1ccc(cc1)Cl)N1CCN(Cc2ccccc2)C)CC1</chem>
C4677	PI	Inhibitor	175	<chem>C1=C2C(C)C[C@H]3[C@H]4CC[C@](C(=O)C)([C@]4(C)CC[C@H]3[C@@]2(C)CCC1=O)O</chem>
C4678	PI	Inhibitor	175	<chem>C1=C2C(=C[C@@H]3[C@H]4CC[C@](C(=O)C)([C@@]4(C)CC[C@H]3[C@@]2(C)CCC1=O)OC(=O)C)C</chem>
C4679	PI	Inhibitor	175	<chem>c1ccc(cc1)C(c1ccccc1)CCNCCCOC(=O)c1cc(c(c1)OC)OC)OC</chem>
C4680	PI	Inhibitor	175	<chem>c12c3ccccc1[C@@H]1C[C@@H](CNC(=O)OCc4ccccc4)CN([C@H]1Cc2cn3C)C</chem>
C4681	PI	Inhibitor	175	<chem>c1ccc(cc1)C(c1ccccc1)(C(=O)CC)C[C@H](C)N(C)C</chem>
C4682	PI	Inhibitor	175	<chem>c1ccc(cc1)CN(CC)CCOc1ccc(cc1)NC(=O)c1ccc2c1[nH]c1ccccc1c2=O</chem>
C4683	PI	Inhibitor	175	<chem>c1cc2c(cc1)/C=C/[C@H]1CC(=CC(=O)O1)OC)OCO2</chem>
C4684	PI	Inhibitor	175	<chem>c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCN1CCN(CC1)CCOC(=O)c1cc(c(c1)OC)OC)OC</chem>
C4685	PI	Inhibitor	175	<chem>c12c(cc1)OC[nH]c1c2CCN2[C@@H]1C[C@H]1[C@H](C(=O)OC)[C@H](C(C[C@@H]1C2)OC)OC</chem>
C4686	PI	Inhibitor	175	<chem>c1ccc2c(c1)C=C(c1cc(ccc1O2)OC)N1CCN(CC1)C</chem>
C4687	PI	Inhibitor	175	<chem>c12c(ccc1)nc(CCCN(CC[C@@H]1[C@H](c3ccc(cc3CC1OC(=O)COC)F)C(C)C)[nH]2</chem>
C4688	PI	Inhibitor	175	<chem>C(#C[C@]1(CC[C@H]2[C@H]3C(=C4C(=CC(=O)CC4)CC3)[C@@H](c3ccc(cc3)N(C)C)C[C@]12C)O)C</chem>
C4689	PI	Inhibitor	175	<chem>c1cc(ccc1C(=O)C1CCN(CC1)CCCN1c2ccc(cc2[nH]c1=O)Cl)F</chem>
C4690	PI	Inhibitor	175	<chem>c12c(cc(c1)OC)OC)[nH]c(c2CCN1CCN(c2ccccc2OC)CC1)C</chem>

C4691	PI	Inhibitor	175	<chem>c1ccc(c(c1)Cl)NC(=O)CN1C[C@@H](C(=O)N)N(CCCC(c2ccc(cc2)F)c2ccc(cc2)F)CC1)Cl</chem>
C4692	PI	Inhibitor	175	<chem>c1ccc2c(c1)c(=O)c1ccc(c1[nH]2)C(=O)Nc1ccc(cc1)OCCCN(CCCc1ccc(c1)OC)OC)C</chem>
C4693	PI	Inhibitor	175	<chem>C(=O)([C@H](C)[C@@H]([C@H](C)C1[C@H](C)[C@@H]2CC[C@](C)([C@H]3CC[C@@](C)([C@@H]4[C@@H](C)C[C@@H](C5[C@@H](C)C[C@@H](C)[C@@](CO)O5)O4)O3)O2)O1)O)OC)O</chem>
C4694	PI	Inhibitor	175	<chem>c1ccc(cc1)N([C@@H]1Cc2ccc2[C@H]1OC)CCCN(CC)CC</chem>
C4695	PI	Inhibitor	175	<chem>c12c(cccc2)c(c2c(c1)ccc2)C(=O)OCCCCCN(CCCCO(=O)/C=C/c1ccc(c(c1)OC)OC)C</chem>
C4696	PI	Inhibitor	175	<chem>c1ccc(cc1)C(=CC(=O)OCCCN(CCCOC(=O)/C=C/c1ccc(c(c1)OC)OC)OC)C)c1ccc1</chem>
C4697	PI	Inhibitor	175	<chem>c1ccc(cc1)c1ccc(cc1)/C=C/C(=O)OCCCN(CCCOC(=O)/C=C/c1ccc(c(c1)OC)OC)OC)C</chem>
C4698	PI	Inhibitor	175	<chem>c1cc(ccc1C(c1ccc(cc1)OC)C(=O)OCCCN(CCCOC(=O)/C=C/c1ccc(c(c1)OC)OC)OC)OC)C</chem>
C4699	PI	Inhibitor	175	<chem>c1c(cc(c(c1OC)OC)OC)/C=C/C(=O)O[C@H]1CC[C@@H](CC1)N([C@H]1CC[C@H](CC1)OC(=O)c1ccc(c(c1)OC)OC)OC)C</chem>
C4700	PI	Inhibitor	175	<chem>c12c(cccc2)c(c2c(c1)ccc2)C(=O)OC1CCC(CC1)N(C1CCC(CC1)OC(=O)c1ccc(c(c1)OC)OC)OC)C</chem>
C4701	PI	Inhibitor	175	<chem>c1c(cc(c(c1OC)OC)OC)/C=C/C(=O)OCCCN(CCCOC(=O)c1ccc(c(c1)OC)OC)OC)C</chem>
C4702	PI	Inhibitor	175	<chem>c12c(cccc2)c(c2c(c1)ccc2)C(=O)OCCCN(CCCOC(=O)c1ccc(c(c1)OC)OC)OC)C</chem>
C4703	PI	Inhibitor	175	<chem>c1ccc2c(c1)c(=O)c1ccc(c1[nH]2)C(=O)Nc1ccc(cc1)OCCCN1Cc2cc(c(cc2CC1)OC)OC</chem>
C4704	PI	Inhibitor	175	<chem>c1cc(c(c1C[C@@H]1c2cc(c(cc2CCN1)OC)OC)OC)OC</chem>
C4705	PI	Inhibitor	175	<chem>c1cc2c(c(c1)OC)C(=O)c1c(c(c3c(c1O)[C@H](C[C@](C(=O)C)(C3)O)O[C@H]1C[C@@H]([C@@H]([C@H](C)O1)O)NC(=O)C)O)C2=O</chem>
C4706	PI	Inhibitor	175	<chem>c1ccc(cc1)OC(=O)N1C=C[C@H](c2ccc(cc2)OC)C(=C1)C(=O)CC</chem>
C4707	PI	Inhibitor	175	<chem>c1ccc(cc1)OC(=O)N1C=C[C@H](c2ccc(cc2)C)C(=C1)C(=O)C</chem>
C4708	PI	Inhibitor	175	<chem>c1ccc(cc1)OC(=O)N1C=C[C@H](c2cccc2OC)C(=C1)C(=O)C</chem>
C4709	PI	Inhibitor	175	<chem>c1ccc(cc1)OC(=O)N1C=C[C@H](c2ccc(cc2)OC)C(=C1)C(=O)C</chem>
C4710	PI	Inhibitor	175	<chem>c1ccc(cc1)OC(=O)N1C=C[C@H](c2ccc(cc2)C)C(=C1)C(=O)CC</chem>
C4711	PI	Inhibitor	175	<chem>c1ccc(cc1)OC(=O)N1C=C[C@H](c2cccc2OC)C(=C1)C(=O)CC</chem>
C4712	PI	Inhibitor	175	<chem>c1ccc(cc1)/C=C(/c1ccc1)CCCl)/c1ccc(cc1)OCCNC</chem>
C4713	PI	Inhibitor	175	<chem>c1cc(ccc1[C@@H](C1(CCCCC1)O)CNC)OC</chem>
C4714	PI	Inhibitor	175	<chem>c1ccc2c(c1)c(=O)c1ccc(c1[nH]2)C(=O)Nc1ccc(cc1)CN(Cc1ccc(c(c1)OC)OC)C</chem>
C4715	PI	Inhibitor	175	<chem>c1ccc(cc1)/C=C(/c1ccc1)CC)/c1ccc(cc1)OCCNC</chem>
C4716	PI	Inhibitor	175	<chem>c1ccc(cc1)C(c1ccc1)CCN(C(=O)CN(C(=O)CNCCC(C)C)CCc1ccc(cc1)Cl)CC(=O)N</chem>
C4717	PI	Inhibitor	175	<chem>c1ccc2c(c1)[C@@H](c1ccc(cc1)OCCN(CC)CC)C(c1ccc(cc1)OC)C(=O)O2</chem>
C4718	PI	Inhibitor	175	<chem>c1ccc(cc1)C(=O)OCCN(Cc1ccc(cc1)OC)CCN(Cc1ccc(cc1)OC)CCOC(=O)c1ccc1</chem>
C4719	PI	Inhibitor	175	<chem>c1ccc(cc1)COc1cc(cc1OCc1ccc1)OCc1ccc1)C(=O)OCCN(CC)CC</chem>
C4720	PI	Inhibitor	175	<chem>c1c(cc(C)nc1C)c1c(cc2c(c1F)n(cc1c2nn(c1=O)C1CCC(CC1)N(C)C)C1CC1)F</chem>
C4721	PI	Inhibitor	175	<chem>c1ccc2c(c1)c(=O)cc1ccc(c(c1OC)OC)OC)o2</chem>
C4722	PI	Inhibitor	175	<chem>C(#N)c1c(c2ccc(cc2)Cl)c2c(CC(C)C)CC2=O)n(c1=S)C1[C@@H]([C@H]([C@@H]([C@@H](COC(=O)C)O1)OC(=O)C)OC(=O)C)OC(=O)C</chem>
C4723	PI	Inhibitor	175	<chem>c12c(cccc2)c(ccc1)[C@@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@H](c1c2c(ccc1)ccc2)C)C</chem>
C4724	PI	Inhibitor	175	<chem>c1ccc2c(c1)c(=O)c1ccc(c1[nH]2)C(=O)Nc1ccc(cc1)CCN(Cc1ccc(c(c1)OC)OC)C</chem>
C4725	PI	Inhibitor	175	<chem>c1ccc(cc1)C1=C(c2ccc(cc2)OCCN2CCCC2)c2ccc(cc2CC1)OC</chem>
C4726	PI	Inhibitor	175	<chem>c12c(cccc2)c(ccc1)OC[C@@H](CN1CCN(c2cccc2OC)CC1)O</chem>
C4727	PI	Inhibitor	175	<chem>c1ccc(cc1)CN(CCO(=O)C1=C(C)NC(=C(C(=O)OC)[C@@H]1c1ccc(c1)[N+](=O)[O-])C)C</chem>
C4728	PI	Inhibitor	175	<chem>c12c3ccc1[C@]1(C[C@H](CN([C@@H]1Cc2en3C)C)COC(=O)c1cc(cnc1)Br)OC</chem>
C4729	PI	Inhibitor	175	<chem>c12c(cccc1)n(c(CN1CCN(CC(=O)NC(C)C)CC1)n2)CCC(=O)c1ccc1 c1cc(cc(c1)[N+](=O)[O-])C1C(=C(C)NC(=C1C(=O)OCCOC)C(=O)OCCOC</chem>
C4730	PI	Inhibitor	175	<chem>c1ccc2c(c1)c(=O)c1ccc(c1[nH]2)C(=O)Nc1ccc(cc1)CCCN(Cc1ccc(c(c1)OC)OC)C</chem>
C4731	PI	Inhibitor	175	<chem>c1ccc(cc1)/C=C(/c1ccc(cc1)OC)\c1ccc(cc1)OCCN1CCCC1/[N+](=O)[O-]</chem>
C4732	PI	Inhibitor	175	<chem>c1ccc(cc1)[C@H](CCN)Oe1ccc(cc1)C(F)(F)F</chem>
C4733	PI	Inhibitor	175	<chem>c1ccc2c(c1)C(=CCNC)c1ccc1CC2</chem>
C4734	PI	Inhibitor	175	<chem>c1cc(c(c2c1[C@@H]([C@@H]1c3c(cc4c(c3OC)OCO4)CCN1C)OC2=O)OC)OC</chem>
C4735	PI	Inhibitor	175	<chem>c12c(cc(c(c1)OC)OC)nenc2Nc1ccc(c1)Br</chem>



C4737	PI	Inhibitor	175	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)CCCCN(Cc1ccc(c(c1)OC)OC)C
C4738	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1[S@]2=O)Cl)CCCN(C)C
C4739	PI	Inhibitor	175	C(#CCOC(=O)[C@](c1ccccc1)(C1CCCC1)O)CN(CC)CC
C4740	PI	Inhibitor	175	c12c(cc(c(c1)OC)OC)[nH]c(c2CCN1CCN(c2ccccc2)CC1)C
C4741	PI	Inhibitor	175	c12c(cccc1)nc1c(c2NC(=O)Cc2ccccc2)CCN1Cc1ccccc1
C4742	PI	Inhibitor	175	c1cc(ccc1C(c1ccc(cc1)F)CCCN1CCC(c2ccc(c(c2)C(F)(F)F)Cl)(CC1)O)F
C4743	PI	Inhibitor	175	c1ccc(c(c1)CCNCC(=O)N(CC(=O)N(CC(=O)N)CCc1ccc(cc1Cl)Cl)CCc1ccc(cc1Cl)Cl)F
C4744	PI	Inhibitor	175	c1cc(ccc1CCNCC(=O)N(CC(=O)N(CC(=O)N)CCc1ccc(cc1Cl)Cl)CCc1ccc(cc1Cl)Cl)F
C4745	PI	Inhibitor	175	c1cc(cc(c1)OC)/C=N\OC[C@@H](CN1CCN(c2ccccc2OC)CC1)O
C4746	PI	Inhibitor	175	c1ccc2c(c1)C(=Nc1ccccc1C2)N1CCN(CC1)C
C4747	PI	Inhibitor	175	c1cc(cc(c1)Cl)CN1C(=S)NC(=S)N(Cc2ccccc2)Cl)CC1
C4748	PI	Inhibitor	175	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)CCCCN(Cc1ccc(c(c1)OC)OC)C
C4749	PI	Inhibitor	175	c1ccc2c(c1)N(c1ccccc1O2)CCCN1CCOCC1
C4750	PI	Inhibitor	175	c1ccc2c(c1)N(c1ccccc1O2)CCCN1CCCCC1
C4751	PI	Inhibitor	175	c1ccc2c(c1)N(c1ccccc1O2)C(=O)CN1CCCCC1
C4752	PI	Inhibitor	175	c1ccc2c(c1)N(c1ccccc1O2)CCCN(CC)CC
C4753	PI	Inhibitor	175	c1ccc2c(c1)N(c1ccccc1O2)CCCN(CCO)CCO
C4754	PI	Inhibitor	175	c1ccc2c(c1)N(c1ccccc1O2)CCCN1CCOCC1
C4755	PI	Inhibitor	175	c1ccc2c(c1)N(c1ccccc1O2)CCCN1CCCCC1
C4756	PI	Inhibitor	175	c1ccc(cc1)NC(=N)NC(=O)c1c(nc(c(n1)Cl)N)N
C4757	PI	Inhibitor	175	c1c2c(ccc1OC(=O)NC)N([C@H]1[C@@]2(C)CCN1C)C
C4758	PI	Inhibitor	175	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)OCCCN(Cc1ccc(c(c1)OC)OC)C
C4759	PI	Inhibitor	175	c1cc2c(cc1CN1CCN(C/C=C(\C)/CC/C=C(\C)/CCC=C(C)C)CC1)OCO2
C4760	PI	Inhibitor	175	c1ccc2c(c1)/C(=C/CCN1CCN(CC1)CCO)/c1cc(ccc1OC2)Cl
C4761	PI	Inhibitor	175	c1cc(ccc1C(=O)CCCN1CCC(C(=O)N)(CC1)N1CCCCC1)F
C4762	PI	Inhibitor	175	c1cc2c(cc1/C=C/C1[C@@H](c3ccc4c(c3)OCO4)C=C[C@H](C(=O)N3CCCCC3)[C@H]1C(=O)N1CCCCC1)OCO2
C4763	PI	Inhibitor	175	c1ccc(cc1)C(=C1CCN(CC1)CCOCCOCCO)c1ccccc1
C4764	PI	Inhibitor	175	c1ccc2c(c1)C(=C1CCN([C@@H]1C)CC)c1ccccc1CC2
C4765	PI	Inhibitor	175	c1ccc(cc1)/C(=C\1/CCN(CC)C1)/c1ccc(cc1)F
C4766	PI	Inhibitor	175	C1(=O)C(=O)C[C@@]2(C)[C@@H](C1)CC[C@H]1[C@H]3CC[C@H](CC)[C@]3(C)CC[C@@H]21
C4767	PI	Inhibitor	175	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)/C=C/CN(Cc1ccc(c(c1)OC)OC)C
C4768	PI	Inhibitor	175	c1ccc(cc1)C[C@H](C)NCCC(c1ccccc1)c1ccccc1
C4769	PI	Inhibitor	175	c1ccc(cc1)[C@H]1C(=O)O[C@@H](C)[C@H](C)[C@H](C(=O)N[C@@H](C(=O)N2[C@@H](C(=O)N([C@@H](C(=O)N3[C@@H](C(=O)N1)CC(=O)CC3)Cc1ccc(cc1)N(C)C)CCC2)CC)NC(=O)c1c(cccn1)O
C4770	PI	Inhibitor	175	c1ccc(cc1)C(c1ccccc1)(C(=O)OCCN(CC)CC)CCC
C4771	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCN1CCN(CC1)C
C4772	PI	Inhibitor	175	c1cc(ccc1/C(=N\CCCC(=O)N)/c1cc(ccc1O)F)Cl
C4773	PI	Inhibitor	175	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CNCCC)O
C4774	PI	Inhibitor	175	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN(CCC)C)O
C4775	PI	Inhibitor	175	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN(C)C)O
C4776	PI	Inhibitor	175	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CN(C(C)C)C(C)C)O
C4777	PI	Inhibitor	175	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)C/C=C/CN(Cc1ccc(c(c1)OC)OC)C
C4778	PI	Inhibitor	175	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CNCc1ccccc1)O
C4779	PI	Inhibitor	175	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN1CCCC1)O
C4780	PI	Inhibitor	175	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CN1CCN(c2ccccc2C)CC1)O
C4781	PI	Inhibitor	175	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN1CCN(c2ccc(cc2)OC)CC1)O
C4782	PI	Inhibitor	175	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CCC)O

C4783	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN(CC)CC)O</chem>
C4784	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN1CCCC1)O</chem>
C4785	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccc(cc1)OC[C@H](CN1CCN(c2ccc(cc2)F)CC1)O</chem>
C4786	PI	Inhibitor	175	<chem>c1ccc(cc1)CC[C@H](c1ccccc1OC[C@H](CN1CCN(c2ccc(cc2)F)CC1)O)O</chem>
C4787	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccc(cc1)OC[C@@H](CN(C(C)C)C(C)C)O</chem>
C4788	PI	Inhibitor	175	<chem>c1cc2c(c(c1)C(=O)Nc1cc(ccc1)CCN1Cc3cc(c(cc3CC1)OC)OC)[nH]c1ccccc1c1c2=O)OC</chem>
C4789	PI	Inhibitor	175	<chem>c1ccc(cc1)CC[C@@H](c1ccccc1OC[C@H](CN(C(C)C)C(C)C)O)O</chem>
C4790	PI	Inhibitor	175	<chem>c1ccc(cc1)CC[C@@H](c1ccccc1OC[C@@H](CN(C(C)C)C(C)C)O)OC</chem>
C4791	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CNc1ccccc1)O</chem>
C4792	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN1CCN(Cc2ccccc2)CC1)O</chem>
C4793	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN1CCN(c2ccc(cc2)F)CC1)O</chem>
C4794	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CNc1ccc(cc1)C(=O)OC)O</chem>
C4795	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CNc1ccc(cc1)C(F)(F)F)O</chem>
C4796	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CNc1ccc(cc1)[N+](=O)[O-])O</chem>
C4797	PI	Inhibitor	175	<chem>c1ccc(cc1)C(=O)N(CCC)C[C@H](COc1ccccc1C(=O)CCc1ccccc1)O</chem>
C4798	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CN(Cc1ccccc1)CCC)O</chem>
C4799	PI	Inhibitor	175	<chem>c1ccc(c(c1)CCN1Cc2cc(c(cc2CC1)OC)OC)NC(=O)c1ccccc1c1c2=O)OC</chem>
C4800	PI	Inhibitor	175	<chem>c1ccc(cc1)C1(CCN(CC1)C[C@H](COc1ccccc1C(=O)CC)O)O</chem>
C4801	PI	Inhibitor	175	<chem>c1ccc(cc1)C(=O)N1CCN(C[C@@H](COc2ccccc2C(=O)CCc2ccccc2)O)CC1</chem>
C4802	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CN1CCOCC1)O</chem>
C4803	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CN1CCC(c2ccccc2)(CC1)O)O</chem>
C4804	PI	Inhibitor	175	<chem>c1ccc(cc1)CC[C@H](c1ccccc1OC[C@H](CN1CCCC1)O)O</chem>
C4805	PI	Inhibitor	175	<chem>c1ccc(cc1)CC[C@@H](c1ccccc1OC[C@H](CN1CCCC1)O)OC</chem>
C4806	PI	Inhibitor	175	<chem>c1ccc(cc1)CC[C@@H](c1ccccc1OC[C@H](CN1CCOCC1)O)OC</chem>
C4807	PI	Inhibitor	175	<chem>c1ccc(cc1)CC[C@@H](c1ccccc1OC[C@@H](CNCCC(c1ccccc1)c1ccccc1)O)OC</chem>
C4808	PI	Inhibitor	175	<chem>c1ccc(cc1)C1(CCN(CC1)C[C@H](COc1ccccc1C(=O)C)O)O</chem>
C4809	PI	Inhibitor	175	<chem>c12c(cccc2)c(ccc1)CCC(=O)c1ccccc1OC[C@@H](CN1CCCC1)O</chem>
C4810	PI	Inhibitor	175	<chem>c1cc2c(c(c1)C(=O)Nc1cc(ccc1)CCCN1Cc3cc(c(cc3CC1)OC)OC)[nH]c1ccccc1c1c2=O)OC</chem>
C4811	PI	Inhibitor	175	<chem>c12c(cccc2)c(ccc1)CCC(=O)c1ccccc1OC[C@H](CN(C(C)C)C(C)C)O</chem>
C4812	PI	Inhibitor	175	<chem>c12c(cccc2)c(ccc1)CCC(=O)c1ccccc1OC[C@H](CN1CCOCC1)O</chem>
C4813	PI	Inhibitor	175	<chem>c12c(cccc2)c(ccc1)CCC(=O)c1ccccc1OC[C@H](CN1CCC(c2ccccc2)(CC1)O)O</chem>
C4814	PI	Inhibitor	175	<chem>c12c(cccc2)c(ccc1)CCC(=O)c1ccccc1OC[C@@H](CNCCC(c1ccccc1)c1ccccc1)O</chem>
C4815	PI	Inhibitor	175	<chem>c1ccc(cc1)C(=O)c1ccccc1OC[C@@H](CN1CCN(c2ccc(cc2)F)CC1)O</chem>
C4816	PI	Inhibitor	175	<chem>c1ccc(cc1)C(=O)c1ccccc1OC[C@H](CN1CCC(c2ccccc2)(CC1)O)O</chem>
C4817	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccc(ccc1OC[C@@H](CN1CCN(Cc2ccccc2)CC1)O)O</chem>
C4818	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccc(ccc1OC[C@H](CNCCC)O)OCc1ccccc1</chem>
C4819	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccc(ccc1OC[C@@H](CN1CCCC1)O)OCc1ccccc1</chem>
C4820	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccc(ccc1OC[C@@H](CN(C(C)C)C(C)C)O)OCc1ccccc1</chem>
C4821	PI	Inhibitor	175	<chem>c1cc2c(c(c1)C(=O)Nc1cc(ccc1)CCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1ccccc1c1c2=O)OC</chem>
C4822	PI	Inhibitor	175	<chem>c1ccc(cc1)CCC(=O)c1ccc(ccc1OC[C@H](CN1CCN(Cc2ccccc2)CC1)O)OCc1ccccc1</chem>
C4823	PI	Inhibitor	175	<chem>c1ccc(cc1)CC[C@H](c1ccccc1OC[C@@H](CN1CCN(c2ccc(cc2)F)CC1)O)OC</chem>
C4824	PI	Inhibitor	175	<chem>c1ccc(cc1)[C@@](C(=O)O)[C@@H]1CCCN(C1)C(C1CCCCC1)O</chem>
C4825	PI	Inhibitor	175	<chem>c1ccc(cc1)C[C@@](c1ccccc1)([C@@H](C)CN(C)C)OC(=O)CC</chem>
C4826	PI	Inhibitor	175	<chem>c1ccc2c(c1)C=Cc1ccccc1C2CCCN</chem>
C4827	PI	Inhibitor	175	<chem>c12c(nc(nc1N1CCC(CC1)NC[C@H]1c3ccccc3COc3ccccc13)NCC=C)n(cn2)CC=C</chem>
C4828	PI	Inhibitor	175	<chem>c12c(nc(nc1NCC=C)N1CCC(CC1)NCC(c1ccc(cc1)F)c1ccc(cc1)F)n(cn2)CC=C</chem>

C4829	PI	Inhibitor	175	c12c(nc(nc1NCC=C)N1CCC(CC1)NC[C@@H]1c3ccccc3COc3ccccc13)n(cn2)CC=C
C4830	PI	Inhibitor	175	c12c(nc(nc1NCC=C)N1CCC(CC1)NC[C@@H]1c3ccccc3CCc3cc(ccc13)OC)n(cn2)CC=C
C4831	PI	Inhibitor	175	c1cc2c(c(c1)C(=O)Nc1ccc(cc1)OCCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)C
C4832	PI	Inhibitor	175	c12c(cc(cc1)Cl)nc1c(cc(cc1)OC)c2N[C@H](C)CCCN(CC)CC
C4833	PI	Inhibitor	175	c12c(ccc(c1)OC)ncce2[C@@H]([C@H]1C[C@@H]2CCN1C[C@H]2C=C)O
C4834	PI	Inhibitor	175	c1ccc2c(c1)CCc1cccc1N2[C@H]1C2CCN(CC2)C1
C4835	PI	Inhibitor	175	c1cc(cc(c1[C@@@]1(Cn2ccnc2)OC[C@@H](COc2ccc(cc2)n2ccnc2)O1)Cl)Cl
C4836	PI	Inhibitor	175	c1cc(cc(c1[C@@@]1(Cn2ccnc2)OC[C@H](COc2ccc(cc2)N2CCN(C(=O)OCC)CC2)O1)Cl)Cl
C4837	PI	Inhibitor	175	c1cc(cc(c1[C@@@]1(Cn2ccnc2)OC[C@H](COc2ccc(cc2)N2CCN(C(=O)C)CC2)O1)Cl)Cl
C4838	PI	Inhibitor	175	c1ccc2c(c1)n(c(=O)[nH]2)C1CCN(CCCCc2ccc(cc2)F)CC1
C4839	PI	Inhibitor	175	c12c(nc(c3ccccc3)n2)N2[C@H](C)COCC2)nc(nc1N(C[C@@H](C)O)CCO)N1[C@@H](C)COCC1
C4840	PI	Inhibitor	175	c12c(nc(c3ccccc3)n2)N2CCOCC2)nc(nc1N1CCOCC1)N1CCOCC1
C4841	PI	Inhibitor	175	c12c(nc(c3ccccc3)n2)N2CCOCC2)nc(nc1N(CCO)C)N1CCOCC1
C4842	PI	Inhibitor	175	c1cc2c(c(c1)C(=O)Nc1ccc(cc1)OCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)OC
C4843	PI	Inhibitor	175	c12c(nc(c3ccccc3)n2)N2CCOCC2)nc(nc1N(CC)CCO)N1CCOCC1
C4844	PI	Inhibitor	175	c12c(nc(c3ccccc3)n2)N2CCOCC2)nc(nc1N(Cc1cccc1)CCO)N1CCOCC1
C4845	PI	Inhibitor	175	c12c(c(nc(n2)N(CCOC)CO)N(CC)CC)nc(nc1N(CC)CC)N(CCOC)CCO
C4846	PI	Inhibitor	175	c1ccc(cc1)CNc1c(nc2c(n1)O[C@@H](N[C@@H]2N1CCSCC1)N1CCNCC1)Cl
C4847	PI	Inhibitor	175	c1ccc(cc1)C[C@@H](C)N[C@@H](C)COc1cccc1
C4848	PI	Inhibitor	175	c1c2c(c(c1OC)OC)OC)mnn(c2=O)C[C@@H](CN1CCOCC1)OC(=O)c1cc(c(c1)OC)OC)OC
C4849	PI	Inhibitor	175	c1ccc(cc1)[C@H]([C@H]1CNCCO1)Oe1cccc1OCC
C4850	PI	Inhibitor	175	c12c(cc(cc1)OC)[nH]c1c2CCN2[C@@H]1C[C@H]1[C@H](C(=O)OC)[C@H](C(C[C@@H]1C2)OC(=O)/C=C/c1cc(c(c1)OC)OC)OC)OC
C4851	PI	Inhibitor	175	c12c(cc(cc1)OC)[nH]c1c2CCN2[C@@H]1C[C@@H]1[C@H](C(=O)OC)[C@H](C(C[C@@H]1C2)OC(=O)c1cc(c(c1)OC)OC)OC)OC
C4852	PI	Inhibitor	175	c1ccc(cc1)COC(=O)C[C@@H](C(=O)N[C@@H](C(=O)OC(C)C)CCCCNC(=O)OCc1cccc1)NC(=O)OC(C)C)C
C4853	PI	Inhibitor	175	c1cc(ccc1CN1C(=S)NC(=S)N(Cc2ccc(cc2)Cl)CC1)Cl
C4854	PI	Inhibitor	175	c1cc2c(c(c1)C(=O)Nc1ccc(cc1)OCCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)F
C4855	PI	Inhibitor	175	c1ccc(cc1)COC(=O)CC[C@@H](C(=O)NCCCC[C@H](C(=O)OC)NC(=O)[C@@H](CC(=O)OCc1cccc1)NC(=O)OC(C)C)NC(=O)OC(C)C)C
C4856	PI	Inhibitor	175	c12c3e4c(c(c1O)O)[C@@](C4=O)(O)O/C=C/[C@@H]([C@@H](C)[C@H]([C@H](C)[C@H]([C@H]([C@H]/C=C/C(=O)Nc1cc3O)/C=N1CCN(CC1)C)c2O)/C)O)OC(=O)C)OC
C4857	PI	Inhibitor	175	C(#N)C[C@@H]1c2cccc2C(=Nc2cc(ccc12)Cl)C1CCN(CC1)C
C4858	PI	Inhibitor	175	c12c(cc(cc1)F)onc2C1CCN(CCc2c(C)nc3CCCCn3c2=O)CC1
C4859	PI	Inhibitor	175	c1c2c(cc(c1OC)OC)[C@H]1C[C@](C)(CC)[C@H](CC(C)C)CN1CC2
C4860	PI	Inhibitor	175	c1cc(ccc1CC[C@H]1c2cc(c(cc2CCN1)OC)OC)OC
C4861	PI	Inhibitor	175	c1cc(ccc1CC[C@H]1c2cc(c(cc2CCN1)OC)OC)OC
C4862	PI	Inhibitor	175	c1cc(ccc1C)CC[C@@H]1c2cc(c(cc2CCN1)OC)OC
C4863	PI	Inhibitor	175	c1cc(ccc1CC[C@H]1c2cc(c(cc2CCN1)OC)OC)O
C4864	PI	Inhibitor	175	c1cc(c(cc1CC[C@H]1c2cc(c(cc2CCN1)OC)OC)OC)OC
C4865	PI	Inhibitor	175	c1cc2c(c(c1)C(=O)Nc1ccc(cc1)CCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)F
C4866	PI	Inhibitor	175	c1cc2c(cc1CC[C@@H]1c3cc(c(cc3CCN1)OC)OC)OCO2
C4867	PI	Inhibitor	175	c1cc(ccc1CC)CC[C@H]1c2cc(c(cc2CCN1)OC)OC
C4868	PI	Inhibitor	175	c1cc(ccc1)C1CCN(CC1)CCCN1C(=O)[C@](c2cccc2)(c2ccc(cc2)OC)NC1=O
C4869	PI	Inhibitor	175	C1(=N)OCCOC[C@@H](C)C[C@@](C)[C@@H](C)C[C@@H](C(=O)O[C@H](CC)[C@](C)([C@@H]([C@H]1C)O)OC)OC1[C@](C)([C@H](C)O1)OC)OC1[C@@H]([C@H](C)[C@@H](C)O1)N(C)O)O
C4870	PI	Inhibitor	175	c1cc(ccc1C(c1ccc(cc1)F)CNC1CCN(Cc2nc(nc(n2)NCC=C)NCC=C)CC1)F
C4871	PI	Inhibitor	175	c1ccc(c(c1)N1CCN(C[C@@H](COc2cc3c(cc2)N(C(=O)C3)O)CC1)OC
C4872	PI	Inhibitor	175	c1ccc(c(c1)N1CCN(C[C@H](COc2cc3c(cc2)NC(=O)CC3)O)CC1)OC
C4873	PI	Inhibitor	175	c12c(cccc1)c(c1cccc1O)nc(c2)N1CCN(CCCC(=O)c2ccc(cc2)F)CC1
C4874	PI	Inhibitor	175	c12c(cccc1)c(c1cccc1OC)nc(c2)N1CCN(CCCC(=O)c2ccc(cc2)F)CC1



C4921	PI	Inhibitor	175	c1ccc(cc1)C(=O)O[C@H]1[C@@]2([C@@]3([C@H](C)C[C@H]([C@@H]2OC(=O)C)OC(=O)C)[C@@H]([C@H](C)C)O3)[C@@H]1OC(=O)c1ccccc1)OC(=O)C)COC(=O)C
C4922	PI	Inhibitor	175	c1ccc(cc1)C(=O)O[C@H]1[C@@]2(C)[C@@]3([C@@]([C@H](C)C[C@H]1OC(=O)C)O)[C@H]([C@H](C)C)O3)[C@@H]([C@H]2OC(=O)c1ccccc1)OC(=O)c1ccccc1)OC(=O)C
C4923	PI	Inhibitor	175	c1ccc(cc1)C(=O)O[C@H]1[C@@]2(C)[C@@]3([C@@]([C@H](C)C[C@H]([C@@H]2OC(=O)c2ccccc2)OC(=O)c2ccccc2)O)[C@@H]([C@H](C)C)O3)[C@@H]1O)OC(=O)C
C4924	PI	Inhibitor	175	c1ccc(cc1)C(=O)O[C@H]1C(=O)[C@H]2C(C)O[C@@]3([C@@]1([C@@H]([C@H](C)C[C@@]3(C)O)OC(=O)c1ccccc1)OC(=O)c1ccccc1)COC(=O)C)[C@H]2OC(=O)C
C4925	PI	Inhibitor	175	c1ccc(cc1)[C@](c1ccc(cc1)C1)(C)OCCN1CCCCC1
C4926	PI	Inhibitor	175	c1cc(c(cc1[C@@H]1C(CO)O)c2ccc(cc2O1)[C@@H]1[C@H](C(=O)c2c(ccc2O1)O)O)O)OC)O
C4927	PI	Inhibitor	175	c1cc(c(cc1CCC)OC)OCC(=O)N1CCN(C(=O)CO)c2ccc(cc2OC)CCC)CC1
C4928	PI	Inhibitor	175	c1=C=C=C(C)[C@H](C)[C@@H]2CC[C@H](C)[C@](C(=O)C)N3[C@H](C(=O)O)[C@H](C)C[C@@H](C=C1)C)OC)O)[C@H](C)C[C@@H]1CC[C@H]([C@@H](C)OC)O)CCCC3)O)O2)OC
C4929	PI	Inhibitor	175	c12c(cc3c(c1)OCO3)[nH]cc2CCN1CCN(c2cccc2OC)CC1
C4930	PI	Inhibitor	175	c1cc2c(c(c1)C(=O)Nc1ccc(cc1OC)OCCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)C
C4931	PI	Inhibitor	175	c1ccc(cc1)N1C2(C(=O)NC1)CCN(CC2)CCCOc1ccc(cc1)F
C4932	PI	Inhibitor	175	c1ccc(cc1)N1C2(C(=O)NC1)CCN(CC/C=C/c1ccc(cc1)F)\C)CC2
C4933	PI	Inhibitor	175	c12c(cc(cc1OC)[nH]c1c2CCN2[C@H]1C[C@@H]1[C@@H](C(=O)OC)[C@@H](C(C[C@H]1C2)OC(=O)c1cc(c(c1)OC)OC(=O)OCC)OC)OC
C4934	PI	Inhibitor	175	C(#N)[C@](c1ccccc1)C(F)(F)F(CCCN(CCCc1ccc(c(c1)OC)OC)C)C(C)C
C4935	PI	Inhibitor	175	c1cc(c(c(c1OC)OC)OC)C(=O)OCCCCCCCCN(CC)CC
C4936	PI	Inhibitor	175	C=CC[C@@H]1C=C(C)C[C@H](C)CC([C@@H]2[C@H](C)[C@@H](C)[C@@H](C(=O)C(=O)N3[C@H](C(=O)O)[C@H](C=C/C4CC[C@H](C4)OC)O)C)[C@H](C)[C@H](CC1=O)O)CCCC3)O)O2)OC)OC
C4937	PI	Inhibitor	175	c1ccc(cc1)[C@@H]1c2ccc(cc2[C@@H](C1)N1CCN(CC1)CCO)C(F)F)F
C4938	PI	Inhibitor	175	[C@@H]1(C(=O)C[C@H](C)[C@@]2(C)[C@@H]([C@H](C(=O)[C@H](C)C[C@](C)[C@@H]([C@H](C1=O)C)OC1[C@@H]([C@H](C)[C@@H](C)O1)N(C)O)OC)N(C(=O)O2)CCCCn1cc(c2ccccc2)nc1)C
C4939	PI	Inhibitor	175	c1cc2c(c(c1)C(=O)Nc1ccc(cc1OC)CCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)F
C4940	PI	Inhibitor	175	c1cc(cc(c1[C@@]1(Cn2en2)OC[C@H](CO)c2ccc(cc2)N2CCN(C(C)C)CC2)O1)Cl)Cl
C4941	PI	Inhibitor	175	c1ccc(cc1)C(c1ccccc1)C[C@@H](C)NC(C)C)C
C4942	PI	Inhibitor	175	c1ccc(cc1C(C)C)OCCCCCN1CCN(c2ccc(c(c2)Cl)C)CC1
C4943	PI	Inhibitor	175	c1ccc2c(c1)[C@@H](C([C@H](C)N2)OC(=O)c1ccc(cc1)C)N1CCCC1
C4944	PI	Inhibitor	175	c1ccc2c(c1)[C@@H](C([C@H](C)N2)OC(=O)c1ccc(cc1)C)N[C@H](C)CCCN(CC)CC
C4945	PI	Inhibitor	175	c1ccc(cc2c1Cc1c(ccs1)C(=N2)C1CCN(CC1)C)Cl
C4946	PI	Inhibitor	175	c12C=C3/C(=O)[C@](C(=N3)/C=c3/cc(/c(=C/C4=N/C=C/c(c1)C)[nH]2)/[C@@](C4=O)C)C1[C@@H](C[C@H](C)C)O1)OC(=O)C)/[nH]3)C(C)[C@H]1[C@@H](C[C@H](C)C)O1)OC(=O)C
C4947	PI	Inhibitor	175	c1ccc(c(c1)C)N1CCN(CCCO)c2cccn2)CC1
C4948	PI	Inhibitor	175	c1cc2c(c(c1)C(=O)Nc1ccc(cc1)CCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1c(ccc1OC)OC)c2=O
C4949	PI	Inhibitor	175	c1ccc(cc1C(c1ccc(cc1)F)NC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)F
C4950	PI	Inhibitor	175	c1ccc(cc1C(c1ccc(cc1)F)N(C1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)CC)F
C4951	PI	Inhibitor	175	c1ccc(cc1C(c1ccc(cc1)F)N(C1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)CC=C)F
C4952	PI	Inhibitor	175	c1ccc(cc1C(c1ccc(cc1)F)NC1CCN(c2nc(nc(n2)NCCC)NCC=C)CC1)F
C4953	PI	Inhibitor	175	c1ccc(c(c1)C)[C@H](c1ccc(cc1)OC)OC)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C4954	PI	Inhibitor	175	c1ccc(cc1[C@H](C1CCCC1)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)F
C4955	PI	Inhibitor	175	c1ccc2c(c1)C(c1ccccc1O2)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C4956	PI	Inhibitor	175	c1ccc2c(c1)[C@H](c1ccccc1OC2)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C4957	PI	Inhibitor	175	c1ccc(cc(c1)Cl)CN1C(=O)N[C@H](N(Cc2cccc(c2)Cl)CC1)SC
C4958	PI	Inhibitor	175	c1ccc2c(c1)c(=O)c1ccc(c1n2C)C(=O)Nc1ccc(cc1)CCN(Cc1ccc(c(c1)OC)OC)C
C4959	PI	Inhibitor	175	c1ccc2c(c1)[C@H](c1ccc(cc1S(=O)(=O)N2C)Cl)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C4960	PI	Inhibitor	175	c1ccc2c(c1)CCc1ccccc1C2CNC1CCN(c2nc(nc(n2)Cl)NCC=C)CC1
C4961	PI	Inhibitor	175	c1ccc2c(c1)CCc1ccccc1C2CNC1CCN(c2nc(nc(n2)OC)NCC=C)CC1
C4962	PI	Inhibitor	175	c1ccc2c(c1)CCc1ccc(cc1)[C@H]2CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)OC
C4963	PI	Inhibitor	175	c1ccc(cc1C(c1ccc(cc1)F)N1CCN(CC1)Nc1nc(nc(n1)NCC=C)NCC=C)F
C4964	PI	Inhibitor	175	c1ccc2c(c1)CCc1ccccc1C2C(=O)NN1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C4965	PI	Inhibitor	175	c1ccc(cc(c1)C(F)(F)F)C1(CCN(CCCC(=O)c2ccc(cc2)F)CC1)O
C4966	PI	Inhibitor	175	c1ccc(cc1)[C@](CC)(COC(=O)c1ccc(c(c1)OC)OC)OC)N(C)C



C5013	PI	Inhibitor	175	<chem>c1ccc(cc1)CN1CCN([C@H]2c3cccc3N(C(=O)c3ccc(cc3)C)[C@@H](C)[C@@H]2O)CC1</chem>
C5014	PI	Inhibitor	175	<chem>c1ccc2c(c1)[C@@H]([C@H]([C@H](C)N2C(=O)c1ccc(cc1)C)O)N[C@H](C)CCCN(CC)CC</chem>
C5015	PI	Inhibitor	175	<chem>c1ccc(cc1)CN[C@H]1c2cccc2N(C(=O)c2ccc(cc2)C)[C@@H](C)[C@@H]1O</chem>
C5016	PI	Inhibitor	175	<chem>c12c(cccc1)[nH]c1c2CCN2[C@H]1C[C@H]1[C@H](C(=O)OC)[C@H](CC[C@H]1C2)O</chem>
C5017	PI	Inhibitor	175	<chem>C1=C2CC[C@H]3[C@@H]4CC[C@H]([C@@]4C)CC[C@H]3[C@@]2(C)CCC1=O)O</chem>
C5018	PI	Inhibitor	175	<chem>C1(=O)CC[C@H]2[C@H]3CC[C@H]4C[C@@H](CC[C@]4(C)[C@H]3CC[C@@]12C)O</chem>
C5019	PI	Inhibitor	175	<chem>c12c(c(nc(n2)N(CCO)CCO)N2CCCC2)nc(nc1N1CCCC1)N(CCO)CCO</chem>
C5020	PI	Inhibitor	175	<chem>c1cc2c(c(e1)C(=O)Nc1ccc(cc1)CCCN(Cc1ccc(c(e1)OC)OC)C)[nH]c1ccc(cc1e2=O)OC</chem>
C5021	PI	Inhibitor	175	<chem>c12c(c(nc(n2)N2CCCC2)N2CCCC2)nc(nc1N1CCCC1)N(CCO)CCO</chem>
C5022	PI	Inhibitor	175	<chem>c12c(c(nc(n2)N2CCN(CC2)C)N2CCCC2)nc(nc1N1CCCC1)N(CCO)CCO</chem>
C5023	PI	Inhibitor	175	<chem>c12c(c(ncn2)N2CCCC2)nc(nc1N1CCCC1)N(CCO)CCO</chem>
C5024	PI	Inhibitor	175	<chem>c12c(c(nc(n2)N(CCO)CCO)N2c3cccc3CCC2)nc(nc1N1c2cccc2CCC1)N(CCO)CCO</chem>
C5025	PI	Inhibitor	175	<chem>c12c(c(nc(n2)N2CCCC2)N(CCO)CCO)nc(nc1N(CCO)CCO)N1CCCC1</chem>
C5026	PI	Inhibitor	175	<chem>c12c(nc(c3cccc3n2)N2CCCC2)nc(nc1N(CCO)CCO)N1CCCC1</chem>
C5027	PI	Inhibitor	175	<chem>c1ccc(cc1)[C@](CCN1CCCC1)(C1CCCC1)O</chem>
C5028	PI	Inhibitor	175	<chem>C(#N)c1c([nH]nc1/C(=C\c1cc(c(e1)C(C)C)O)C(C)C)/C#N)N</chem>
C5029	PI	Inhibitor	175	<chem>c1ccc(cc1)C(c1cc(c(e1)CN1CCCC1)O)CN1CCCC1)C</chem>
C5030	PI	Inhibitor	175	<chem>c1ccc(cc1)CN1[C@H](c2nc3cccc3e(=O)n2[C@@H]1c1ccc(c(e1)O)O)C</chem>
C5031	PI	Inhibitor	175	<chem>c1cc2c(c(e1)C(=O)Nc1ccc(cc1)CCN1Cc3cc(c(cc3CC1)OC)OC)[nH]c1c(cccc1F)c2=O</chem>
C5032	PI	Inhibitor	175	<chem>c1ccc(c(e1)C)N1CCN([C@H]2Cc3ccc(cc3CC2)O)CC1</chem>
C5033	PI	Inhibitor	175	<chem>c1cc(cc2c1C[C@@H]1[C@@H](C)[C@@]2(C)CCN1CC=C(C)C)O</chem>
C5034	PI	Inhibitor	175	<chem>c1cc(ccc1/C(=C/c1ccc(cc1)O)/CC)/CCO</chem>
C5035	PI	Inhibitor	175	<chem>c1ccc(cc1)CN(CCOC(=O)C1=C(C)NC(=C([C@@H]1c1cccc(c1)[N+](=O)[O-])[P@@](=O)N(C)C)OCC)C</chem>
C5036	PI	Inhibitor	175	<chem>c1ccc(cc1)CN(c1cccc1)CCOC(=O)C1=C(C)NC(=C([C@@H]1c1cccc(c1)[N+](=O)[O-])P1(=O)OCC(C)C)CO1C</chem>
C5037	PI	Inhibitor	175	<chem>c1ccc(cc1)CN(c1cccc1)[C@]1(C)[C@H](C(=O)O)[C@H](c2cccc(c2CC)[N+](=O)[O-])C(=C(N)CCN1CCOCC1)P1(=O)OCC(C)C)CO1</chem>
C5038	PI	Inhibitor	175	<chem>c1ccc(cc1)[C@H]1[C@H](CCCN1)Nc1cc(ccc1OC)N(C)S(=O)C</chem>
C5039	PI	Inhibitor	175	<chem>c1ccc(cc1)C[C@@H]([C@H](CN(CC(C)C)S(=O)(=O)c1ccc(cc1)N)O)NC(=O)O[C@H]1CCOC1</chem>
C5040	PI	Inhibitor	175	<chem>c1ccc(cc1)OCCCN(CCN(CCCOc1cccc1)S(=O)(=O)c1cccc1)S(=O)(=O)c1cccc1</chem>
C5041	PI	Inhibitor	175	<chem>c1ccc2c(c1)CCc1cccc1C12c2cccc2CN1C</chem>
C5042	PI	Inhibitor	175	<chem>c12c(ccc(c1)NS(=O)(=O)C)[nH]c(c2)C(=O)N1CCN(c2cc(cen2)NC(C)C)CC1</chem>
C5043	PI	Inhibitor	175	<chem>c1ccc(cc1)CC[C@H](/C=C/S(=O)(=O)c1cccc1)NC(=O)[C@H](Cc1cccc1)NC(=O)N1CCOCC1</chem>
C5044	PI	Inhibitor	175	<chem>c12c(cc(cc1)OC)nc([nH]2)[S@](=O)Cc1c(c(en1)C)OC)C</chem>
C5045	PI	Inhibitor	175	<chem>c12c(cccc2)c(ccc1)N(C(=S)Sc1nc2c(cccc2)o1)C</chem>
C5046	PI	Inhibitor	175	<chem>c1cc(ccc1C)S[C@H](c1ccc(c(e1)OCCc1cnc[nH]1)OC)CCCCCN1Cc2cc(c(cc2CC1)OC)OC</chem>
C5047	PI	Inhibitor	175	<chem>c1cc(c(e1)[C@@H](CCCCN1Cc2cc(c(cc2CC1)OC)OC)SC1CCCC1)OC)OC</chem>
C5048	PI	Inhibitor	175	<chem>c1cc(c(e1)[C@@H](CCCCN1Cc2cc(c(cc2CC1)OC)OC)SCCCCC)OC)OC</chem>
C5049	PI	Inhibitor	175	<chem>c1cc(ccc1C)S[C@H](c1ccc(c(e1)OC)OC)CCCCCN1Cc2cc(c(cc2CC1)OC)OC</chem>
C5050	PI	Inhibitor	175	<chem>c1cc(ccc1C)S[C@H](c1ccc2c(c1)OCO2)CCCCCN1Cc2cc(c(cc2CC1)OC)OC</chem>
C5051	PI	Inhibitor	175	<chem>c1ccc(cc1)C(c1cccc1)SC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1</chem>
C5052	PI	Inhibitor	175	<chem>c1cc(ccc1C(c1cccc1)F)N1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)F</chem>
C5053	PI	Inhibitor	175	<chem>C(=C(C)C)CC/C(=C/CC/C(=C/CC/C(=C/CSC[C@@H](C(=O)OC)N)/C)/C</chem>
C5054	PI	Inhibitor	175	<chem>C(=C(C)C)CC/C(=C/CC/C(=C/CSC[C@@H](C(=O)N)NC(=O)C)/C</chem>
C5055	PI	Inhibitor	175	<chem>C(=C(C)C)CC/C(=C/CC/C(=C/CSC[C@@H](C(=O)NC)NC(=O)C)/C</chem>
C5056	PI	Inhibitor	175	<chem>C(=C(C)C)CC/C(=C/CC/C(=C/CSC[C@@H](C(=O)OC)NC(=O)C)/C</chem>
C5057	PI	Inhibitor	175	<chem>c1ccc(cc1)SC[C@H]([C@@H](CN1[C@H](C(=O)NC(C)C)C)[C@H]2CCCC[C@H]2C1)O)NC(=O)c1cccc(c1)C</chem>
C5058	PI	Inhibitor	175	<chem>c1ccc2c(c1)c(=O)n(c(=O)[nH]2)CCCCN1CCN(c2cccc2S)CC1</chem>

C5059	PI	Inhibitor	175	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)SCCCN(Cc1ccc(c1)OC)OC)C
C5060	PI	Inhibitor	175	c12c(nc(c(n2)SCc2ccccc2)N(C)C)nc(nc1N(C)C)N1CCNCC1
C5061	PI	Inhibitor	175	c12c(c(ncn2)SCc2ccccc2)nc(nc1N1CCOCC1)N1CCNCC1
C5062	PI	Inhibitor	175	C(#N)[C@@](c1ccc(c1)OC)OC)(CCCCCCCCN1Cc2cc(c(cc2CC1)OC)OC)Sc1ccc(cc1)C
C5063	PI	Inhibitor	175	c1cc(ccc1CN1C(=O)N[C@H](N(Cc2ccc(cc2)C1)CC1)SC)C1
C5064	PI	Inhibitor	175	c12c(cc(c1)OC)OC)[nH]c(c2CCN1CCN(c2ccccc2)CC1)C(=O)OCC
C5065	PI	Inhibitor	175	C(#N)[C@@](c1ccc(c1)OC)OC)(CCCCCN1Cc2cc(c(cc2CC1)OC)OC)Sc1ccc(cc1)C
C5066	PI	Inhibitor	175	C(#N)[C@@](c1ccc(c1)OC)OC)(CCCCCN1Cc2cc(c(cc2CC1)OC)OC)SC1CCCCC1
C5067	PI	Inhibitor	175	C(#N)[C@](c1ccc(c1)OC)OC)(CCCCCN1Cc2cc(c(cc2CC1)OC)OC)Sc1ccc(cc1)C
C5068	PI	Inhibitor	175	C(#N)[C@@](c1ccc(c1)OC)OC)(CCCCCN1Cc2cc(c(cc2C1)OC)OC)SC1CCCCC1
C5069	PI	Inhibitor	175	C(#N)[C@](c1ccc(c1)OC)OC)(CCCCCN1Cc2cc(c(cc2C1)OC)OC)Sc1ccc(cc1)C
C5070	PI	Inhibitor	175	c1ccc(cc1)C1(CCCN(CCc2ccc(c2)OC)OC)C)S(=O)(=O)CCCS1(=O)=O
C5071	PI	Inhibitor	175	c1ccc(cc1)NC(=O)OCCN(C(=O)N1c2ccccc2Sc2ccc(cc12)OC)CCOC(=O)Nc1ccccc1
C5072	PI	Inhibitor	175	c1ccc(c1)CC=C)OC[C@@H](CNC(C)C)O
C5073	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)C)[C@@H](C)CN(C)C
C5074	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)OC)C[C@@H](C)CN(C)C
C5075	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)OC)C[C@@H](C)CN1CCC(CC1)O
C5076	PI	Inhibitor	175	c1ccc2c(c1)N(c1ccccc1S2)C[C@@H](C)CN1CCN(CC1)CCOCCO
C5077	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)C)C[C@@H](C)N(C)C
C5078	PI	Inhibitor	175	c1ccc2c(c1)N(c1ccccc1S2)C[C@@H](C)N(C)C
C5079	PI	Inhibitor	175	c1ccc2c(c1)N(c1ccccc1S2)C[C@@H]1C2CCN(CC2)C1
C5080	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)S(=O)(=O)C)CC[C@@H]1CCCCN1C
C5081	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)[S@](=O)C)CC[C@@H]1CCCCN1C
C5082	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)SC)CC[C@@H]1CCCCN1C
C5083	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)C)CCCN(C)C
C5084	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)C)CCCN1CCC(C(=O)c2ccc(cc2)F)CC1
C5085	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)C(F)(F)F)CCCN1CCC(C(=O)c2ccc(cc2)F)CC1
C5086	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)C(F)(F)F)CCCN1CCN(C2CC2)CC1
C5087	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)S(=O)(=O)N(C)C)CCCN1CCN(CC1)C
C5088	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)CCC)CCCN1CCN(CC1)C
C5089	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)C(F)(F)F)CCCN1CCN(C2CC2)CC1
C5090	PI	Inhibitor	175	c1ccc2c(c1)C(=CCCN(C)C)c1ccccc1CC2
C5091	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)C)CCCN1CCN(CC1)CCO
C5092	PI	Inhibitor	175	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)CC)CCCN1CCN(CC1)CCO
C5093	PI	Inhibitor	175	c1ccc2c(c1)N(c1ccccc1S2)CCN1CCCC1
C5094	PI	Inhibitor	175	c1cc(c2c(c1)Sc1ccccc1N2)C(=O)Nc1ccc(cc1)OCCN(CCc1ccc(c1)OC)OC)C
C5095	PI	Inhibitor	175	c1ccc2c(c1)C(=C/CCN1CCN(CC1)C)/c1cc(ccc1S2)S(=O)(=O)N(C)C
C5096	PI	Inhibitor	175	C(#N)c1ccc2c(c1)C1=C(c3ccccc3S2)CCN(CC1)C
C5097	PI	Inhibitor	175	c1ccc2c(c1)N=C(c1cc(ccc1S2)C)N1CCN(CC1)C
C5098	PI	Inhibitor	175	c1ccc2c(c1)C(=C1CCN(CC1)C)c1ccccc1S2
C5099	PI	Inhibitor	175	c1ccc(c1)[C@H]1C(=C(C)NC(=C1C(=O)OCC)COCCN)C(=O)OC)C1
C5100	PI	Inhibitor	175	c1ccc2c(c1)c(=O)c1cccc(c1s2)C(=O)Nc1ccc(cc1)OCCN(CCc1ccc(c1)OC)OC)C
C5101	PI	Inhibitor	175	c1cc2c(cc1C(F)(F)F)/C(=C/CCN1CCN(CC1)CCO)/c1ccc(cc1S2)F
C5102	PI	Inhibitor	175	C(#N)[C@H]1C(=S)N(C(=C(C(=O)C)[C@@H]1c1ccc(cc1)OC)c1ccccc1)C1[C@@H]([C@H]([C@@H]([C@@H](COC(=O)C)O1)OC(=O)C)OC(=O)C)OC(=O)C
C5103	PI	Inhibitor	175	C(#N)[C@H]1C(=S)N(C(=C[C@@H]1c1ccccc1)c1ccccc1)C1[C@@H]([C@H]([C@@H]([C@@H](COC(=O)C)O1)OC(=O)C)OC(=O)C)OC(=O)C
C5104	PI	Inhibitor	175	C(#N)[C@H]1C(=S)N(C(=C[C@@H]1c1ccccc1)c1ccccc1)C1[C@@H]([C@H]([C@@H]([C@@H](COC(=O)C)O1)OC(=O)C)OC(=O)C)OC(=O)C



C5105	PI	Inhibitor	175	C(#N)c1c(c2ccc(cc2)OC)c2c(CC(C)(C)CC2=O)n(c1=S)C1[C@@H]([C@H]([C@@H]([C@@H](COC(=O)C)O1)OC(=O)C)OC(=O)C)OC(=O)C
C5106	PI	Inhibitor	175	c1cc(c(cc1CN1C(=S)NC(=S)N(Cc2ccc(c(c2)OC)OC)CC1)OC)OC
C5107	PI	Inhibitor	175	c1cc(ccc1[N+](=O)[O-])OP(=S)(OC)OC
C5108	PI	Inhibitor	175	c1ccc2c(c1)CCC1=C(C[Cl+][C=C]1)N2CCCN(C)C
C5109	PI	Inhibitor	175	c12e3c(ccc1)CCc1ccccc1n3cc2CN(Cc1ccccc1)C
C5110	PI	Inhibitor	175	c1cc(ccc1C(=C(c1ccc(cc1)OC)CN(C)C)c1ccc(cc1)OC)OC
C5111	PI	Inhibitor	175	c12c(nc(nc1N1CCC(CC1)NCC1c3ccccc3CCc3ccccc13)NCC=C)n(en2)CC=C
C5112	PI	Inhibitor	175	c12een(c1nc(nc2NCC=C)N1CCC(CC1)NCC1c2ccccc2CCc2ccccc12)CC=C
C5113	PI	Inhibitor	175	c12c(nc(nc1NCC=C)N1CCC(CC1)NCC(c1ccccc1)c1ccccc1)n(en2)CC=C
C5114	PI	Inhibitor	175	c12c(nc(nc1NCC=C)N1CCC(CC1)NCC1c3ccccc3CCc3ccccc13)n(en2)CC=C
C5115	PI	Inhibitor	175	c12c(nc(nc1NCC=C)N1CCC(CC1)NCC1c3ccccc3CCc3ccccc13)n(en2)CCC
C5116	PI	Inhibitor	175	c12c(cccc2)c(ccc1)CNC1CCN(c2nc3c(c(n2)NCC=C)nen3CC=C)CC1
C5117	PI	Inhibitor	175	c12c(nc(nc1NCCC)N1CCC(CC1)NCC1c3ccccc3CCc3ccccc13)n(en2)CCC
C5118	PI	Inhibitor	175	c1ccc(cc1)C(c1ccccc1)N1CCN(CC1)/N=C/c1ccc(C)n1
C5119	PI	Inhibitor	175	c1ccc2c(c1)CCc1ccccc1C2CNC1CCN(c2nc(nc(n2)N(C)C)N(C)C)CC1
C5120	PI	Inhibitor	175	c1ccc2c(c1)CCc1ccccc1C2CNC1CCN(c2nc(nc(n2)NCC=C)NCC)CC1
C5121	PI	Inhibitor	175	c1ccc(cc1)C(c1ccccc1)CN(C1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)C
C5122	PI	Inhibitor	175	c1ccc(cc1)C(c1ccccc1)NC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C5123	PI	Inhibitor	175	c1ccc2c(c1)CCc1ccccc1C2NC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C5124	PI	Inhibitor	175	c1cc(c(c(c1)C)C(c1c(cccc1C)C)C)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)C
C5125	PI	Inhibitor	175	c1ccc(cc1)C(c1ccccc1)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C5126	PI	Inhibitor	175	c1ccc2c(c1)[C@H]1c3ccccc3[C@]2(CC1)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C5127	PI	Inhibitor	175	c1ccc2c(c1)c1ccccc1C2CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C5128	PI	Inhibitor	175	c1ccc2c(c1)C=Cc1ccccc1C2CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C5129	PI	Inhibitor	175	c1ccc2c(c1)CCc1ccccc1C2CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C5130	PI	Inhibitor	175	c1ccc(cc1)C(c1ccccc1)CCNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C5131	PI	Inhibitor	175	c1cc(ccc1C(c1ccc(cc1)F)CCCN1CCN(C(=O)NCC)CC1)F
C5132	PI	Inhibitor	175	c1ccc2c(c1)CCc1ccccc1C2CN1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C5133	PI	Inhibitor	175	c1ccc2c(c1)CCc1ccccc1C2CNN1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C5134	PI	Inhibitor	175	c1ccc(cc1)C(c1ccccc1)CNC1CCN(c2nc(nc(n2)NCCC)NCC=C)CC1
C5135	PI	Inhibitor	175	c1ccc2c(c1)CCc1ccccc1C2CNC1CCN(c2nc(nc(n2)NCCC)NCC=C)CC1
C5136	PI	Inhibitor	175	c1ccc(cc1)C(c1ccccc1)CCNC1CCN(c2nc(nc(n2)NCCC)NCC=C)CC1
C5137	PI	Inhibitor	175	c1ccc(cc1)C1=Ne2ccenc2N(c2ccccc12)CCCN(C)C
C5138	PI	Inhibitor	175	c12c(ccc(c1)CN1CCN(C(c3ccccc3)c3ccccc3)CC1)n(c(CCCC)n2)CC
C5139	PI	Inhibitor	175	c1ccnc(c1)/C(=C/CN1CCCC1)/c1ccc(cc1)C
C5140	PI	Inhibitor	175	c1ccc2c(c1)C(=C(C2)CCN(C)C)[C@H](c1ccccc1)C
C5141	PI	Inhibitor	175	c1ccc(cc1)c1ccc(cc1)[C@H](c1ccccc1)n1ccn1
C5142	PI	Inhibitor	175	C1=C2CC(=O)CC[C@]2(C)[C@H]2CC[C@]3(C(=O)CC[C@H]3[C@H]2C1)C
C5143	PI	Inhibitor	175	c12c(c(ccc1)CC)oc(e2)[C@H](CNC(C)(C)C)O
C5144	PI	Inhibitor	175	c12c(cccc1)oc(e2CCc1ccccc1)C(=O)CN1CCN(c2ccccc2OC)CC1
C5145	PI	Inhibitor	175	c12c(cccc1)oc(e2CCc1ccccc1)[C@H](CN1CCN(c2ccccc2OC)CC1)O
C5146	PI	Inhibitor	175	c12c(cccc1)oc(e2CCc1ccccc1)CCNC(C)C
C5147	PI	Inhibitor	175	c1ccc(cc1)C(c1ccccc1)Cc1nc(CCN2CCCCC2)on1
C5148	PI	Inhibitor	175	c12c(c(ccc1)[C@H]1C(=C(C)NC(=C1C(=O)OC(C)C)C(=O)OC)non2
C5149	PI	Inhibitor	175	c12c(c(ccc1)C1C(=C(C)NC(=C1C(=O)OCC)C)C(=O)OCC)non2
C5150	PI	Inhibitor	175	c1ccc2c(c1)C(=C1CCN(CC1)C)c1ccse1CC2









C5335	PI	Noninhibitor	175	c1ccc(c(c1)c1ccc(cc1)Cn1c(c(nc1CCCC)Cl)CO)c1n[nH]nn1
C5336	PI	Noninhibitor	175	C1=C[C@H](C)C(CC[C@H])(C[C@H](CC(=O)O)O)[C@@H]2C1=CC(C)CC2OC(=O)[C@@H](C)CC
C5337	PI	Noninhibitor	175	c1cc(c(cc1c1cc(=O)c2c(cc2o1)O)O)OC1[C@@H](C([C@@H](C(CO)O1)O)O)
C5338	PI	Noninhibitor	175	c1ccc(cc1)C1(c2ccccc2)C(=O)N(C(=O)N1)CC(=O)O
C5339	PI	Noninhibitor	175	c1ccc(cc1)C1(c2ccccc2)C(=O)N(C(=O)N1)CCC(=O)O
C5340	PI	Noninhibitor	175	c1ccc(cc1)C1(c2ccccc2)C(=O)N(CC(=O)O)[C@H](C)N1
C5341	PI	Noninhibitor	175	c12c(cc2)Cl)nc(cc1)/C=C/c1ccc(c1)[C@H](SCCC(=O)N(CC)CC)SCCC(=O)O
C5342	PI	Noninhibitor	175	c1ccc2c(c1)C1=C(c3ccccc3O2)CCN(CC1)C
C5343	PI	Noninhibitor	175	c1ccc(cc1)[C@](c1ccc(cc1)Cl)(C)O[C@H](C)CN(C)C
C5344	PI	Noninhibitor	175	c1cc(ccc1C(=O)O)CCNC(=O)c1cc(ccc1OC)Cl
C5345	PI	Noninhibitor	175	c1ccc2c(c1)C(=NCC2)COc1ccc(cc1)OC
C5346	PI	Noninhibitor	175	c1ccc(cc1)CC(C)(C)NC
C5347	PI	Noninhibitor	175	C(=O)(N)OCC(C)(CCC)COC(=O)N
C5348	PI	Noninhibitor	175	c1cc(ccc1C(c1ccc(cc1)OC)C(Cl)(Cl)Cl)OC
C5349	PI	Noninhibitor	175	C(=O)(C)OCCOC
C5350	PI	Noninhibitor	175	c1c(c(cc1Cl)N)OC)C(=O)NCCN(CC)CC
C5351	PI	Noninhibitor	175	c1cc(c(c1)C)OC[C@@H](C)N)C
C5352	PI	Noninhibitor	175	c1(c(nc1c1)NC)N1CCN(CC1)C)SC
C5353	PI	Noninhibitor	175	c1ccc2c(c1)Cc1ccccc1N1[C@H]2CN(CC1)C
C5354	PI	Noninhibitor	175	c1cc(cc1[C@H](Cn1ccnc1)OCc1ccc(cc1Cl)Cl)Cl
C5355	PI	Noninhibitor	175	C12(C3(C4(C5(C(C1(C4(Cl)Cl)Cl)(C2(C(C35Cl)(Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl
C5356	PI	Noninhibitor	175	C1(=C(C(=O)C2=C(C1=O)N1[C@@]([C@@H]2COC(=O)N)([C@@H]2[C@H](C1)N2)OC)N)
C5357	PI	Noninhibitor	175	c1cc(c(cc1CC=N/C1/CCCN1C)OC)OC
C5358	PI	Noninhibitor	174	O[C@H](COc1ccc(cc1)NC(=O)C)CNC(C)C
C5359	PI	Inhibitor	174	COc1ccc(CCN(C)CC#CCN2C(=O)[C@H]3[C@H](C4c5ccccc5C3c3ccccc43)C2=O)cc1OC
C5360	PI	Inhibitor	174	COc1ccc(CCN(C)CCCN2C(=O)[C@H]3[C@H](C4c5ccccc5C3c3ccccc43)C2=O)cc1OC
C5361	PI	Inhibitor	174	COc1ccc(CCN(C)CCN2C(=O)[C@H]3[C@H](C4c5ccccc5C3c3ccccc43)C2=O)cc1OC
C5362	PI	Inhibitor	174	CCCCCCC[C@@H]1[C@@H](C(=O)O[C@H](C(=O)N([C@H](C(CC(=O)O1)OCOC)Cc1ccccc1)C)C(C)C
C5363	PI	Inhibitor	174	CC1COC(=O)C[C@H]([C@@H](N(C(=O)[C@@H](OC1=O)C(C)C)Cc1ccccc1)O
C5364	PI	Inhibitor	174	CC1COC(=O)C[C@H]([C@H](N(C(=O)[C@@H](OC1=O)C(C)C)Cc1ccccc1)OCOC
C5365	PI	Inhibitor	174	CCCCCCC[C@@H]1[C@@H](C(=O)O[C@H](C(=O)N([C@H](CCC(=O)O1)Cc1ccccc1)C)C(C)C
C5366	PI	Inhibitor	174	CCCCCCC[C@@H]1[C@@H](C(=O)O[C@H](C(=O)N([C@H](C(CC(=O)O1)O)Cc1ccccc1)C)C(C)C
C5367	PI	Inhibitor	174	CCCCCCC[C@@H]1[C@@H](C(=O)OC(C(=O)N([C@H](C(CC(=O)O1)O)Cc1ccccc1)C)C(C)C
C5368	PI	Inhibitor	174	CCCCCCC[C@@H]1[C@@H](C(=O)OC(C(=O)N([C@H](C(CC(=O)O1)OCOC)Cc1ccccc1)C)C(C)C
C5369	PI	Inhibitor	174	CCCC[C@@H]1[C@@H](C(=O)OCC(=O)N([C@H](C(CC(=O)O1)O)Cc1ccccc1)C)C
C5370	PI	Inhibitor	174	CCCCCCC[C@@H]1[C@@H](C(=O)O[C@H](C(=O)N([C@H](C(CC(=O)O1)O)Cc1ccccc1)C)C(C)C
C5371	PI	Inhibitor	174	CCCC[C@@H]1[C@@H](C(=O)OCC(=O)N([C@H](C(CC(=O)O1)OCOC)Cc1ccccc1)C)C
C5372	PI	Inhibitor	174	CN([C@@H](Cc1ccccc1)[C@@H](CC(=O)OC)OCOC)C(=O)OCc1ccccc1
C5373	PI	Inhibitor	174	CN([C@@H](Cc1ccccc1)[C@@H](CC(=O)OC)O)C(=O)OCc1ccccc1
C5374	PI	Inhibitor	174	CCCCCCC[C@@H]([C@H](C)C(=O)O[C@@H](C(C)C)C(=O)OC)O
C5375	PI	Inhibitor	174	CCCCCCC[C@@H]1[C@@H](C(=O)O[C@H](C(=O)N([C@H](C(CC(=O)O1)OCOC)Cc1ccccc1)C)C(C)C
C5376	PI	Inhibitor	174	CCCCCCC[C@@H]1[C@@H](C(=O)OCC(=O)N([C@H](C(CC(=O)O1)O)Cc1ccccc1)C)C
C5377	PI	Inhibitor	174	CCCCCCC[C@@H]1[C@@H](C(=O)OCC(=O)N([C@H](C(CC(=O)O1)OCOC)Cc1ccccc1)C)C
C5378	PI	Inhibitor	174	CCCCCCCC1CC(=O)O[C@H](C(=O)N([C@H](C(CC(=O)O1)O)Cc1ccccc1)C)C(C)C
C5379	PI	Inhibitor	174	CCCCCCCC1CC(=O)O[C@H](C(=O)N([C@H](C(CC(=O)O1)OCOC)Cc1ccccc1)C)C(C)C
C5380	PI	Inhibitor	174	C[C@H]1[C@H](OC(=O)C[C@H]([C@@H](N(C(=O)[C@@H](OC1=O)C(C)C)Cc1ccccc1)O)C

C5381	PI	Inhibitor	174	<chem>C[C@H]1[C@H](OC(=O)C[C@H]([C@@H](N(C(=O)[C@@H](OC1=O)C(C)C)C)Cc1cccc1)OCOC)C</chem>
C5382	PI	Inhibitor	174	<chem>c1ccc2c(c1)c(=O)c1cccc1n2CCCCN1CCCC1</chem>
C5383	PI	Inhibitor	174	<chem>COc1cccc2c1n(c1cccc1c2=O)CCCCN1CCCC1</chem>
C5384	PI	Noninhibitor	174	<chem>O[C@H]1CC[C@H]2CN3CCc4c([nH]c5ccccc45)[C@H]3C[C@@H]2C1C(=O)OC</chem>
C5385	PI	Inhibitor	174	<chem>c1ccc2c(c1)c(=O)c1cccc1n2CCCCN1CCOCC1</chem>
C5386	PI	Inhibitor	174	<chem>COc1cccc2c1n(c1cccc1c2=O)CCCCN1CCOCC1</chem>
C5387	PI	Inhibitor	174	<chem>c1ccc2c(c1)c(=O)c1cccc1n2CCCCN(CCO)CCO</chem>
C5388	PI	Inhibitor	174	<chem>COc1cccc2c1n(c1cccc1c2=O)CCCCN(CCO)CCO</chem>
C5389	PI	Inhibitor	174	<chem>c1ccc2c(c1)c(=O)c1cccc1n2CCCCN1CCN(CC1)CCO</chem>
C5390	PI	Inhibitor	174	<chem>COc1cccc2c1n(c1cccc1c2=O)CCCCN1CCN(CC1)CCO</chem>
C5391	PI	Inhibitor	174	<chem>COc1cccc2c1[nH]c1cccc1c2=O</chem>
C5392	PI	Inhibitor	174	<chem>c1ccc2c(c1)c(=O)c1cccc1n2CCCC1</chem>
C5393	PI	Inhibitor	174	<chem>COc1cccc2c1n(c1cccc1c2=O)CCCC1</chem>
C5394	PI	Inhibitor	174	<chem>CN1CCN(CC1)CCc1c2cccc2c(=O)c2c1ccc2</chem>
C5395	PI	Inhibitor	174	<chem>CN1CCN(CC1)CCc1c2cccc2c(=O)c2c1c(ccc2)OC</chem>
C5396	PI	Inhibitor	174	<chem>c1ccc2c(c1)c(=O)c1cccc1n2CCCN1CCCC1</chem>
C5397	PI	Inhibitor	174	<chem>COc1cccc2c1n(c1cccc1c2=O)CCCN1CCCC1</chem>
C5398	PI	Inhibitor	174	<chem>c1ccc2c(c1)c(=O)c1cccc1n2CCCN1CCOCC1</chem>
C5399	PI	Inhibitor	174	<chem>COc1cccc2c1n(c1cccc1c2=O)CCCN1CCOCC1</chem>
C5400	PI	Inhibitor	174	<chem>c1ccc2c(c1)c(=O)c1cccc1n2CCCN(CCO)CCO</chem>
C5401	PI	Inhibitor	174	<chem>COc1cccc2c1n(c1cccc1c2=O)CCCN(CCO)CCO</chem>
C5402	PI	Inhibitor	174	<chem>c1ccc2c(c1)c(=O)c1cccc1n2CCCN1CCN(CC1)CCO</chem>
C5403	PI	Inhibitor	174	<chem>COc1cccc2c1n(c1cccc1c2=O)CCCN1CCN(CC1)CCO</chem>
C5404	PI	Inhibitor	174	<chem>c1ccc2c(c1)c(=O)c1cccc1n2CCCC1</chem>
C5405	PI	Inhibitor	174	<chem>COc1cccc2c1n(c1cccc1c2=O)CCCC1</chem>
C5406	PI	Inhibitor	174	<chem>CN1CCN(CC1)CCc1c2cccc2c(=O)c2c1ccc2</chem>
C5407	PI	Inhibitor	174	<chem>CN1CCN(CC1)CCc1c2cccc2c(=O)c2c1c(ccc2)OC</chem>
C5408	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)CCC(=O)OC)c1ccc(cc1)N(C)C</chem>
C5409	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C#N)c1ccc(cc1)N(C)C</chem>
C5410	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/COC)c1ccc(cc1)N(C)C</chem>
C5411	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)CCOC)c1ccc(cc1)N(C)C</chem>
C5412	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)C(=O)OC)c1ccc(cc1)N(C)C</chem>
C5413	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)CCCCOC)c1ccc(cc1)N(C)C</chem>
C5414	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)[C@@H]1C[C@@H]1C(=O)OC)c1ccc(cc1)N(C)C</chem>
C5415	PI	Inhibitor	174	<chem>CCCCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C</chem>
C5416	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/COCCOC)c1ccc(cc1)N(C)C</chem>
C5417	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/COCc1cccc1)c1ccc(cc1)N(C)C</chem>
C5418	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/COc1cccc1)c1ccc(cc1)N(C)C</chem>
C5419	PI	Inhibitor	174	<chem>CCN(CC)C(=O)OC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C</chem>
C5420	PI	Inhibitor	174	<chem>CCCCC(=O)OC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C</chem>
C5421	PI	Inhibitor	174	<chem>CN(C)C/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C</chem>
C5422	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/CN1CCCCC1)c1ccc(cc1)N(C)C</chem>
C5423	PI	Inhibitor	174	<chem>CCCCCN1c(c(nc1c1ccc(cc1)C(=O)O)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C</chem>
C5424	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/CN1CCOCC1)c1ccc(cc1)N(C)C</chem>
C5425	PI	Inhibitor	174	<chem>CCCCCN1c(c(nc1c1ccc(cc1)C(=O)OC)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C</chem>
C5426	PI	Inhibitor	174	<chem>CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C(=O)O)c1ccc(cc1)N(C)C</chem>

C5427	PI	Inhibitor	174	CN(C)c1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)N(C)C
C5428	PI	Inhibitor	174	CN(C)c1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)O)c1ccc(cc1)N(C)C
C5429	PI	Inhibitor	174	CN(C)c1ccc(cc1)c1c(n(c(n1)c1ccc(cc1)O)CCc1cccc1)c1ccc(cc1)N(C)C
C5430	PI	Inhibitor	174	CN(C)c1ccc(cc1)c1c(n(c(n1)c1ccc(cc1)C(=O)O)CCc1cccc1)c1ccc(cc1)N(C)C
C5431	PI	Inhibitor	174	CCN(CC)c1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)N
C5432	PI	Inhibitor	174	CNe1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)NC
C5433	PI	Inhibitor	174	CC(C)Ne1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)NC
C5434	PI	Inhibitor	174	CCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C
C5435	PI	Inhibitor	174	CCN(CC)c1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/COCC)c1ccc(cc1)N(CC)CC
C5436	PI	Inhibitor	174	CCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N1CCOCC1)c1ccc(cc1)N1CCOCC1
C5437	PI	Inhibitor	174	CCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)NC)c1ccc(cc1)N(C)C
C5438	PI	Inhibitor	174	CCN(CC)c1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/COCC)c1ccc(cc1)NC
C5439	PI	Inhibitor	174	CCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)NC)c1ccc(cc1)N1CCCC1
C5440	PI	Inhibitor	174	CCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)NC)c1ccc(cc1)NC(C)C
C5441	PI	Inhibitor	174	CCN(CC)c1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)N(CC)CC
C5442	PI	Inhibitor	174	CCNe1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/COCC)c1ccc(cc1)NC(C)C
C5443	PI	Inhibitor	174	CCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)F)c1ccc(cc1)NC(C)C
C5444	PI	Inhibitor	174	CCN(CC)c1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/COCC
C5445	PI	Inhibitor	174	CCCN(CCC)c1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/COCC
C5446	PI	Inhibitor	174	CCOC/C=C/c1ccc(cc1)c1[nH]c(en1)c1ccc(cc1)N1CCOCC1
C5447	PI	Inhibitor	174	CCOC/C=C/c1ccc(cc1)c1[nH]c(en1)c1ccc(cc1)NC(C)C
C5448	PI	Inhibitor	174	CCOC/C=C/c1ccc(cc1)c1[nH]c(en1)c1ccc(cc1)NCC(C)C
C5449	PI	Inhibitor	174	COC(=O)/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N1CCCC1)c1ccc(cc1)N1CCCC1
C5450	PI	Inhibitor	174	COC(=O)/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N(CC=C)CC=C)c1ccc(cc1)N(CC=C)CC=C
C5451	PI	Inhibitor	174	CNe1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)N(C)C
C5452	PI	Inhibitor	174	CCN(CC)c1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)NC
C5453	PI	Inhibitor	174	CCCN(CCC)c1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)NC
C5454	PI	Inhibitor	174	O[C@]12O[C@@](NC(=O)[C@@H]3CN(C)[C@@H]4C5c(Br)[nH]e6cccc(c56)C4=C3)(C(C)C)C(=O)N1[C@@H](CC(C)C)C(=O)N1CCCC21
C5455	PI	Inhibitor	174	CCCCN(CCCC)c1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)NC
C5456	PI	Inhibitor	174	CN(C)c1ccc(cc1)c1c([nH]e(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)N
C5457	PI	Inhibitor	174	O=C(N[C@@H]1CCCC[C@@H]1N1CCN(CC1)c1cccc1)c1cccc1NC(=O)c1enc2cccc2c1
C5458	PI	Inhibitor	174	COe1cc2CCN(CCc3ccc(NC(=O)c4cccc4[N+](=O)[O-])cc3)Cc2cc1OC
C5459	PI	Inhibitor	174	[O-][N+](=O)c1cccc1C(=O)Ne1ccc(CCN2CCc3cccc3C2)cc1
C5460	PI	Inhibitor	174	COe1cc2CCN(CCc3ccc(NC(=O)c4cccc4N)cc3)Cc2cc1OC
C5461	PI	Inhibitor	174	Ne1cccc1C(=O)Ne1ccc(CCN2CCc3cccc3C2)cc1
C5462	PI	Inhibitor	174	COe1cc2CCN(CCc3ccc(NC(=O)c4ccc(cc4)[N+](=O)[O-])cc3)Cc2cc1OC
C5463	PI	Inhibitor	174	[O-][N+](=O)c1ccc(cc1)C(=O)Ne1ccc(CCN2CCc3cccc3C2)cc1
C5464	PI	Inhibitor	174	COe1cc2CCN(CCc3ccc(NC(=O)c4ccc(N)cc4)cc3)Cc2cc1OC
C5465	PI	Inhibitor	174	Ne1ccc(cc1)C(=O)Ne1ccc(CCN2CCc3cccc3C2)cc1
C5466	PI	Inhibitor	174	COe1cc2CCN(CCc3ccc(NC(=O)c4cnc5cccc5c4)cc3)Cc2cc1OC
C5467	PI	Inhibitor	174	O=C(Ne1ccc(CCN2CCc3cccc3C2)cc1)c1enc2cccc2c1
C5468	PI	Inhibitor	174	COe1ccc(cc1OC)C(=O)Ne1ccc(CCN2CCc3cc(OC)c(OC)cc3C2)cc1
C5469	PI	Inhibitor	174	COe1cc2CCN(CCc3ccc(NC(=O)c4ccc(OC)c(OC)cc4[N+](=O)[O-])cc3)Cc2cc1OC
C5470	PI	Inhibitor	174	COe1cc2CCN(CCc3ccc(NC(=O)c4cnc5cccc45)cc3)Cc2cc1OC
C5471	PI	Inhibitor	174	COe1cc2CCN(CCc3ccc(NC(=O)c4cccc4Br)cc3)Cc2cc1OC
C5472	PI	Inhibitor	174	COe1cc2CCN(CCc3ccc(NC(=O)c4cccc(Br)c4)cc3)Cc2cc1OC



C5473	PI	Noninhibitor	174	OC(=O)COCCN1CCN(CC1)[C@@H](c1cccc1)c1ccc(Cl)cc1
C5474	PI	Inhibitor	174	COe1cc2CCN(CCe3ccc(NC(=O)c4cccc5ccccc45)cc3)Ce2cc1OC
C5475	PI	Inhibitor	174	COe1cc2CCN(CCe3ccc(NC(=O)c4ccc5ccccc5c4)cc3)Ce2cc1OC
C5476	PI	Inhibitor	174	COe1cc2CCN(CCe3ccc(NC(=O)c4cnc5ccccc5n4)cc3)Ce2cc1OC
C5477	PI	Inhibitor	174	COe1cc2CCN(CCe3ccc(NC(=O)c4ccc5ccccc5cn4)cc3)Ce2cc1OC
C5478	PI	Inhibitor	174	COe1cc2CCN(CCe3ccc(NC(=O)c4cccnc4)cc3)Ce2cc1OC
C5479	PI	Inhibitor	174	COe1cc2CCN(CCe3ccc(NC(=O)c4ccc(Br)cc4)cc3)Ce2cc1OC
C5480	PI	Inhibitor	174	COe1cc2CCN(CCe3ccc(NC(=O)c4ccc5ncccc5c4)cc3)Ce2cc1OC
C5481	PI	Inhibitor	174	COe1cc2CCN(CCe3ccc(NC(=O)c4cccc4NC(=O)c4ccc(C)cc4)cc3)Ce2cc1OC
C5482	PI	Inhibitor	174	O=C(Nc1cccc1C(=O)Nc1ccc(CCN2CCc3ccccc3C2)cc1)c1cnc2ccccc2c1
C5483	PI	Noninhibitor	174	C1NCCN(C1)Cc1ccccc1
C5484	PI	Noninhibitor	174	C1NCc1ccccc1Cl
C5485	PI	Noninhibitor	174	CCN(CC)CCOC(=O)C(c1ccccc1)c1ccccc1
C5486	PI	Noninhibitor	174	CN(C)CCCOCl(CCCCC1)Cc1ccccc1
C5487	PI	Noninhibitor	174	C[C@H](NC1=C(C=C1)O)[C@@H](Cc1ccc(Cl)cc1)c1ccc(Cl)cc1
C5488	PI	Noninhibitor	174	COe1c(OC)cc/C=C/C2=C(CN3CCN2CC3)N2CCCC2)cc1OC
C5489	PI	Noninhibitor	174	COe1c(OC)cc/C=C/C2=C(NC(C)C)CN3CCN2CC3)cc1OC
C5490	PI	Noninhibitor	174	N(C1=NCCN1)c1c(Cl)ccccc1Cl
C5491	PI	Noninhibitor	174	COC1CC2CC3N(CCC4CC(OC)C(OC)CC34)C(C)C2CC1OC
C5492	PI	Noninhibitor	174	CC(c1ccc(OC#N)cc1)c1ccc(OC#N)cc1
C5493	PI	Noninhibitor	174	[N]=C(N)N/N=C/c1c(Cl)ccccc1Cl
C5494	PI	Noninhibitor	174	OC(=O)CN1C2=C1C(N2)(c1ccccc1)c1ccccc1
C5495	PI	Noninhibitor	174	COe1ccc(cc1)C(OCCN(C)C)c1ccccc1
C5496	PI	Noninhibitor	174	COe1ccc(cc1)OC1=NCc2ccccc12
C5497	PI	Noninhibitor	174	[N]=C(N)NC(=O)Cc1c(Cl)ccccc1Cl
C5498	PI	Noninhibitor	174	COCCNCc1cc(OC)c(OC)c(OC)c1
C5499	PI	Noninhibitor	174	c1(NC)c(NCC[C@H](O)CCC)nc(nc1[C@@H](NCCN(CCO)CCO)N1CCCC(O)C1)N(CCO)CCO
C5500	PI	Noninhibitor	174	CCN(CC)CCOC(=O)[C@H](Cc1ccccc1)c1ccccc1
C5501	PI	Noninhibitor	174	CC[C@@H](c1ccccc1)/C/I=C(/OCCCN2CCN(CCCO1)CC2)\[C@H](CC)c1ccccc1
C5502	PI	Noninhibitor	174	NCCCCCNSe1ccccc2c(Cl)ccccc12
C5503	PI	Noninhibitor	174	C1CN(CCN1CCe1[nH]nnn1)c1ccccc1
C5504	PI	Inhibitor	174	c1ccc(cc1c1ccc(=O)c2c(cc(cc2o1)O)O)OCCOCCOCCOCCO
C5505	PI	Noninhibitor	174	Oe1c2O[C@H]3C(=O)CC[C@@]4(O)[C@@H]5Cc(cc1)c2[C@]34CCN5CC1CC1
C5506	PI	Noninhibitor	174	N(C)CC[C@H](c1ccccc1)c1ccccc1
C5507	PI	Inhibitor	174	Oe1ccc2[nH]cc(CCCCN3CCC(=CC3)c3ccccc3)c2c1
C5508	PI	Inhibitor	174	Oe1cc(CCCCC)cc(O)c1[C@H]1C=C(C)CC[C@H]1C(=C)C
C5509	PI	Inhibitor	174	O[C@H]1C=C[C@@H]2C(=O)O[C@H]3C[C@H](C/C=C/C[C@H](/C=C/C=C/4CO[C@H]1[C@@]24O)C)O[C@]1(C3)C/C(=N/OC)[C@H](C)C(O1)C(=C/C(C)C)/C
C5510	PI	Inhibitor	174	OCC(=O)[C@]1(O)CC[C@@H]2[C@@H]3CCCC4=CC(=O)CC[C@H]4[C@@H]3C(=O)C[C@]12C
C5511	PI	Noninhibitor	174	[N]=C(N)N1CCc2ccccc2C1
C5512	PI	Noninhibitor	174	CC(C)NC[C@H](COe1c(cc(cc1)NC(=O)C)C(=O)C)O
C5513	PI	Inhibitor	174	c1c(ccc2c1sc(c1ccc(cc1)S(=O)(=O)CCCC)c2C(=O)c1ccc(OCCN2CCCCC2)cc1)OS(=O)(=O)CCCC
C5514	PI	Inhibitor	174	C1(c2ccccc2C2C(c3c1ccc3)C2(F)F)N1CCN(CC1)C[C@@H](COe1c2c(ccc1)nc2)O
C5515	PI	Inhibitor	174	CCOe1c(OC)cc2c(c1)[C@H]1CN(C)CC[C@H]1N=C2c1ccc(cc1)C(=O)N(C(C)C)C(C)C
C5516	PI	Inhibitor	174	N(c1ccc(cc1)C1=N[C@@H]2CCN(C)C[C@H]2c2c1cc(OC)c(OC)c2)S(=O)(=O)c1ccc(C)cc1
C5517	PI	Noninhibitor	174	OC(=O)[C@@]1(C)CCc2c(C)c(O)c(C)c2O1
C5518	PI	Noninhibitor	174	Oe1c([C@H](CC(=O)C)c2ccc(cc2)[N+](=O)[O-])c(=O)c2ccccc2o1

C5519	PI	Noninhibitor	174	Oc1ccc(cc1)NC(=O)C
C5520	PI	Noninhibitor	174	ONC(=O)C
C5521	PI	Noninhibitor	174	N(CC(=O)OCc1ccccc1)C(=O)[C@@H](CSC(=O)C)Cc1ccccc1
C5522	PI	Noninhibitor	174	NS(=O)(=O)c1c(Cl)cc2N[C@H](CSCC=C)NS(=O)(=O)c2c1
C5523	PI	Noninhibitor	174	oc[C@H]1O[C@@H](O[C@H]2[C@@H](C[C@@H](N)[C@@H](O[C@H]3O[C@@H](CN)[C@@H](O)[C@H](O)[C@@H]3O)[C@@H]2O)NC(=O)[C@@H](O)CCN)[C@@H](O)[C@H](N)[C@@H]1O
C5524	PI	Noninhibitor	174	[nH]1cnc2c1c(=O)n(C)c(=O)n2C
C5525	PI	Noninhibitor	174	CN(C)c1c(C)n(C)n(c1=O)c1ccccc1
C5526	PI	Noninhibitor	174	OC(=O)[C@H]1N2[C@@H](SC1(C)C)[C@@H](NC(=O)[C@@H](N)c1ccc(O)cc1)C2=O
C5527	PI	Noninhibitor	174	Ne1cc(c[nH]c1=O)c1cnccl
C5528	PI	Noninhibitor	174	Oc1c(cccc1NC=O)C(=O)N[C@@H]1[C@H](C)OC(=O)[C@@H](CCCCC)[C@H](OC(=O)CC(C)C)[C@H](C)OC1=O
C5529	PI	Noninhibitor	174	CN1[C@H]2CC(C[C@@H]1[C@H]1O[C@@H]21)OC(=O)C(=C)c1ccccc1
C5530	PI	Noninhibitor	174	Oc1ccc(cc1)[N+](=O)[O-]
C5531	PI	Noninhibitor	174	OC[C@@H](O)[C@@H]1OC(=C(O)C1=O)O
C5532	PI	Noninhibitor	174	O[C@@H]1CC(=C2[C@H]([C@@H]3OC(=O)[C@H](C)[C@H]13)C(=CC2=O)C)C
C5533	PI	Noninhibitor	174	OC(=O)[C@@H]1N2[C@H](SC1(C)C)C(NC(=O)[C@@H](NC(=O)N1CCNC1=O)c1ccccc1)C2=O
C5534	PI	Noninhibitor	174	CC(C)(C)NC[C@H](c1cc(cc(c1)OC(=O)N(C)C)OC(=O)N(C)C)O
C5535	PI	Noninhibitor	174	NS(=O)(=O)c1cc2c(cc1C(F)(F)F)N[C@@H](Cc1ccccc1)NS2(=O)=O
C5536	PI	Inhibitor	174	NS(=O)(=O)c1c(Cl)cc2NC(=NS(=O)(=O)c2c1)CSCc1ccccc1
C5537	PI	Noninhibitor	174	O[C@H](CC[C@H]1[C@H](C)C=CC2=C[C@@H](O)C[C@H](OC(=O)[C@H](C)CC)[C@H]12)[C@@H](O)CC(=O)O
C5538	PI	Noninhibitor	174	OC[C@@H]1O[C@@H]2[C@H](OC(=O)c3cc(O)c(OC)c(O)c23)C(O)[C@@H]1O
C5539	PI	Noninhibitor	174	N(C)CCc1cccn1
C5540	PI	Noninhibitor	174	C1C[C@@H]2C([C@@]3(C1=CC(=C)C=C3)C)([C@H](C[C@]1([C@H]2C[C@@H]([C@@]1(C(=O)CO)O)C)C)O)F
C5541	PI	Noninhibitor	174	O[C@@H](COc1ccc(CCOC2CC2)cc1)CNC(C)C
C5542	PI	Noninhibitor	174	O[C@@H]1CC[C@@]2(C)[C@H](CC[C@@]3(C)[C@@H]2CC[C@@H]2[C@H]4[C@@H](CC[C@]4(CC[C@@]32C)C(=O)O)C(=C)C)C1(C)C
C5543	PI	Noninhibitor	174	CN1CCc2cc3c(OCO3)cc2[C@@H]1[C@H]1OC(=O)c2c1ccc1c2OCO1
C5544	PI	Noninhibitor	174	CC(=O)Oc1ccc(cc1)C(c1ccc(OC(=O)C)cc1)c1cccn1
C5545	PI	Noninhibitor	174	CS(=O)(=O)OCCCCOS(=O)(=O)C
C5546	PI	Inhibitor	174	[nH]1c2cc(OC)ccc2c2c1[C@H]1C[C@@H]3[C@@H](C[C@H](OC(=O)c4cc(OC)c(OC)c(OC)c4)[C@H](OC)C3C(=O)OC)CN1CC2
C5547	PI	Noninhibitor	174	Ne1c(Br)cc(C(=O)NCCN(CC)CC)c(OC)c1
C5548	PI	Noninhibitor	174	N(C(=O)[C@@H]1CCCCN1CCCC)c1c(C)cccc1C
C5549	PI	Noninhibitor	174	N1[C@@H]2N(C)CC[C@@]3([C@H]4Ne5c(cccc5)[C@@]23CCN4C)c2ccccc12
C5550	PI	Noninhibitor	174	O[C@]1(CC)C(=O)OCc2c1cc1n(Cc3c1nc1ccccc1c3)c2=O
C5551	PI	Noninhibitor	174	COc1c(OC)c2c(C[C@@H]3N(CCc4cc5c(OCO5)cc34)C2)cc1
C5552	PI	Noninhibitor	174	OC(=O)[C@@H](C(=O)N[C@H]1[C@@H]2SC(C)(C)[C@H](N2C1=O)C(=O)O)c1ccccc1
C5553	PI	Inhibitor	174	OC(=O)CCC(=O)O[C@@H]1CC[C@@]2(C)[C@H](CC[C@@]3(C)[C@@H]2C(=O)C=C2[C@@H]4C[C@@](C)(CC[C@@]4C)CC[C@]32C)C(=O)O)C1(C)C
C5554	PI	Noninhibitor	174	N(CCC1)C(=O)N(CCC1)N=O
C5555	PI	Noninhibitor	174	OC(=O)C1=C(Cl)CS[C@@H]2[C@H](NC(=O)[C@H](N)c3ccccc3)C(=O)N12
C5556	PI	Noninhibitor	174	OC(=O)C1=C(CSc2nnnn2C)CS[C@@H]2N1C(=O)[C@]2(OC)NC(=O)CSCC#N
C5557	PI	Inhibitor	174	OC(=O)C1=C(COC(=O)C)CS[C@@H]2[C@@H](NC(=O)/C(=N/OC)/c3csc(n3)N)C(=O)N12
C5558	PI	Noninhibitor	174	OC(=O)C1=C(COC(=O)N)CS[C@@H]2N1C(=O)[C@H]2NC(=O)/C(=N/OC)/c1ccco1
C5559	PI	Noninhibitor	174	OC(=N)c1cc(=O)c(=O)c2=c1[nH]c1c(o2)cc(cc1)N(CC)CC
C5560	PI	Noninhibitor	174	OC(=O)C1=C(COC(=O)C)CS[C@@H]2[C@@H](NC(=O)Cc3ccccc3)C(=O)N12
C5561	PI	Noninhibitor	174	OC(=O)C1=C(COC(=O)C)CS[C@@H]2[C@@H](NC(=O)CSc3ccccc3)C(=O)N12
C5562	PI	Inhibitor	174	O[C@@H]1CC[C@@]2(C)[C@H](C1)C[C@H](O)C1[C@@H]3CC[C@@H]([C@H](C)CCC(=O)O)[C@@]3(C)CC[C@H]21
C5563	PI	Noninhibitor	174	CN1[C@H](c2ccc(Cl)cc2)S(=O)(=O)CCC1=O
C5564	PI	Noninhibitor	174	COc1ccc(cc1)C(=C(c1ccc(OC)cc1)c1ccc(OC)cc1)Cl

C5565	PI	Inhibitor	174	O[C@H](COC(=O)N)COc1ccc(Cl)cc1
C5566	PI	Noninhibitor	174	N(CCC)C(=O)NS(=O)(=O)c1ccc(Cl)cc1
C5567	PI	Noninhibitor	174	O[C@@]1(NC(=O)c2ccccc12)c1cc(c(Cl)cc1)S(=O)(=O)N
C5568	PI	Noninhibitor	174	NS(=O)(=O)c1c(Cl)cc2NC=NS(=O)(=O)c2c1
C5569	PI	Noninhibitor	174	O=C1C=CC(=O)c2c1ccc1c2ccc2ccccc12
C5570	PI	Noninhibitor	174	N(CCCCN1CCN(CC1)c1ccccc1OC)C(=O)c1cc2ccccc2cc1
C5571	PI	Noninhibitor	174	OC(=O)c1nn(CC)c2cc3c(OCC3)cc2c1=O
C5572	PI	Noninhibitor	174	N([C@@H]1CCSC1=O)C(=O)C
C5573	PI	Noninhibitor	174	O[C@H](CNC(C)(C)C)c1cc(Cl)c(N)c(Cl)c1
C5574	PI	Inhibitor	174	O[C@H]1[C@@H](O[C@@H]([C@@H]([C@@H](NC(=O)[C@H]2C[C@@H](CCC)CN2C)[C@@H](C)Cl)[C@@H](O)[C@@H]1O)SC
C5575	PI	Noninhibitor	174	OC1C[C@@]2(C)[C@H](C[C@@H](C)[C@]2(OC(=O)CC)C(=O)CC1)[C@H]2CCC3=CC(=O)C=C[C@@]3(C)[C@@]12F
C5576	PI	Noninhibitor	174	OC(=O)C(C)(C)Oe1ccc(Cl)cc1
C5577	PI	Noninhibitor	174	NS(=O)(=O)c1c(Cl)ccc(c1)C(=O)NN1[C@H](C)CCC[C@H]1C
C5578	PI	Noninhibitor	174	C#CCN(C)CCCOc1c(Cl)cc(Cl)cc1
C5579	PI	Inhibitor	174	O[C@@H]1C[C@H](CCn2c(C(C)C)c(C(=O)Nc3ccccc3)c(c2c2ccc(F)cc2)c2ccccc2)OC(=O)C1
C5580	PI	Noninhibitor	174	COe1c(OC)cc(cc1)C(=O)OC1C[C@@H]2CC[C@H](C1)N2C
C5581	PI	Noninhibitor	174	OCC(=O)[C@]1(O)CC[C@@H]2[C@H]3CCCC=CC(=O)CC[C@@]4(C)[C@@H]3C(O)C[C@]12C
C5582	PI	Noninhibitor	174	O[C@H](CC1CC(=O)NC(=O)C1)[C@H]1CC(C)C[C@@H](C)C1=O
C5583	PI	Inhibitor	174	OC1C[C@@]2(C)[C@H](C[C@H](C)[C@]2(O)C(=O)COC(=O)C)[C@H]2CCC3=CC(=O)C=C[C@@]3(C)[C@]12F
C5584	PI	Noninhibitor	174	ON(CCCCCNC(=O)CCC(=O)N(O)CCCCNC(=O)CCC(=O)N(O)CCCCCN)C(=O)C
C5585	PI	Noninhibitor	174	O[C@@H]1[C@@H]2C34[C@H]5[C@@H]6[C@@H](OC)[C@H]5[C@@]5(C)[C@H]6OC)OCO[C@@]15[C@@H]3N(CC)C[C@@]2(COC)CC[C@H]4OC
C5586	PI	Noninhibitor	174	O[C@@H]1CC[C@@]2(COC)CN(CC)[C@H]3[C@@]4(O)[C@@H](OC)[C@@H]2[C@@]13[C@H]1C[C@@H]2[C@@H](OC)[C@@H]1[C@@]4(O)C[C@H]2OC
C5587	PI	Noninhibitor	174	O[C@@]12C[C@H]3[C@@H](OC)[C@]1(O)[C@@]1(C[C@@H]3OC)OCO[C@@]31[C@@H]([C@H]1[C@@]42[C@H]3N(CC)C[C@@]1(C)CC[C@@H]4OC)C(=O)C
C5588	PI	Inhibitor	174	O[C@H]1C[C@@H](CC[C@H]2[C@H](C)C=CC3=C[C@@H](C)C[C@H](OC(=O)C(C)(C)CC)[C@H]23)OC(=O)C1
C5589	PI	Noninhibitor	174	O[C@H]1[C@H]2C[C@@H]3[C@H](N(C)C)C(=O)C(=O)N(C(=O)N)[C@@]3(O)C(=O)C2=C(O)c2c(O)ccc(Cl)c12
C5590	PI	Noninhibitor	174	N(C(=O)OCC)C1=C(N2CC2)C(=O)C(=C(N2CC2)C1=O)NC(=O)OCC
C5591	PI	Noninhibitor	174	CCN(CC)C(=O)N1CCN(C)CC1
C5592	PI	Noninhibitor	174	Oe1ccc(cc1)/C(=C/CC)c1ccc(O)cc1/CC
C5593	PI	Noninhibitor	174	N1C(=O)OC(C)(C)C1=O
C5594	PI	Noninhibitor	174	Oe1ccc(cc1)/C(=C/C)/C(=C/C)/c1ccc(O)cc1
C5595	PI	Inhibitor	174	N(C(=O)OC[C@@H](CN1CCCC1)OC(=O)Ne1ccccc1)c1ccccc1
C5596	PI	Noninhibitor	174	OS(=O)(=O)CN(C)c1c(C)n(C)n(c1=O)c1ccccc1
C5597	PI	Noninhibitor	174	O[C@H](CN(CC(C)S(=O)(=O)c1ccc(cc1)N)[C@@H](Cc1ccccc1)NC(=O)O[C@H]1CCOC1
C5598	PI	Inhibitor	174	Oe1c(OC)cc2CCN3C4c(C[C@H]3c2c1)ccc(OC)c4O
C5599	PI	Noninhibitor	174	O[C@H]1[C@H]2[C@@H](C)c3ccccc(O)c3C(=C2C(=O)[C@@]2(O)[C@H]1[C@H](N(C)C)C(=O)C(=C(/O)\N)/C2=O)O
C5600	PI	Noninhibitor	174	CC[C@@]12CCCN3CCc4c([C@H]13)n(c1ccccc41)C(=O)C2
C5601	PI	Noninhibitor	174	Oe1cc(O)c2c(=O)cc(oc2c1)c1ccc(OC)cc1
C5602	PI	Noninhibitor	174	C1[C@H](C(Oc2cc(cc(c12)O)O)c1cc(c(cc1)O)O)O
C5603	PI	Noninhibitor	174	O[C@@]12O[C@@](NC(=O)[C@@H]3CN(C)[C@H]4Cc5c[nH]c6ccccc56)C4=C3)(C(C)C)C(=O)N1[C@@H](C(C)C)C(=O)N1CCC[C@@H]21
C5604	PI	Inhibitor	174	O[C@@]12O[C@@](NC(=O)[C@@H]3CN(C)[C@H]4Cc5c[nH]c6ccccc56)C4=C3)(C(C)C)C(=O)N1[C@@H](Cc1ccccc1)C(=O)N1CCCC21
C5605	PI	Noninhibitor	174	N([C@@H]1CCc2cc(OC)c(OC)c(OC)c2[C@H]2CCCC(OC)C(=O)C[C@H]12)C(=O)C
C5606	PI	Inhibitor	174	O[C@@]12O[C@@](NC(=O)[C@@H]3CN(C)[C@H]4Cc5c[nH]c6ccccc56)C4=C3)(C(C)C)C(=O)N1[C@@H](CC(C)C)C(=O)N1CCCC21
C5607	PI	Noninhibitor	174	N(C)C(=O)Oe1ccc2N(C)[C@H]3N(C)CC[C@@]3(C)c2c1
C5608	PI	Noninhibitor	174	NC(=S)c1cc(CC)ncc1
C5609	PI	Noninhibitor	174	N1c2c(cc(OCC)cc2)C(=CC1(C)C)C
C5610	PI	Noninhibitor	174	OC(=O)CN(CC(=O)O)CC(=O)Ne1c(CC)ccccc1CC

C5611	PI	Noninhibitor	174	O[C@@H](COc1c(OC)c2nc3c(cco3)c(OC)c2cc1)C(C)(C)O
C5612	PI	Noninhibitor	174	N(CC)[C@@H](C)Cc1cc(ccc1)C(F)(F)F
C5613	PI	Noninhibitor	174	OC(=O)[C@@H](C)c1cc(Oc2ccccc2)ccc1
C5614	PI	Inhibitor	174	O[C@@H](CN[C@H](C)Cc1ccc(O)cc1)c1cc(O)cc(O)c1
C5615	PI	Inhibitor	174	Clc1ccc(OCC(=O)N2CCN(Cc3cc4c(OCO4)cc3)CC2)cc1
C5616	PI	Inhibitor	174	Cc1c(oc2c(cccc2c1=O)C(=O)OCCN1CCCCC1)c1ccccc1
C5617	PI	Noninhibitor	174	O[C@@H]1C[C@@]2(C)[C@@H](C[C@@H]3OC(C)(C)O[C@@]23C(=O)COC(=O)C)[C@@H]2C[C@@H](F)C3=CC(=O)C=C[C@@]3(C)[C@@]12F
C5618	PI	Noninhibitor	174	OCC(=O)[C@]1(O)CC[C@@H]2[C@H]3CCCC4=CC(=O)CC[C@@]4(C)[C@]3(F)C(O)C[C@]12C
C5619	PI	Noninhibitor	174	OCC(=O)[C@]12OC(C)(C)O[C@@H]1C[C@@H]1[C@H]3C[C@@H](F)C4=CC(=O)C=C[C@@]4(C)[C@@H]3C(O)C[C@]21C
C5620	PI	Noninhibitor	174	CN(C)CCOC(c1ccccc1)c1ccccc1
C5621	PI	Noninhibitor	174	OC1C[C@@]2(C)[C@H](CC[C@]2(O)C(=O)C)[C@H]2C[C@H](C)C3=CC(=O)C=C[C@@]3(C)[C@]12F
C5622	PI	Noninhibitor	174	OC(=O)CC[C@H](NC(=O)c1ccc(cc1)NCc1cnc2nc([nH]c(=O)e2n1)N)C(=O)O
C5623	PI	Noninhibitor	174	O[C@@H](COc1cccc2c1n(C)c(=O)cc2OC)C(C)(C)O
C5624	PI	Noninhibitor	174	[O-][N+](=O)c1ccc(o1)/C=N/N1C[C@H](CN2CCOCC2)OC1=O
C5625	PI	Noninhibitor	174	OC(=O)c1cc(c(Cl)cc1NCc1ccco1)S(=O)(=O)N
C5626	PI	Noninhibitor	174	OC(=O)CC1(CN)CCCCC1
C5627	PI	Noninhibitor	174	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@H]1[C@H](O)Cc2ccccc12)CN1CCN(Cc2ccccc2)C[C@@H]1C(=O)NC(C)(C)C
C5628	PI	Noninhibitor	174	O[C@@H]1C[C@@H]2Oc3c(OC)ccc4c3[C@@]2(CCN(C)C4)C=C1
C5629	PI	Noninhibitor	174	N1=c2c(=C3C1=CC(=O)C=C3)ccnc2C
C5630	PI	Noninhibitor	174	OCC(CO)OCn1cnc2c1nc([nH]c2=O)N
C5631	PI	Noninhibitor	174	N1C(=O)[C@@]2([C@@H]3OC[C@@H]4[C@@H]5[C@H]2[C@]([C@H]4C3)(CN5C)C=C)c2ccccc12
C5632	PI	Noninhibitor	174	N(N1C[C@H]2CCC[C@H]2C1)C(=O)NS(=O)(=O)c1ccc(C)cc1
C5633	PI	Noninhibitor	174	Cn1c2ccccc2c(=O)cc1c1cc2c(OCO2)cc1
C5634	PI	Noninhibitor	174	OC[C@H](O)COc1ccccc1OC
C5635	PI	Noninhibitor	174	Clc1cc(Cl)c(Cl)cc1OCC#Cl
C5636	PI	Inhibitor	174	CC(=O)N1CCN(CC1)c1ccc(OC[C@@H]2CO[C@](Cn3ccnc3)(O2)c2ccc(Cl)cc2Cl)cc1
C5637	PI	Inhibitor	174	[nH]1c2=CC(=O)C=Cc2c2CCNC(=c12)C
C5638	PI	Noninhibitor	174	n1c2ccccc2c2c1c(C)[nH]cc2
C5639	PI	Noninhibitor	174	[nH]1c2ccccc2c2c1[C@@H](C)NCC2
C5640	PI	Noninhibitor	174	O[C@H]1C[C@]2(C)[C@H](C[C@H]3OC(C)(C)O[C@@]23C(=O)CC1)[C@H]2CCC3=CC(=O)CC[C@@]3(C)[C@@]12F
C5641	PI	Noninhibitor	174	O[C@H]1CCN2CC=C(COC(=O)[C@@](O)(C(C)C)[C@H](C)OC)C12
C5642	PI	Noninhibitor	174	OCCN1CCN(CCS(=O)(=O)O)CC1
C5643	PI	Noninhibitor	174	N1CCC2=c3ccc(OC)cc3=NC2=C1C
C5644	PI	Noninhibitor	174	O[C@H]1[C@@H](C)O[C@@H](OC[C@H]2O[C@@H](Oc3cc(O)c4C(=O)C[C@H](Oc4c3)c3cc(O)c(OC)cc3)[C@@H](O)[C@@H](O)[C@@H]2O)[C@@H](O)[C@@H]1O
C5645	PI	Noninhibitor	174	O[C@@H]1C=C2CCN(C)[C@H]2[C@H]2[C@H]1OC(=O)c1cc3c(OCO3)cc21
C5646	PI	Inhibitor	174	COc1c(OC)c2c(cc1)[C@H](OC2=O)[C@@H]1N(C)CCc2cc3c(OCO3)cc12
C5647	PI	Noninhibitor	174	O[C@@H]1N(C)CCc2cc3c(OCO3)cc12
C5648	PI	Noninhibitor	174	O[C@@H]([C@@H](C)N1CCC(Cc2ccccc2)CC1)c1ccc(O)cc1
C5649	PI	Noninhibitor	174	Oc1c2c(C[C@@H]3N(C)CCc4cc(OC)c(OC)c2c34)ccc1OC
C5650	PI	Noninhibitor	174	NC(=O)C(CCN(C(C)C)C(C)C)c1ccccc1)c1ccccc1
C5651	PI	Noninhibitor	174	N(C(C)C)c1c(C)n(C)n(c1=O)c1ccccc1
C5652	PI	Noninhibitor	174	[O-][N+](=O)O[C@H]1CO[C@H]2[C@H](CO[C@@H]12)O[N+](=O)[O-]
C5653	PI	Noninhibitor	174	OC[C@H]1O[C@H](O[C@H]2C(O)[C@H](O[C@H]3O[C@@H](CN)[C@@H](O)[C@@H](O)[C@H]3O)[C@@H](C[C@@H]2N)N)[C@H](O)[C@H](N)[C@H]1O
C5654	PI	Noninhibitor	174	O[C@@H]1[C@@H]2C[C@@H]3[C@H]1[C@](O)(C[C@@H]2OC)[C@H]1C[C@H]2[C@]43[C@H]1N(CC)C[C@]2(C)CC[C@H]4O
C5655	PI	Noninhibitor	174	COC1=CC(=O)O[C@H](C1)/C=C/c1ccccc1
C5656	PI	Noninhibitor	174	[nH]1c(=O)n(CCN2CCC(CC2)C(=O)c2ccc(F)cc2)c(=O)c2ccccc12

C5657	PI	Noninhibitor	174	<chem>N(Cc1cccc1)c1[nH]cnc2c1nnc2</chem>
C5658	PI	Inhibitor	174	<chem>COc1c(OC)cc(C[C@@H]2N(C)CCc3cc(OC)c(OC)cc23)c(Br)c1</chem>
C5659	PI	Noninhibitor	174	<chem>N(C(=O)c1c(C)onc1)c1ccc(cc1)C(F)(F)F</chem>
C5660	PI	Noninhibitor	174	<chem>OC(=O)CC[C@H](NC(=O)c1ccc(cc1)NCC1CNc2c(N1C=O)c(=O)[nH]c(N)n2)C(=O)O</chem>
C5661	PI	Noninhibitor	174	<chem>O[C@H](COc1cccc2c1CCCC2=O)CNC(C)(C)C</chem>
C5662	PI	Noninhibitor	174	<chem>O[C@]1(CC[C@H]2[C@H]3CCCC4=CC(=O)CC[C@H]4[C@H]3CC[C@@]12CC)C#C</chem>
C5663	PI	Inhibitor	174	<chem>O[C@@H]1CC[C@@]2(C)[C@@H](CCC3[C@@H]4CC[C@@H]([C@H](C)CCC(=O)O)[C@@]4(C)CC[C@H]23)C1</chem>
C5664	PI	Noninhibitor	174	<chem>O[C@@H](C[C@H]1CCC[C@H](CC(=O)c2cccc2)N1C)c1cccc1</chem>
C5665	PI	Noninhibitor	174	<chem>OC(=O)c1cn(CC)c2c(cc(F)c(N3CCN[C@H](C)C3)c2F)c1=O</chem>
C5666	PI	Noninhibitor	174	<chem>CCN(CC)CCOCCOC(=O)C1(CCCC1)c1cccc1</chem>
C5667	PI	Noninhibitor	174	<chem>CN1c2ccc(Cl)cc2C(=NCC1=O)c1cccc1</chem>
C5668	PI	Inhibitor	174	<chem>O[C@H]1C[C@H](CC[C@H]2[C@@H](C)C=CC3=C[C@@H](C)C[C@@H](OC(=O)[C@H](C)CC)[C@H]23)OC(=O)C1</chem>
C5669	PI	Noninhibitor	174	<chem>CN(C)CCOC(=O)COc1ccc(Cl)cc1</chem>
C5670	PI	Noninhibitor	174	<chem>O[C@H]1C=C2CCN3C4cc5c(OCO5)cc4[C@@H]([C@H]23)[C@@H]1O</chem>
C5671	PI	Inhibitor	174	<chem>OC[C@H]1CN(C)[C@H]2Cc3c[nH]c4cccc(c34)C2=C1</chem>
C5672	PI	Inhibitor	174	<chem>N([C@@H]1CN(C)[C@@H]2Cc3c[nH]c4cccc(c34)C2=C1)C(=O)N(CC)CC</chem>
C5673	PI	Inhibitor	174	<chem>NCc1ccc(cc1)S(=O)(=O)N</chem>
C5674	PI	Noninhibitor	174	<chem>CN(CCC1)CCCl</chem>
C5675	PI	Noninhibitor	174	<chem>Cc1cc(CN2CCN(CC2)[C@H](c2cccc2)c2ccc(Cl)cc2)ccc1</chem>
C5676	PI	Noninhibitor	174	<chem>N1C(=O)C[C@@](C)(CC)C1=O</chem>
C5677	PI	Noninhibitor	174	<chem>OC(=O)c1cccc1Nc1c(Cl)ccc(C)c1Cl</chem>
C5678	PI	Noninhibitor	174	<chem>N(CCN(CC)CC)C(=O)COc1ccc(OC)cc1</chem>
C5679	PI	Noninhibitor	174	<chem>OS(=O)(=O)CCS</chem>
C5680	PI	Noninhibitor	174	<chem>O[C@]1(CC[C@H]2[C@@H]3CCc4cc(OC)ccc4[C@H]3CC[C@@]12C)C#C</chem>
C5681	PI	Noninhibitor	174	<chem>OC(=O)[C@@H]1[C@H]2[C@@H]2[C@H](SC1(C)C)[C@H](NC(=O)[C@H](N=C)c1cccc1)C2=O</chem>
C5682	PI	Inhibitor	174	<chem>O[C@H](CNC)c1cc(OC)c(O)cc1</chem>
C5683	PI	Noninhibitor	174	<chem>CN(C)CCN(Cc1cccs1)c1cccn1</chem>
C5684	PI	Noninhibitor	174	<chem>CN1CC[C@]23[C@@H]4[C@H]1Cc1c2c(c(cc1)OC)O[C@H]3C(=O)CC4</chem>
C5685	PI	Noninhibitor	174	<chem>[nH]1ccn(C)c1=S</chem>
C5686	PI	Noninhibitor	174	<chem>OC(=O)[C@H](CCS(=O)(=N)C)N</chem>
C5687	PI	Inhibitor	174	<chem>CN1CCCC(CC2c3cccc3Sc3c2cccc3)C1</chem>
C5688	PI	Noninhibitor	174	<chem>O[C@H](COC(=O)N)COc1cccc1OC</chem>
C5689	PI	Noninhibitor	174	<chem>O[C@@H]([C@H](C)N)c1c(OC)ccc(OC)c1</chem>
C5690	PI	Noninhibitor	174	<chem>OC[C@@H](CC)NC(=O)[C@H]1CN(C)[C@@H]2Cc3c[nH]c4cccc(c34)C2=C1</chem>
C5691	PI	Inhibitor	174	<chem>OCC(=O)[C@]1(O)CC[C@@H]2[C@@H]3C[C@@H](C)C4=CC(=O)C=C[C@]4(C)[C@@H]3C(O)C[C@]12C</chem>
C5692	PI	Noninhibitor	174	<chem>OCCn1c(C)ncc1[N+](=O)[O-]</chem>
C5693	PI	Noninhibitor	174	<chem>Nc1nc(N)c(mn1)c1c(Cl)c(Cl)ccc1</chem>
C5694	PI	Inhibitor	174	<chem>O[C@@]1(CC[C@@H]2[C@H]3CCCC4=CC(=O)CCC4=C3[C@H](C[C@@]12C)c1ccc(cc1)N(C)C)C#CC</chem>
C5695	PI	Noninhibitor	174	<chem>OC(=O)[C@@H](Cn1ccc(=O)c(O)c1)N</chem>
C5696	PI	Noninhibitor	174	<chem>ClC(Cl)[C@H](c1ccc(Cl)cc1)c1cccc1Cl</chem>
C5697	PI	Noninhibitor	174	<chem>O[C@]1(C)[C@H](C)C(=O)O[C@@H]2CCN3CC=C(COC(=O)[C@]1(C)O)C23</chem>
C5698	PI	Noninhibitor	174	<chem>OC(=O)CC/C(=C/Cc1c(O)c2c(COC2=O)c(C)c1OC)/C</chem>
C5699	PI	Noninhibitor	174	<chem>Oc1cc(O)c2c(=O)c(O)c(oc2c1)c1cc(O)c(O)c(O)c1</chem>
C5700	PI	Noninhibitor	174	<chem>OC(=O)C[C@@H](NC(=O)C)C(=O)O</chem>
C5701	PI	Noninhibitor	174	<chem>OC[C@H]1O[C@H](O)[C@@H](NC(=O)C)[C@@H](O[C@@H](C)C(=O)O)C1O</chem>
C5702	PI	Noninhibitor	174	<chem>N1[C@H](C)CCC[C@@H]1C</chem>

C5703	PI	Noninhibitor	174	<chem>O[C@@H]1C(=C)[C@@H]2C[C@@]31[C@H]1C[C@H]4[C@@]5([C@H]1N(CC)C[C@]4(C)CC[C@H]5O)[C@@H]3C[C@H]2O</chem>
C5704	PI	Noninhibitor	174	<chem>OC(=O)[C@@H](C)c1cc2c(cc1)cc(OC)cc2</chem>
C5705	PI	Inhibitor	174	<chem>Oc1ccc(cc1)[C@H]1CC(=O)c2c(O)cc(O)cc2O1</chem>
C5706	PI	Noninhibitor	174	<chem>OC[C@@H]1O[C@H](Oe2cc(O)c3C(=O)C[C@H](Oe3c2)e2ccc(O)cc2)[C@@H](O[C@H]2O[C@@H](C)[C@H](O)[C@@H](O)[C@H]2O)[C@H](O)[C@@H]1O</chem>
C5707	PI	Noninhibitor	174	<chem>O[C@@H]1[C@@H](CN)O[C@@H](O[C@H]2[C@@H](O)[C@@H](O)[C@@H](C[C@H]2N)N)[C@H](N)[C@H]1O</chem>
C5708	PI	Noninhibitor	174	<chem>OC[C@@H]1O[C@H](O[C@H]2C(O)[C@H](O[C@H]3O[C@@H](CN)[C@H](O)C[C@@H]3N)[C@H](C[C@@H]2N)N)[C@@H](O)[C@@H](N)[C@H]1O</chem>
C5709	PI	Noninhibitor	174	<chem>CN1CCO[C@@H](c2cccc2)c2c(C1)cccc2</chem>
C5710	PI	Noninhibitor	174	<chem>N(C(=O)c1ncccc1)c1c(C)n(C)n(c1=O)c1cccc1</chem>
C5711	PI	Noninhibitor	174	<chem>OC(=O)c1c(nccc1)Nc1cccc(c1)C(F)F</chem>
C5712	PI	Noninhibitor	174	<chem>[nH]1c2cccc2c2c1[C@H]1[C@@H]3CC[C@@H]([C@H]4CCNC34)N1CC2</chem>
C5713	PI	Noninhibitor	174	<chem>O[C@@H]([C@H](C)N)c1cc(O)c(O)cc1</chem>
C5714	PI	Noninhibitor	174	<chem>O[C@@H](CNC(C)C)c1cc(O)cc(O)c1</chem>
C5715	PI	Noninhibitor	174	<chem>O[C@H](CC)Cn1c(C)nc1[N+](=O)[O-]</chem>
C5716	PI	Noninhibitor	174	<chem>CN(C)CCO[C@H](c1cccc1)c1cccc1C</chem>
C5717	PI	Noninhibitor	174	<chem>CCN(CC)CCc1nc(no1)c1cccc1</chem>
C5718	PI	Noninhibitor	174	<chem>OC(=O)c1cc2c(ccc2)c(Cc2cc3cccc3c(C(=O)O)c2O)c1O</chem>
C5719	PI	Noninhibitor	174	<chem>N1CCCC[C@@H]1[C@H](C(=O)OC)c1cccc1</chem>
C5720	PI	Inhibitor	174	<chem>N1CCCCC1CC(C1CCCC1)C1CCCC1</chem>
C5721	PI	Noninhibitor	174	<chem>oc[C@@H]1O[C@@H](O[C@@H]2C(O)[C@@H](C[C@H](N)[C@@H]2O[C@H]2O[C@H](CO)[C@@H](O)[C@@H](O)[C@H]2N)N)[C@H](O)[C@H]1O[C@@H]1O[C@@H](CN)[C@H](O)[C@H](O)[C@H]1N</chem>
C5722	PI	Noninhibitor	174	<chem>C/C1=C/CC[C@@]2(C)O[C@H]2[C@@H]2OC(=O)C(=C)[C@@H]2CC1</chem>
C5723	PI	Noninhibitor	174	<chem>CN1C(C)(C)CCCC1(C)C</chem>
C5724	PI	Inhibitor	174	<chem>C1CCn2nnc2CC1</chem>
C5725	PI	Noninhibitor	174	<chem>O[C@@H](CC(=O)O)[C@@H](CC(C)C)NC(=O)[C@@H](C)NC(=O)C[C@@H](O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)[C@H](NC(=O)CC(C)C)(C)C)(C)C</chem>
C5726	PI	Noninhibitor	174	<chem>N(C(=O)C)c1ccc(OCC)cc1</chem>
C5727	PI	Noninhibitor	174	<chem>Nc1nc(N)c(cc1)/N=N/c1cccc1</chem>
C5728	PI	Noninhibitor	174	<chem>Oc1c(OC)cc(cc1)C(=O)OC1C[C@H]2CC[C@@H](C1)N2C</chem>
C5729	PI	Noninhibitor	174	<chem>N(Cc1ncccc1)C(=O)c1cc(C(=O)NCc2ncccc2)c(OC)cc1</chem>
C5730	PI	Noninhibitor	174	<chem>O[C@@]12C[C@@H]3O[C@@]43C(=O)O[C@H]([C@H]3OC(=O)[C@H]1[C@H]3C(=C)C)[C@@]24C</chem>
C5731	PI	Noninhibitor	174	<chem>O/C(=C\1/N(C)S(=O)(=O)c2cccc2C1=O)/Nc1cccc1</chem>
C5732	PI	Noninhibitor	174	<chem>O[C@@H]1[C@H]2COC(=O)C2[C@@H](c2cc(OC)c(OC)c(OC)c2)c2c1cc1OCOc1c2</chem>
C5733	PI	Noninhibitor	174	<chem>CCCCOc1ccc(OCCCN2CCOCC2)cc1</chem>
C5734	PI	Noninhibitor	174	<chem>O[C@@H]1CC[C@]2(C)[C@H]3CC[C@@]4(C)[C@H](CC[C@H]4C(=O)C)[C@@H]3CC=C2C1</chem>
C5735	PI	Noninhibitor	174	<chem>OC(CCN1CCCCC1)(c1cccc1)c1cccc1</chem>
C5736	PI	Noninhibitor	174	<chem>Oc1c(cc(SC(C)(C)Se2cc(c(O)c(e2)C(C)(C)C(C)C)cc1C(C)(C)C(C)C)C(C)C)</chem>
C5737	PI	Noninhibitor	174	<chem>CCN(CC)[C@H](C)CN1c2cccc2Sc2c1cccc2</chem>
C5738	PI	Noninhibitor	174	<chem>[nH]1c(=O)cc(CCC)[nH]c1=S</chem>
C5739	PI	Noninhibitor	174	<chem>NC(=O)c1ncnc1</chem>
C5740	PI	Noninhibitor	174	<chem>OCc1enc(C)c(O)c1CO</chem>
C5741	PI	Noninhibitor	174	<chem>COc1c(C#N)c(=O)n(C)cc1</chem>
C5742	PI	Noninhibitor	174	<chem>CN1CCc2cc3c(OCO3)c3c2[C@@H]1Cc1cccc31</chem>
C5743	PI	Noninhibitor	174	<chem>N1CCc2cc(OC)c(OC)cc2[C@H]1C</chem>
C5744	PI	Noninhibitor	174	<chem>O=C1O[C@@]23C[C@@H](C=CC2=C1)N1CCCC[C@@H]31</chem>
C5745	PI	Noninhibitor	174	<chem>N(C1CCC(C)CC1)C(=O)N(CCC1)N=O</chem>
C5746	PI	Noninhibitor	174	<chem>O[C@]1(C)C(=C)C/C(=C)/C(=O)O[C@H]2CCN3CC=C(COC1=O)C23</chem>
C5747	PI	Noninhibitor	174	<chem>O[C@@]12CC[C@H]3[C@H](C)[C@H]4CC[C@@H](C)CN4C[C@@H]3[C@@H]1C[C@@H]1[C@@H]2CC(=O)[C@@H]2CC(=O)CC[C@@]12C</chem>
C5748	PI	Noninhibitor	174	<chem>O[C@H]1[C@@H](O[C@H]2[C@@H](C[C@@H](N)[C@@H](O[C@H]3OC(=CC[C@@H]3N)CN)[C@@H]2O)N)OC[C@@](C)(O)[C@@H]1NC</chem>

C5749	PI	Noninhibitor	174	COe1c(OC)c2nc3c(cco3)c(OC)c2cc1
C5750	PI	Noninhibitor	174	OC[C@H]1O[C@H](O)[C@H](NC(=O)N(C)N=O)[C@@H](O)C1O
C5751	PI	Noninhibitor	174	OC(=O)CCCC(=O)Nc1ccc(cc1)S(=O)(=O)Nc1nccs1
C5752	PI	Noninhibitor	174	Nc1ccc(cc1)S(=O)(=O)NC(=O)c1cccc1
C5753	PI	Noninhibitor	174	Nc1ccc(cc1)S(=O)(=O)Nc1nnc(Cl)cc1
C5754	PI	Noninhibitor	174	Nc1ccc(cc1)S(=O)(=O)Nc1cc(OC)nc(OC)n1
C5755	PI	Noninhibitor	174	Nc1ccc(cc1)S(=O)(=O)Nc1nccc(C)n1
C5756	PI	Noninhibitor	174	OCC(=O)[C@]1(O)CC[C@@H]2[C@@H]3CCCC4=CC(=O)C=C[C@@]4(C)[C@@H]3C(=O)C[C@@]12C
C5757	PI	Noninhibitor	174	Nc1ccc(cc1)S(=O)(=O)Nc1ncc(OC)cn1
C5758	PI	Noninhibitor	174	Nc1ccc(cc1)S(=O)(=O)Nc1nc(C)cc(C)n1
C5759	PI	Noninhibitor	174	Nc1ccc(cc1)S(=O)(=O)Nc1nnc(C)s1
C5760	PI	Noninhibitor	174	Nc1ccc(cc1)S(=O)(=O)Nc1cccc1
C5761	PI	Noninhibitor	174	Nc1ccc(cc1)S(=O)(=O)Nc1cc2ncnc2cc1
C5762	PI	Noninhibitor	174	Nc1ccc(cc1)S(=O)(=O)Nc1c(C)c(C)no1
C5763	PI	Noninhibitor	174	[nH]1c2ccccc2nc1c1c(OC)cc(cc1)S(=O)C
C5764	PI	Noninhibitor	174	OC(=O)[C@H](C)c1ccc(cc1)C(=O)c1cccs1
C5765	PI	Noninhibitor	174	OC(=O)CCCC(=O)OCC1(CCCC)C(=O)N(N(C1=O)c1cccc1)c1cccc1
C5766	PI	Noninhibitor	174	[nH]1c2cc(OC)ccc2c2c1[C@H]1C[C@H]3[C@H](C[C@@H](OC(=O)c4cc(OC)c(OC(=O)OCC)c(OC)c4)[C@@H](OC)C3C(=O)OC)CN1CC2
C5767	PI	Noninhibitor	174	O[C@@H]1[C@H]2[C@@H]3N4C[C@@]5(C)C[C@H](OC(=O)c6cccc6)[C@@H](OC(=O)C)[C@]63[C@@H]5[C@H]4C[C@@]32CC(=C)[C@H]1[C@H](OC(=O)C)[C@@H]63
C5768	PI	Noninhibitor	174	Nc1nc(nc2cc(OC)c(OC)cc12)N1CCN(CC1)C(=O)[C@H]1CCCCO1
C5769	PI	Noninhibitor	174	O[C@@H](CNC(C)(C)C)c1cc(O)cc(O)c1
C5770	PI	Noninhibitor	174	[nH]1c2ccccc2c2c1[C@H]1C[C@H]3[C@H](CN1CC2)C(C)OC=C3C(=O)OC
C5771	PI	Noninhibitor	174	N1CCN=C1[C@H]1CCCc2ccccc12
C5772	PI	Noninhibitor	174	C1CN2C[C@H](N=C2S1)c1cccc1
C5773	PI	Noninhibitor	174	C1CCC2=Nc3ccccc3CN2C1
C5774	PI	Noninhibitor	174	O=c1n2CCCCc2nc2ccccc12
C5775	PI	Noninhibitor	174	[nH]1c2ccccc2nc1c1cscn1
C5776	PI	Noninhibitor	174	NS(=O)(=O)c1ccc(OC)c(c1)C(=O)NC[C@@H]1CCCN1CC
C5777	PI	Noninhibitor	174	OC(=O)c1cccc1S
C5778	PI	Inhibitor	174	N(CCN(CC)CC)C(=O)c1c(OC)ccc(c1)S(=O)(=O)C
C5779	PI	Noninhibitor	174	CCS(=O)(=O)CCn1c(C)ncc1[N+](=O)[O-]
C5780	PI	Noninhibitor	174	N(N1CCCCC1)C(=O)NS(=O)(=O)c1ccc(C)cc1
C5781	PI	Noninhibitor	174	C(C#CCN1CCCC1)N1CCCC1
C5782	PI	Noninhibitor	174	OCC(=O)[C@]1(O)[C@@H](O)C[C@H]2[C@@H]3CCCC4=CC(=O)C=C[C@]4(C)[C@]3(F)C(O)C[C@@]12C
C5783	PI	Noninhibitor	174	NS(=O)(=O)c1c(Cl)cc2N[C@H](NS(=O)(=O)c2c1)C(Cl)C1
C5784	PI	Noninhibitor	174	OC(=O)[C@@H](Cc1cc(I)c(Oc2cc(I)c(O)cc2)c(I)c1)N
C5785	PI	Noninhibitor	174	N1CCN(Cc2c(OC)c(OC)c(OC)cc2)CC1
C5786	PI	Noninhibitor	174	CN1C(=O)OC(C)(C)C1=O
C5787	PI	Noninhibitor	174	Cc1cc2c(o1)c(C)c1oc(=O)cc(C)c1c2
C5788	PI	Noninhibitor	174	CO[C@@H]1C=C2CCN(C)[C@H]2[C@H]2[C@@H]1OC(=O)c1cc3c(OCO3)cc21
C5789	PI	Inhibitor	174	Fc1ccc(cc1)C(OCCN1CCN(CCCc2ccccc2)CC1)c1ccc(F)cc1
C5790	PI	Noninhibitor	174	O[C@H]1[C@@H](O)[C@@]2(O)[C@H](C[C@@]34O[C@@]5(O)[C@H](CC[C@@H]23)[C@]4(C)CC[C@@H]5OC(=O)c2cc(OC)c(OC)cc2)[C@H]2CN3[C@@H](C)CC[C@H]3[C@@](O)(O)[C@@H]12
C5791	PI	Noninhibitor	174	OC[C@H]1O[C@H](O)[C@H](O)[C@H]1O)n1cnc2c1nnc2N
C5792	PI	Noninhibitor	174	O[C@@]1(C[C@@]2(CC)CCCN3CCc4c([C@H]23)n1c1cccc41)C(=O)OC
C5793	PI	Inhibitor	174	CCOC(=O)C1=C[C@@]2(CC)CCCN3CCc4c([C@H]23)n1c1cccc41
C5794	PI	Noninhibitor	174	N(C1=NCCCS1)c1c(C)cccc1C

C5795	PI	Noninhibitor	174	O[C@@H]1CC[C@H]2CN3CCc4c([nH]e5ccccc45)[C@H]3C[C@@H]2C1C(=O)O
C5796	PI	Inhibitor	174	O[C@H]1[C@H](C)/C=C(\C)/[C@@H](OC(=O)N)[C@H](OC)/C=C/C=C(\C)/C(=O)NC2=CC(=O)C(=C(C[C@H](C)C[C@@H]1OC)C2=O)OC
C5797	PI	Inhibitor	174	Oc1cc2c(O)c(c1)NC(=O)/C=C/C=C[C@@H](C)[C@@H](OC(=O)N)/C=C/[C@@H](C)[C@H](OC)[C@H](C[C@@H](C)[C@H]2OC)OC)/C)
C5798	PI	Inhibitor	174	O[C@H]1[C@H](C)/C=C(\C)/[C@H](OC(=O)N)[C@@H](OC)/C=C/C=C(\C)/C(=O)NC2=CC(=O)C(=C(C[C@H](C)C[C@@H]1OC)C2=O)NCC=C
C5799	PI	Inhibitor	174	N1c2c(cc(C)s2)C(=Nc2ccccc12)N1CCN(C)CC1
C5800	PI	Inhibitor	174	OCCOCCN1CCN(CC1)C1=Nc2ccccc2Sc2ccccc12
C5801	PI	Noninhibitor	174	N(C)C(=O)O/N=C/C(C)(C)SC
C5802	PI	Inhibitor	174	N1C(=C([C@@H](c2ccccc2)[N+](=O)[O-])C(=C1C)C(=O)O[C@H]1CCCN(Cc2ccccc2)C1)C(=O)OC)C
C5803	PI	Inhibitor	174	N(/N=C(/C=C/c1ccc(cc1)C(F)(F)F)\C=C/c1ccc(cc1)C(F)(F)F)C1=NCC(C)(C)CN1
C5804	PI	Noninhibitor	174	N(CC)C(=O)Oe1ccccc1[N+](=O)[O-]
C5805	PI	Noninhibitor	174	CC1(C)[C@H](C=C(C)Cl)[C@H]1C(=O)OCc1cc(Oc2ccccc2)ccc1
C5806	PI	Noninhibitor	174	ClCC1(CCl)[C@@H]2C[C@H](C(Cl)(Cl)[C@@H]2Cl)/C1=C/Cl
C5807	PI	Inhibitor	174	COe1cc2c(SCCN(C2)C(=O)CCN2CCC(Cc3ccccc3)CC2)cc1
C5808	PI	Inhibitor	174	CCCCCCCCCCCC(CCCN(C)CCc1cc(OC)ccc1)(C#N)c1cc(OC)ccc1
C5809	PI	Inhibitor	174	n1c(NCCc2ccccc2OC)c2OC)nc(c2c1cc(OC)c(OC)c2)N1CCc2cc(OC)c(OC)cc2C1
C5810	PI	Inhibitor	174	n1c(c2c(nc1NCCc1ccc(c(c1)OC)OC)ccc(c2)C)N(Cc1ccccc1)C
C5811	PI	Inhibitor	174	c1ccccc2c1oc(cc2=O)C(=O)Nc1cc(OC)c(OC)cc1c1nnn(n1)c1ccc(CCN2CCc3cc(OC)c(OC)cc3C2)cc1
C5812	PI	Inhibitor	174	OC[C@H]1Oe2c(OC1c1ccc(OC)c(OC)c1)cc(cc2)c1c(O)c(=O)c2c(O)cc(OC)cc2o1
C5813	PI	Inhibitor	174	OC[C@H]1Oe2c(OC1c1ccc(OC)c(OC)c1)cc(cc2)c1c(OC)c(=O)c2c(O)cc(O)cc2o1
C5814	PI	Inhibitor	174	OC[C@H]1Oe2c(OC1c1ccc(OC)c(OC)c1)cc(cc2)c1c(OC)c(=O)c2c(O)cc(OC)cc2o1
C5815	PI	Inhibitor	174	OC[C@H]1Oe2c(OC1c1ccc(OC)c(OC)c1)cc(cc2)c1c(O)c(=O)c2c(OC)cc(OC)cc2o1
C5816	PI	Inhibitor	174	OC[C@H]1Oe2c(OC1c1ccc(O)c(O)c1)cc(cc2)c1c(O)c(=O)c2c(O)cc(O)cc2o1
C5817	PI	Inhibitor	174	OC[C@@H]1Oe2ccc(cc2OC1c1ccc(O)c(OC)c1)[C@H]1Oe2c(C(=O)[C@@H]1O)c(O)cc(OCc1ccccc1)e2
C5818	PI	Inhibitor	174	OC[C@H]1Oe2c(OC1c1ccc(O)c(OC)c1)cc(cc2)c1c(O)c(=O)c2c(O)cc(O)cc2o1
C5819	PI	Inhibitor	174	OC[C@H]1Oe2c(OC1c1ccc(O)c(OC)c1)cc(cc2)c1c(O)c(=O)c2c(O)cc(OCc3ccccc3)cc2o1
C5820	PI	Inhibitor	174	OC[C@H]1Oe2c(OC1c1ccc(O)c(OC)c1)cc(cc2)c1c(O)c(=O)c2c(O)cc(OC)cc2o1
C5821	PI	Inhibitor	174	OC[C@H]1Oe2c(OC1c1ccc(OC)c(OC)c1)cc(cc2)c1c(O)c(=O)c2c(O)cc(O)cc2o1
C5822	PI	Inhibitor	174	OC[C@H]1Oe2c(OC1c1ccc(O)c(OC)c1)cc(cc2)c1c(OC)c(=O)c2c(O)cc(OC)cc2o1
C5823	PI	Inhibitor	174	CC(=O)Oe1c(O)cc2oc(cc(=O)c2c1O)c1ccccc1
C5824	PI	Noninhibitor	174	OC(=O)CCC(=O)O[C@H]1O[C@H]2O[C@@]3(C)CC[C@H]4[C@H](C)CC[C@@H]([C@H]1C)[C@@]24OO3
C5825	PI	Inhibitor	174	COe1c(OC)c(OC)c2c(=O)cc(oc2c1)c1ccccc1
C5826	PI	Inhibitor	174	COe1c(OC)c(O)c2c(=O)cc(oc2c1)c1ccccc1
C5827	PI	Inhibitor	174	Oe1c2c(=O)ccc(oc2cc2c1OCO2)c1ccccc1
C5828	PI	Inhibitor	174	COe1c2c(=O)ccc(oc2cc2c1OCO2)c1ccccc1
C5829	PI	Inhibitor	174	c1(c2c(cc(c1OC(=O)C)Oe1ccccc1)oc(cc2=O)c1ccccc1)OC(=O)C
C5830	PI	Inhibitor	174	c1(c2c(cc(c1Oe1ccccc1)O)oc(cc2=O)c1ccccc1)O
C5831	PI	Inhibitor	174	COe1c2c(=O)ccc(oc2cc2c1OC(O2)(c1ccccc1)c1ccccc1)c1ccccc1
C5832	PI	Inhibitor	174	CCCOe1c(O)cc2oc(cc(=O)c2c1O)c1ccccc1
C5833	PI	Inhibitor	174	CCOe1c(O)cc2oc(cc(=O)c2c1O)c1ccccc1
C5834	PI	Inhibitor	174	CC(=O)Oe1c(OC(=O)C)c(O)c2c(=O)cc(oc2c1)c1ccccc1
C5835	PI	Noninhibitor	174	Oe1ccc(cc1)c1coe2cc(O)ccc2c1=O
C5836	PI	Inhibitor	174	CCOe1c(OC)cc2oc(cc(=O)c2c1O)c1ccccc1
C5837	PI	Inhibitor	174	CCCOe1c(OC)cc2oc(cc(=O)c2c1OC)c1ccccc1
C5838	PI	Inhibitor	174	CCCOe1c(OCCC)c(O)c2c(=O)cc(oc2c1)c1ccccc1
C5839	PI	Inhibitor	174	CCOe1c(OCC)c(O)c2c(=O)cc(oc2c1)c1ccccc1
C5840	PI	Inhibitor	174	CCCCCCCCOe1c(OCCCCCCC)c(O)c2c(=O)cc(oc2c1)c1ccccc1



C5841	PI	Inhibitor	174	CCCCCOe1c(OCCCCC)c(O)c2c(=O)cc(oc2c1)c1cccc1
C5842	PI	Inhibitor	174	CCCCOe1c(OCCCC)c(O)c2c(=O)cc(oc2c1)c1cccc1
C5843	PI	Inhibitor	174	CC(=O)Oe1c(OC(=O)C)c(OC(=O)C)c2c(=O)cc(oc2c1)c1cccc1
C5844	PI	Inhibitor	174	CCCCCOe1c(OCCCCC)c(OC)c2c(=O)cc(oc2c1)c1cccc1
C5845	PI	Inhibitor	174	CCCCCOe1c(OCCCCC)c(OC)c2c(=O)cc(oc2c1)c1cccc1
C5846	PI	Inhibitor	174	Oe1c(CNCC)cc(cc1)Nc1cnc2cc(Cl)ccc12
C5847	PI	Inhibitor	174	CCOe1c(OCC)c(OC)c2c(=O)cc(oc2c1)c1cccc1
C5848	PI	Inhibitor	174	CCCCOe1c(OCCCC)c(OC)c2c(=O)cc(oc2c1)c1cccc1
C5849	PI	Inhibitor	174	COe1c(OC(=O)C)c(OC)c2c(=O)cc(oc2c1)c1cccc1
C5850	PI	Inhibitor	174	CC(=O)Oe1c(OCc2cccc2)cc2oc(cc(=O)c2c1OC(=O)C)c1cccc1
C5851	PI	Inhibitor	174	CC(=O)Oe1c(OCc2cccc2)c(O)c2c(=O)cc(oc2c1)c1cccc1
C5852	PI	Inhibitor	174	CC(=O)Oe1c(OC(=O)C)c(OCc2cccc2)c2c(=O)cc(oc2c1)c1cccc1
C5853	PI	Inhibitor	174	CC(=O)Oe1c(OC(=O)C)c(Br)c2oc(cc(=O)c2c1O)c1cccc1
C5854	PI	Inhibitor	174	O[C@@H](COe1c(ccc1)C(=O)CCc1cccc1)CN1CCN(CC1)c1cccc(C)c1C
C5855	PI	Inhibitor	174	Clc1c(ccc1)c1nc2c(ccc2)c(n1)N1CCCC1
C5856	PI	Inhibitor	174	O[C@H](COe1c(ccc1)C(=O)CCc1cccc1)CN(CCC)C(=O)c1cccc1
C5857	PI	Noninhibitor	174	Oe1c2C(=O)C=C(C(=O)c2cc(C)c1)c1c(C)cc2C(=O)C=CC(=O)c2c1O
C5858	PI	Inhibitor	174	O[C@H](COe1c(ccc1)C(=O)CC)CN1CCC(O)(CC1)c1cccc1
C5859	PI	Inhibitor	174	O[C@H](COe1c(ccc1)C(=O)Cc1cccc2c1cccc2)CN1CCC(O)(CC1)c1cccc1
C5860	PI	Inhibitor	174	O[C@@H](COe1cc(ccc1)C(=O)C)CN1CCCCC1
C5861	PI	Inhibitor	174	O[C@@H](COe1cc(ccc1)C(=O)C)CN1CCN(CC1)c1ccc(F)cc1
C5862	PI	Inhibitor	174	O[C@@H](COe1c(ccc1)C(=O)CCc1cccc1)CN1CCN(CC1)C(=O)c1cccc1
C5863	PI	Inhibitor	174	O[C@H](COe1ccc(OC)cc1)CN1CCN(CC1)c1ccc(F)cc1
C5864	PI	Inhibitor	174	NC1=C(C#N)[C@H](c2e(O1)n[nH]c2c1ccc(C)cc1)c1ccc(cc1)N(C)C
C5865	PI	Inhibitor	174	O[C@H](COe1c(ccc1)C(=O)CCc1cccc1)CN[C@H](C(C)C)c1cccc1
C5866	PI	Noninhibitor	174	Oe1cc2c3c(oc(=O)c4cc(O)c(O)c(oc2=O)c34)c1O
C5867	PI	Inhibitor	174	O[C@H](COe1c(cc(Cl)c(Cl)c1)C(=O)CCc1cccc1)CN1CCN(CC1)c1cccc1C
C5868	PI	Inhibitor	174	O[C@H](COe1c(cc(C)cc1)C(=O)C)CN1CCCCC1
C5869	PI	Inhibitor	174	O[C@H](COe1cccc2c1C(=O)CC2=C)CN1CCCCC1
C5870	PI	Inhibitor	174	O[C@H](COe1c(ccc1)C(=O)CCc1cccc1)CN[C@@H](c1cccc1)C(C)(C)C
C5871	PI	Inhibitor	174	O[C@@H](COe1cccc2c1C(=O)CC2=O)CN1CCCCC1
C5872	PI	Inhibitor	174	O[C@H](COe1cccc2c1C(=O)[C@H](C2=C)c1cccc1)CN1CCCCC1
C5873	PI	Inhibitor	174	O[C@H](COe1cccc2c1C(=O)[C@H](C2=O)c1cccc1)CN1CCCCC1
C5874	PI	Inhibitor	174	O[C@@H](COe1cccc2c1C(=O)[C@@H](C2=C)c1cccc1)CN1CCN(CC1)c1cccc(C)c1C
C5875	PI	Noninhibitor	174	O=C1CC(CCN2CCCC2)Oe2cccc12
C5876	PI	Noninhibitor	174	OC(=O)/C=C/c1cc(OC)c(O)cc1
C5877	PI	Noninhibitor	174	OC(=O)COe1cccc1C(=O)CCc1cccc1
C5878	PI	Inhibitor	174	O[C@H](COe1cccc(c1)C(=O)C)CN1CCN(CC1)c1c(C)c(C)ccc1
C5879	PI	Inhibitor	174	O[C@@H](COe1cccc(c1)C(=O)C)CN1CCN(CC1)c1c(C)ccc1
C5880	PI	Inhibitor	174	O[C@H](COe1cccc1C(=O)C)CN1CCN(CC1)c1c(C)c(C)ccc1
C5881	PI	Inhibitor	174	O=C([C@@H]1Oe2cccc2[C@H]1Cc1cccc1)N1CCCCC1
C5882	PI	Noninhibitor	174	C[C@H]1[C@@H](Oe2c1cccc2)C(=O)N1CCCCC1
C5883	PI	Inhibitor	174	C([C@@H]1Oe2cccc2[C@H]1Cc1cccc1)N1CCCCC1
C5884	PI	Inhibitor	174	N(C(=O)c1ccc(OCCCC)cc1)c1cc2c(cc1)nc(SCc1c(C)c(C(=O)C)c(C)cc1C)s2
C5885	PI	Inhibitor	174	N(C(=O)CCc1cccc1)c1cc2c(cc1)nc(SCc1c(C)c(C(=O)C)c(C)cc1C)s2
C5886	PI	Inhibitor	174	N(C(=O)c1cccc2c1cccc2)c1cc2c(cc1)nc(SCc1c(C)c(C(=O)C)c(C)cc1C)s2

C5887	PI	Inhibitor	174	<chem>N(C(=O)C1=C(C)NC(=S)N[C@H]1c1cccc1)c1c(OCC)cccc1</chem>
C5888	PI	Inhibitor	174	<chem>O[C@@H](COc1ccc(cc1)C(=O)CCc1cccc1)CN1CCN(CC1)c1cccc(C)c1C</chem>
C5889	PI	Inhibitor	174	<chem>c1(cc(ccc1C(=O)CCc1cccc1)OC)OCC(=O)CN1CCN(CC1)c1c(cccc1)C</chem>
C5890	PI	Inhibitor	174	<chem>O[C@H](COc1c(cc(C)cc1)C(=O)C)CN1CCN(CC1)c1cccc1C</chem>
C5891	PI	Inhibitor	174	<chem>O[C@@H](COc1c(cccc1)C(=O)C)CN1CCN(CC1)c1cccc1C</chem>
C5892	PI	Inhibitor	174	<chem>O[C@@H](COc1c(ccc(C)c1)C(=O)C)CN1CCN(CC1)c1cccc1C</chem>
C5893	PI	Inhibitor	174	<chem>O[C@@H](COc1c(cc(Cl)c(Cl)c1)C(=O)C)CN1CCN(CC1)c1cccc1C</chem>
C5894	PI	Noninhibitor	174	<chem>N(NC(=O)c1nn(C)cc1)C(=C)c1ccnn1C</chem>
C5895	PI	Inhibitor	174	<chem>O[C@H](COc1c(ccc(OC)c1)C(=O)CCc1ccc(cc1)N(C)C)CN1CCN(CC1)c1cccc1C</chem>
C5896	PI	Noninhibitor	174	<chem>Oc1ccc(cc1)c1coc2cc(O)cc(O)c2c1=O</chem>
C5897	PI	Inhibitor	174	<chem>O[C@H](COc1ccc(cc1)C(=O)C)CNCCC(c1cccc1)c1cccc1</chem>
C5898	PI	Inhibitor	174	<chem>O[C@H](COc1cc(ccc1)C(=O)CCc1cccc1)CN1CCN(CC1)c1cccc1C</chem>
C5899	PI	Inhibitor	174	<chem>O[C@@H](COc1cc(ccc1)C(=O)CCc1cccc1)CNCCC(c1cccc1)c1cccc1</chem>
C5900	PI	Inhibitor	174	<chem>O[C@@H](COc1cc(ccc1)C(=O)CCc1cccc1)CN1CCOCC1</chem>
C5901	PI	Inhibitor	174	<chem>O[C@H](COc1ccc(cc1)C(=O)CCc1cccc1)CNCCC(c1cccc1)c1cccc1</chem>
C5902	PI	Noninhibitor	174	<chem>N(/N=C/c1ccnc1)c1nnc(nn1)n1nc(C)cc1C</chem>
C5903	PI	Noninhibitor	174	<chem>OC[C@H](O)Cc1cc(OC)c(OC)cc1</chem>
C5904	PI	Noninhibitor	174	<chem>N(C(=O)C(=O)N1CCCCC1)/N=C/c1c(F)cccc1Cl</chem>
C5905	PI	Inhibitor	174	<chem>O[C@@H](COc1c(cccc1)C(=O)CCc1ccc(cc1)N(C)C)CN1CCN(CC1)c1cccc1C</chem>
C5906	PI	Noninhibitor	174	<chem>Nc1ccc(cc1)C(=O)OCCOCC</chem>
C5907	PI	Noninhibitor	174	<chem>OC[C@H]1O[C@@H](Oc2cccc3cc4c(C(=O)OC4)c(O)c23)[C@@H](O)[C@H](O)[C@@H]1O</chem>
C5908	PI	Noninhibitor	174	<chem>CN(C)c1ccc(cc1)c1nc(nc(n1)C(F)(F)F)C(F)(F)F</chem>
C5909	PI	Inhibitor	174	<chem>O[C@@H](COc1c(cccc1)C(=O)CCc1cccc1)CN1CCCCC1</chem>
C5910	PI	Inhibitor	174	<chem>O[C@H](COc1c(cccc1)C(=O)CCc1cccc1)CN(C(C)C)C(C)C</chem>
C5911	PI	Inhibitor	174	<chem>O[C@@H](COc1c(cccc1)C(=O)CC)CN1CCCCC1</chem>
C5912	PI	Inhibitor	174	<chem>O[C@H](COc1c(cccc1)C(=O)CCc1cccc1)CN1CCN(CC1)c1cccc1</chem>
C5913	PI	Inhibitor	174	<chem>c1cc(c(cc1)OC[C@@H](CN1CCN(CC1)c1c(cccc1)OC)O)C(=O)CCc1cccc1</chem>
C5914	PI	Inhibitor	174	<chem>O[C@H](COc1c(cccc1)C(=O)CCc1cccc1)CN1CCN(CC1)c1cccc(OC)c1</chem>
C5915	PI	Noninhibitor	174	<chem>O[C@H](C(Cl)(Cl)Cl)P(=O)(OC)OC</chem>
C5916	PI	Inhibitor	174	<chem>O[C@H](COc1c(cccc1)C(=O)CCc1cccc1)CN1CCN(CC1)c1ccc(OC)cc1</chem>
C5917	PI	Inhibitor	174	<chem>O[C@H](COc1c(cccc1)C(=O)CCc1cccc1)CN1CCN(CC1)c1cccc1C</chem>
C5918	PI	Inhibitor	174	<chem>O[C@@H](COc1c(cccc1)C(=O)CCc1cccc1)CN(C)CCC</chem>
C5919	PI	Inhibitor	174	<chem>O[C@H](COc1c(cccc1)C(=O)CCc1cccc1)CN1CCOCC1</chem>
C5920	PI	Inhibitor	174	<chem>O[C@H](COc1c(cccc1)C(=O)CCc1cccc1)CN1CCC(O)(CC1)c1cccc1</chem>
C5921	PI	Inhibitor	174	<chem>O[C@@H](COc1ccc(cc1)C(=O)CCc1cccc1)CN1CCCCC1</chem>
C5922	PI	Inhibitor	174	<chem>C(Cc1c(CCc2ccccc2)c2c(o1)cccc2)N1CCCCC1</chem>
C5923	PI	Inhibitor	174	<chem>O[C@H](CNCCC)c1c(CC)c2c(o1)cccc2</chem>
C5924	PI	Inhibitor	174	<chem>O[C@@H](CNCCC)c1c(CCc2ccccc2)c2c(o1)cccc2</chem>
C5925	PI	Inhibitor	174	<chem>O[C@H](COc1c(cccc1)C(=O)CCc1cccc1)CN1CCC(Cc2ccccc2)CC1</chem>
C5926	PI	Noninhibitor	174	<chem>O[C@@H](COc1cc(ccc1)C(=O)C)CN1CCOCC1</chem>
C5927	PI	Inhibitor	174	<chem>O[C@@H](COc1c(cc(O)cc1)C(=O)CCc1cccc1)CN(CCC)CCC</chem>
C5928	PI	Inhibitor	174	<chem>O[C@@H](COc1cc(ccc1)C(=O)CCc1cccc1)CN1CCCCC1</chem>
C5929	PI	Inhibitor	174	<chem>O[C@H](COc1cccc2c1cccn2)CN1CCN(CC1)C1c2ccccc2[C@H]2[C@H](c3c1cccc3)C2(F)F</chem>
C5930	PI	Inhibitor	174	<chem>O[C@@H](COc1ccc(cc1)C(=O)CCc1cccc1)CN1CCOCC1</chem>
C5931	PI	Inhibitor	174	<chem>O[C@@H](COc1ccc(cc1)C(=O)CCc1cccc1)CN(CCC)CCC</chem>
C5932	PI	Inhibitor	174	<chem>O[C@H](COc1cccc1[C@@H](O)CCc1cccc1)CN(CCC)CCC</chem>

C5933	PI	Inhibitor	174	<chem>O[C@@H](COc1cccc1[C@H](CCc1cccc1)OC)CN(CCC)CCC</chem>
C5934	PI	Inhibitor	174	<chem>O[C@H](COc1cccc1C(=O)CCc1cccc1)CNCC(c1cccc1)c1cccc1</chem>
C5935	PI	Inhibitor	174	<chem>O[C@H](COc1cccc1C(=O)CCc1cccc2c1cccc2)CNCCC(c1cccc1)c1cccc1</chem>
C5936	PI	Inhibitor	174	<chem>O[C@@@H](CN1CCN(CC1)C(c1cccc1)c1cccc1)c1cc(OC)c(OC)cc1</chem>
C5937	PI	Inhibitor	174	<chem>O=C(CCc1cccc1)c1cccc1OCCCN1CCCCC1</chem>
C5938	PI	Inhibitor	174	<chem>O=C(CCc1cccc1)c1cccc1OCCN1CCCCC1</chem>
C5939	PI	Inhibitor	174	<chem>O=C(CCc1cccc1)c1cccc1OCCCCN1CCCCC1</chem>
C5940	PI	Inhibitor	174	<chem>O=C(CCc1cccc1)c1cccc1OCCCCCN1CCCCC1</chem>
C5941	PI	Inhibitor	174	<chem>O=C(CCc1cccc1)c1cccc1OCCCCCN1CCCCC1</chem>
C5942	PI	Inhibitor	174	<chem>O=C(CCc1cccc1)c1cccc1OCCCCCCCCN1CCCCC1</chem>
C5943	PI	Inhibitor	174	<chem>O[C@@@H](COc1c(ccc1)[C@H](CCc1cccc1)OC)CNCCCC(c1cccc1)c1cccc1</chem>
C5944	PI	Inhibitor	174	<chem>O[C@@@H](COc1c(ccc1)[C@@H](O)CCc1cccc1)CN1CCOCC1</chem>
C5945	PI	Inhibitor	174	<chem>O[C@@@H](COc1c(cc(Oc2cccc2)cc1)C(=O)CCc1cccc1)CNC(C)C</chem>
C5946	PI	Inhibitor	174	<chem>O[C@H](COc1c(cc(O)cc1)C(=O)CCc1cccc1)CN1CCCCC1</chem>
C5947	PI	Inhibitor	174	<chem>O[C@@@H](COc1c(ccc1)C(=O)CCc1cccc1)CNCCCC(c1cccc1)c1cccc1</chem>
C5948	PI	Inhibitor	174	<chem>O[C@H](COc1c(ccc1)C(=O)CCc1cccc1)CNC1CCCCC1</chem>
C5949	PI	Inhibitor	174	<chem>N1[C@@H](N(c2ccc(Oc3cccc3)cc2)C(=O)c2c1cccc2)c1ccc(OC)cc1</chem>
C5950	PI	Inhibitor	174	<chem>N1[C@H](N(c2ccc(cc2)C(C)(C)C)C(=O)c2cccc12)c1ccc2OCc2c1</chem>
C5951	PI	Inhibitor	174	<chem>N1[C@@H](N(c2ccc(CC)cc2)C(=O)c2cccc12)c1ccc(OCC(C)C)cc1</chem>
C5952	PI	Noninhibitor	174	<chem>N1[C@@H](N(c2ccc(CC)cc2)C(=O)c2cccc12)c1ccc(OCc2cccc2)cc1</chem>
C5953	PI	Inhibitor	174	<chem>N1[C@H](N(c2ccc(Cl)cc2)C(=O)c2c1cccc2)c1ccc(cc1)[C@@H](C)CC</chem>
C5954	PI	Inhibitor	174	<chem>N1[C@@H](N(c2ccc(cc2)[C@H](C)CC)C(=O)c2cccc12)c1ccc(cc1)C(C)C</chem>
C5955	PI	Inhibitor	174	<chem>CCCCSe1nc2c(c(=O)n1CC=C)C1(CCCC1)Cc1e2cccc1</chem>
C5956	PI	Inhibitor	174	<chem>O[C@H](COc1c(cc(O)cc1)C(=O)CCc1cccc1)CN(C(C)C)C(C)C</chem>
C5957	PI	Inhibitor	174	<chem>O[C@H](COc1c(ccc1)[C@H](CCc1cccc1)OC(C)C)CN1CCCCC1</chem>
C5958	PI	Inhibitor	174	<chem>O[C@H](COc1c(ccc1)C(=O)C)CN1CCC(Cc2cccc2)CC1</chem>
C5959	PI	Inhibitor	174	<chem>O[C@H](COc1c(ccc1)C(=O)C)CN1CCC(O)(CC1)c1cccc1</chem>
C5960	PI	Inhibitor	174	<chem>O[C@H](COc1c(ccc1)C(=O)CCc1ccc(Cl)cc1)CN1CCN(CC1)c1c(C)cccc1</chem>
C5961	PI	Inhibitor	174	<chem>O[C@@@H](COc1c(ccc1)C(=O)CCc1ccc(OC)cc1)CN1CCN(CC1)c1c(C)cccc1</chem>
C5962	PI	Noninhibitor	174	<chem>N=C(CCC(=O)N)c1n[nH]c(=S)n1c1ccc(OC)cc1</chem>
C5963	PI	Inhibitor	174	<chem>CC(=O)O[C@H](COc1c(ccc1)C(=O)CCc1cccc1)CN1CCCCC1</chem>
C5964	PI	Inhibitor	174	<chem>O[C@H](COc1c(cc(Cl)cc1)C(=O)CCc1cccc1)CN1CCN(CC1)c1cccc1C</chem>
C5965	PI	Inhibitor	174	<chem>c1c(cc(c1)OCC[C@H](CN1CCN(CC1)c1c(ccc1)C)O)C(=O)CCc1cccc1)OC</chem>
C5966	PI	Inhibitor	174	<chem>O[C@@@H](COc1c(cc(C)cc1)C(=O)CCc1cccc1)CN1CCN(CC1)c1cccc1C</chem>
C5967	PI	Inhibitor	174	<chem>O[C@H](COc1c(ccc1)C(=O)CCc1cccc1)CN(C(=O)CC)c1cccc1</chem>
C5968	PI	Inhibitor	174	<chem>O=C(CCc1cccc1)c1c(OCCCN2CCOCC2)cccc1</chem>
C5969	PI	Inhibitor	174	<chem>Fc1ccc(cc1)N1CCN(CCCCc2c(ccc2)C(=O)CCc2cccc2)CC1</chem>
C5970	PI	Inhibitor	174	<chem>O[C@H](CN1C[C@@H]2CCCC[C@H]2CC1C(=O)NC(C)(C)C)[C@H](Cc1cccc1)NC(=O)[C@@H](CC(=O)N)NC(=O)c1nc2cccc2cc1</chem>
C5971	PI	Inhibitor	174	<chem>C[C@H]1CC[C@@H]2COC3=C([C@H]2C1)C(=O)C1=C([C@H]2C[C@@H](C)CC[C@H]2C(C)(C)O1)C3=O</chem>
C5972	PI	Inhibitor	174	<chem>COc1ccc2[C@@H]3[C@H](COc2c1)C(C)(C)OC1=C3C(=O)C(=O)C2=C1OC(C)(C)[C@H]1COc3cc(OC)ccc3[C@@H]21</chem>
C5973	PI	Inhibitor	174	<chem>COc1cccc(CCc2c(OCCN3CCN(C)CC3)cccc2)c1</chem>
C5974	PI	Inhibitor	174	<chem>COc1cccc(CCc2c(OCCCN3CCc4cc(OC)c(OC)cc4C3)cccc2)c1</chem>
C5975	PI	Inhibitor	174	<chem>COc1cccc(CCc2c(OCCN3CCN(CC3)c3cc(Cl)ccc3)cccc2)c1</chem>
C5976	PI	Inhibitor	174	<chem>COc1cccc(CCc2c(OCCCN3CCN(CC3)c3cc(Cl)ccc3)cccc2)c1</chem>
C5977	PI	Inhibitor	174	<chem>COc1cccc(CCc2c(OCCCN3CCN(CC3)c3cc(Cl)ccc3)cccc2)c1</chem>
C5978	PI	Inhibitor	174	<chem>COc1cccc(CCc2c(OCCCN3CCN(CC3)c3cc(Cl)ccc3)cccc2)c1</chem>

C5979	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCN(CC3)e3ce(ccc3)C(F)(F)F)cccc2)c1
C5980	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCN(CC3)e3ce(ccc3)C(F)(F)F)cccc2)c1
C5981	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCN(CC3)e3e(OC)cccc3)cccc2)c1
C5982	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCN(CC3)e3e(OC)cccc3)cccc2)c1
C5983	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCN(CC3)e3e(OC)cccc3)cccc2)c1
C5984	PI	Inhibitor	174	COe1cccc(CCc2e(OCCN3CCN(CC3)e3ecc(F)cc3)cccc2)c1
C5985	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCN(CC3)e3ecc(F)cc3)cccc2)c1
C5986	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCN(CC3)e3ecc(F)cc3)cccc2)c1
C5987	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCN(CC3)e3ecc(F)cc3)cccc2)c1
C5988	PI	Inhibitor	174	COe1cccc(CCc2e(OCCN3CCN(CC3)e3nccn3)cccc2)c1
C5989	PI	Inhibitor	174	COe1cccc(CCc2e(OCCN3CCN(CC3)e3nccn3)cccc2)c1
C5990	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCN(CC3)e3nccn3)cccc2)c1
C5991	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCN(CC3)e3nccn3)cccc2)c1
C5992	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCN(C)CC3)cccc2)c1
C5993	PI	Inhibitor	174	COe1cccc(CCc2e(OCCN3CCe4cccc4C3)cccc2)c1
C5994	PI	Inhibitor	174	COe1cccc(CCc2e(OCCN3CCe4cccc4C3)cccc2)c1
C5995	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCe4cccc4C3)cccc2)c1
C5996	PI	Inhibitor	174	COe1cccc(CCc2e(OCCCCN3CCe4cccc4C3)cccc2)c1
C5997	PI	Inhibitor	174	COe1cccc(CCc2e(OCCN3CCe4cc(OC)c(OC)cc4C3)cccc2)c1
C5998	PI	Inhibitor	174	N([C@H](C)c1ccccc1)C(=O)Nc1ccc(S[C@@H]2CC3=CC(=O)CC[C@]3(C)[C@H]3CC[C@]4(C)[C@H](CC[C@H]4C(=O)C)[C@H]23)cc1
C5999	PI	Inhibitor	174	OCC12[C@@H]3C4[C@H]1N([C@@H]1C([C@H](N3C(=O)OC)C1(CO)[C@@H]4c1ccccc1)[C@@H]2c1ccccc1)C(=O)OC
C6000	PI	Inhibitor	174	OC(=O)CC[C@H](NC(=O)c1ccc(Cl)c(Cl)c1)C(=O)N(CCCCC)CCOC
C6001	PI	Inhibitor	174	OCC12[C@H]3C4[C@@H]1N([C@H]1C([C@@H](N3C(=O)OC(C)(C)C)C1(CO)[C@H]4c1ccccc1)[C@@H]2c1ccccc1)C(=O)OC(C)(C)C
C6002	PI	Inhibitor	174	OCC12[C@H]3C4[C@H](C5([C@@H](N([C@H]14)C(=O)Oe1ccccc1)C([C@H]2c1ccccc1)[C@@H]5N3C(=O)Oe1ccccc1)CO)c1ccccc1
C6003	PI	Inhibitor	174	OCC12[C@@H]3C4[C@H]1N(Cc1ccccc1)[C@@H]1C([C@H](N3Cc3ccccc3)C1(CO)[C@H]4c1ccccc1)[C@@H]2c1ccccc1
C6004	PI	Noninhibitor	174	OC(=O)Cc1ccccc1Nc1c(Cl)cccc1Cl
C6005	PI	Noninhibitor	174	N(C(=O)OC)c1[nH]c2c(cc(SCC)cc2)n1
C6006	PI	Noninhibitor	174	NC(=O)OC[C@](C)(CCC)COC(=O)NC(C)C
C6007	PI	Noninhibitor	174	NCCO/N=C(/CCCCOC)c1ccc(cc1)C(F)F
C6008	PI	Inhibitor	174	N1C(=O)CCe2c1ccc(OCCCCe1nnnn1C1CCCCC1)c2
C6009	PI	Noninhibitor	174	N1C(=S)NC(=O)C(CC)([C@H](C)CCC)C1=O
C6010	PI	Noninhibitor	174	OC(=O)/C=C/c1cc(O)c(O)cc1
C6011	PI	Noninhibitor	174	N(C)CC(C)(C)c1ccccc1
C6012	PI	Noninhibitor	174	OC(=O)C(C)(C)O/N=C(/C(=O)N[C@@H]1[C@H](C)N(C1=O)S(=O)(=O)O)\c1csc(n1)N
C6013	PI	Inhibitor	174	CN(C)CCCOe1nn(Cc2ccccc2)c2c1ccccc2
C6014	PI	Noninhibitor	174	OC(=O)C1=C(CSc2nnc(C)s2)CS[C@H]2N1C(=O)[C@@H]2NC(=O)Cn1cnn1
C6015	PI	Inhibitor	174	Oc1c2nc(Cl)nc2n(C)c(=O)n1C
C6016	PI	Noninhibitor	174	Cc1c2c(c(e3c1cc[nH]e3)C)c1ccccc1n2
C6017	PI	Noninhibitor	174	Oe1c(Cc2e(O)oc3ccccc3e2=O)c(=O)c2ccccc2o1
C6018	PI	Inhibitor	174	O[C@@]12OC(C)(NC(=O)[C@H]3C[C@H]4[C@@H](Cc5c[nH]c6cccc4c56)N(C)C3)C(=O)N1[C@@H](Cc1ccccc1)C(=O)N1CCC[C@@H]21
C6019	PI	Noninhibitor	174	OCCNC(=O)Cn1cnc1[N+](=O)[O-]
C6020	PI	Noninhibitor	174	Oc1cc(O)c2C(=O)C[C@@H](Oe2c1)c1cc(O)c(OC)cc1
C6021	PI	Noninhibitor	174	NS(=O)(=O)c1c(Cl)ccc(c1)C(=O)N[C@@H]1[C@@H](C)Nc2ccccc12
C6022	PI	Inhibitor	174	O[C@H]([C@@H](C)CCc1c(C(=O)c(O)c(C)cc1)[C@H](C)C(=O)[C@@H](CC)[C@H]1O[C@@](CC)(C[C@H]1C)[C@H]1CC[C@@](O)(CC)[C@@H](C)O1
C6023	PI	Noninhibitor	174	N(Cc1ccccc1)c1ncnc2c1[nH]cn2
C6024	PI	Noninhibitor	174	Oc1ccc(cc1)C(=O)N/N=C/c1ccc(o1)[N+](=O)[O-]

C6025	PI	Noninhibitor	174	c1ccc(ccc1O)[C@H](CC)[C@H](CC)c1ccc(O)cc1
C6026	PI	Noninhibitor	174	O[C@@]1(CC[C@@@H]2[C@@@H]3CCCC4=CC(=O)CC[C@@H]4[C@@H]3CC[C@@@]12C)C#C
C6027	PI	Noninhibitor	174	On1cccc1=S
C6028	PI	Inhibitor	174	Oe1c(cc(C)c(CC2=NCCN2)c1C)C(C)(C)C
C6029	PI	Noninhibitor	174	[N]=C(N)c1ccc(OCCCCCOe2ccc(cc2)C(=N)N)cc1
C6030	PI	Noninhibitor	174	O=C1C(C(=O)c2ccccc12)c1ccccc1
C6031	PI	Noninhibitor	174	O[C@@@H]([C@H](C)N)c1ccccc1
C6032	PI	Noninhibitor	174	OC(=O)[C@H]1N2[C@@@H](SC1(C)C)C(NC(=O)[C@H](NC(=O)N1CCN(CC)C(=O)C1=O)c1ccccc1)C2=O
C6033	PI	Noninhibitor	174	Oe1ccc(/C=C/c2cc(O)cc(O)c2)cc1
C6034	PI	Noninhibitor	174	OC[C@@]1(O)[C@H](C)C/C(=C/C)/C(=O)O[C@H]2CCN3CC=C(COC1=O)C23
C6035	PI	Noninhibitor	174	C1CCN2C[C@H]3C[C@@@H](CN4CCCC[C@H]34)C2C1
C6036	PI	Inhibitor	174	CC(=O)S[C@@@H]1CC2=CC(=O)CC[C@@@]2(C)[C@@@H]2CC[C@@@]3(C)[C@H](CC[C@@@]43CCC(=O)O4)[C@H]12
C6037	PI	Noninhibitor	174	OC(=O)c1c(OC(=O)C)cc(cc1)C(F)(F)F
C6038	PI	Noninhibitor	174	O[C@@@H]1CC[C@@@]2(C)[C@H](CC[C@@]3(C)[C@@@H]2CC=C2[C@@@H]4[C@@@H](C)[C@H](C)CC[C@@]4(CC[C@@]32C)C(=O)O)C1(C)C
C6039	PI	Noninhibitor	174	N1CCN=C1Cc1c(C)ccc(cc1C)C(C)(C)C
C6040	PI	Noninhibitor	174	N1=NC2=NC(=NC(=O)C2=N1)c1ccccc1OCCC
C6041	PI	Inhibitor	174	Ne1ccc(cc1)c1cc(cc(c1)C(F)(F)F)C(F)(F)F
C6042	PI	Inhibitor	174	OC1C[C@]2(C)[C@H](C)[C@H](C)[C@]2(OC(=O)c2ccco2)C(=O)C[C@@]1(C)[C@H]2CCC3=CC(=O)C=C[C@@@]3(C)[C@@]12C1
C6043	PI	Noninhibitor	174	N([C@@@H](C(C)C)C(=O)O[C@@@H](C#N)c1cc(Oc2ccccc2)ccc1)c1c(Cl)cc(cc1)C(F)(F)F
C6044	PI	Inhibitor	174	CCCOe1c(OC)cc2oc(cc(=O)c2c1O)c1ccccc1
C6045	PI	Inhibitor	174	COe1c2c(=O)cc(oc2cc(OC(=O)C)c1OC(=O)C)c1ccccc1
C6046	PI	Inhibitor	174	O[C@@@H](COe1ccccc1C(=O)C)CN1CCN(CC1)c1ccccc1C
C6047	PI	Inhibitor	174	O[C@H](COe1c(cc(OC)cc1)C(=O)C)CN1CCN(CC1)c1ccccc1C
C6048	PI	Inhibitor	174	[nH]1c2cc(OC)ccc2c1[C@H]1C[C@H]3[C@@@H](C[C@H](OC(=O)/C=C/c4cc(OC)c(OC)c(OC)c4)[C@@@H](OC)C3C(=O)OC)CN1CC2
C6049	PI	Inhibitor	174	O[C@H](COe1c(cc(C(=O)C)c(C)c1)C(=O)C)CN1CCN(CC1)c1ccccc1C
C6050	PI	Inhibitor	174	O[C@H](COe1cc(ccc1)C(=O)CCe1ccccc1)CN1CCN(CC1)c1ccccc1C
C6051	PI	Noninhibitor	174	Oe1c(cccc1OC)/C=N/NC(=O)C(=O)NC(C)(C)C
C6052	PI	Inhibitor	174	O[C@@@H](COe1c(cccc1)C(=O)c1ccccc1)CN(CC)CC
C6053	PI	Inhibitor	174	O[C@@@H](CN1CCN(CC1)c1ccccc1)C(=O)CCe1ccccc1
C6054	PI	Inhibitor	174	O[C@H](COe1ccccc1C(=O)CCe1ccccc1)CNC(c1ccccc1)c1ccccc1
C6055	PI	Inhibitor	174	O=C(CCc1ccccc1)c1ccccc1OCCCCCCCCN1CCCCC1
C6056	PI	Inhibitor	174	O[C@H](COe1c(cc(Oc2ccccc2)cc1)C(=O)CCe1ccccc1)CN1CCCCC1
C6057	PI	Inhibitor	174	O[C@@@H](COe1c(cc(Oc2ccccc2)cc1)C(=O)CCe1ccccc1)CN1CCN(Cc2ccccc2)CC1
C6058	PI	Noninhibitor	174	N(C)CCC[C@@@](C#N)(C(C)C)c1cc(OC)c(OC)cc1
C6059	PI	Inhibitor	174	O[C@@@H](COe1c(cccc1)C(=O)CCe1ccc(C)cc1)CN1CCN(CC1)c1c(C)ccccc1
C6060	PI	Inhibitor	174	COe1cccc(CCc2c(OCCCCN3CCc4cc(OC)c(OC)cc4C3)cccc2)c1
C6061	PI	Inhibitor	174	COe1cccc(CCc2c(OCCCCN3CCc4cc(OC)c(OC)cc4C3)cccc2)c1
C6062	PI	Inhibitor	174	COe1cccc(CCc2c(OCCCCN3CCN(C)CC3)cccc2)c1
C6063	PI	Inhibitor	174	COe1cccc(CCc2c(OCCCCN3CCN(C)CC3)cccc2)c1
C6064	PI	Inhibitor	174	N(CCC)C(=O)Nc1ccc(S[C@@@H]2CC3=CC(=O)CC[C@@]3(C)[C@H]3CC[C@@@]4(C)[C@H](CC[C@@H]4C(=O)C)[C@H]23)cc1
C6065	PI	Inhibitor	174	N(CC)C(=O)Nc1ccc(S[C@@@H]2CC3=CC(=O)CC[C@@]3(C)[C@@@H]3CC[C@@@]4(C)[C@H](CC[C@@@H]4C(=O)C)[C@H]23)cc1
C6066	PI	Inhibitor	174	CCCCc1ccc(cc1)C(=O)Nc1ccccc1C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC
C6067	PI	Inhibitor	174	Ce1cccc(c1NC(=O)c1ccc(cc1)C(C)C)C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC
C6068	PI	Noninhibitor	174	NCCC[C@@@](C#N)(C(C)C)c1cc(OC)c(OC)cc1
C6069	PI	Inhibitor	174	CC(C)c1ccc(cc1)C(=O)Nc1c(cccc1Cl)C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC
C6070	PI	Inhibitor	174	CC(C)c1ccc(cc1)C(=O)Nc1ccccc1C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC)Cl

C6071	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCNC(=O)c1cccc1NC(=O)c1ccc(cc1)Oe1cccc1
C6072	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCNC(=O)c1cccc1NC(=O)c1ccc(cc1)C(=O)c1cccc1
C6073	PI	Inhibitor	174	CC(C)c1ccc(cc1)C(=O)Nc1ccc(cc1)C(=O)NCCN1CCc2cc(c(cc2C1)OC)OCN
C6074	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCNC(=O)c1cccc1NC(=O)c1ccc(cc1)OC1CCCCC1
C6075	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCNC(=O)c1cccc1NC(=O)c1ccc(cc1)OCe1cccc1
C6076	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1cccc2e1cccc2
C6077	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCNC(=O)c1cccc1NC(=O)c1ccc(cc1)c1cccc1
C6078	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1cces1
C6079	PI	Inhibitor	174	Oe1c(OC)cc(cc1)[C@@](CCCN(C)CCc1cc(OC)c(OC)cc1)(C#N)C(C)C
C6080	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1ccsc1
C6081	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1ccoc1
C6082	PI	Inhibitor	174	Ce1ccc(cc1)C(=O)Nc1cccc1C(=O)Nc1ccc(cc1)CCN1CCc2cc(c(cc2C1)OC)OC
C6083	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1cc2cccc2o1
C6084	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1ccc2cccc2n1
C6085	PI	Inhibitor	174	CCC(=O)c1ncn(en1)C(=O)Nc1cccc1C(=O)Nc1ccc(cc1)CCN1CCc2cc(c(cc2C1)OC)OC
C6086	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCNC(=O)c1cccc1NC(=O)c1ccc2cccc2e1
C6087	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)Cc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1cc2cccc2nc1
C6088	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1ccc2c(nc1)CCCC2
C6089	PI	Inhibitor	174	CN(CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1cnc2cccc2n1)Cc1ccc(c(e1)OC)OC
C6090	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCNC(=O)c1cccc1NC(=O)c1ccc(cc1)C1CCCCC1
C6091	PI	Inhibitor	174	CN(CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1cc2cccc2nc1)Cc1ccc(c(e1)F)F
C6092	PI	Inhibitor	174	CN(CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1cc2cccc2nc1)Cc1ccc(c(e1)O)OC
C6093	PI	Inhibitor	174	CN(CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1cc2cccc2nc1)Cc1ccc(c(e1)OC)O
C6094	PI	Inhibitor	174	Ce1cnc(en1)C(=O)Nc1cccc1C(=O)Nc1ccc(c1)CCN1CCc2cc(c(cc2C1)OC)OC
C6095	PI	Inhibitor	174	CC(C)c1ccc(cc1)C(=O)Nc1cccc1C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC
C6096	PI	Inhibitor	174	CC(C)c1ccc(cc1)C(=O)Nc1ccc(cc1)C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC)Cl
C6097	PI	Inhibitor	174	CC(C)c1ccc(cc1)C(=O)Nc1ccc(cc1)C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC)Cl
C6098	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCNC(=O)c1cccc1NC(=O)c1ccc2cccc2n1
C6099	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCNC(=O)c1cccc1NC(=O)c1cc2cccc2en1
C6100	PI	Inhibitor	174	CCCc1ccc(cc1)C(=O)Nc1cccc1C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC
C6101	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCNC(=O)c1cccc1NC(=O)c1ccc(cc1)Br
C6102	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCNC(=O)c1cccc1NC(=O)c1ccc(cc1)Ce1cccc1
C6103	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1cccn1
C6104	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1cccn1
C6105	PI	Inhibitor	174	COe1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1cncn1
C6106	PI	Inhibitor	174	COe1ccc(c1)C(=O)Nc1cccc1C(=O)Nc1ccc(cc1)CCN1CCc2cc(c(cc2C1)OC)OC
C6107	PI	Inhibitor	174	COe1ccc(cc1OC)CN1CCc2ccc(cc2C1)NC(=O)c1cccc1NC(=O)c1cnc2cccc2n1
C6108	PI	Inhibitor	174	CN(CCc1ccc(cc1)NC(=O)c1cccc1NC(=O)c1cc2cccc2nc1)CCc1ccc(c(e1)OC)OC
C6109	PI	Inhibitor	174	Ce1nc(es1)C(=O)Nc1cccc1C(=O)Nc1ccc(cc1)CCN1CCc2cc(c(cc2C1)OC)OC
C6110	PI	Inhibitor	174	c1ccc(cc1)CCNc1c2c(c(e3n2CCCC3)C#N)ncn1
C6111	PI	Inhibitor	174	c1ccc(cc1)CS(=O)(=O)Nc1c2c(c(e3n2CCCC3)C#N)ncn1
C6112	PI	Inhibitor	174	c1ccc2e(c1)c(c[nH]2)CCN1CCN(CC1)c1c2c(c(e3n2CCCC3)C#N)ncn1
C6113	PI	Inhibitor	174	c1ccc(cc1)CCN1CCN(CC1)c1c2c(c(e3n2CCCC3)C#N)ncn1
C6114	PI	Inhibitor	174	c1ccc(cc1)CCCN1CCN(CC1)c1c2c(c(e3n2CCCC3)C#N)ncn1
C6115	PI	Inhibitor	174	c1ccc(cc1)CS(=O)(=O)N1CCN(CC1)c1c2c(c(e3n2CCCC3)C#N)ncn1
C6116	PI	Inhibitor	174	c1ccc(cc1)C(=O)CN1CCN(CC1)c1c2c(c(e3n2CCCC3)C#N)ncn1

C6117	PI	Inhibitor	174	c1ccc(c(c1)CCN1CCN(CC1)c1e2c(c(c3n2CCCC3)C#N)ncn1)C1
C6118	PI	Inhibitor	174	c1cc(cc(c1)C1)CCN1CCN(CC1)c1e2c(c(c3n2CCCC3)C#N)ncn1
C6119	PI	Noninhibitor	174	OCC(=O)[C@]1(O)CC(O)[C@H]2C[C@@H](N)[C@H](O)[C@@H](C)O2)c2c(O)c3c(C(=O)c4cccc(OC)c4C3=O)c(O)c2C1
C6120	PI	Inhibitor	174	c1cc(ccc1CCN1CCN(CC1)c1e2c(c(c3n2CCCC3)C#N)ncn1)C1
C6121	PI	Inhibitor	174	c1cc(cc(c1)[N+](=O)[O-])CCN1CCN(CC1)c1e2c(c(c3n2CCCC3)C#N)ncn1
C6122	PI	Inhibitor	174	c1cc(ccc1CCN1CCN(CC1)c1e2c(c(c3n2CCCC3)C#N)ncn1)[N+](=O)[O-]
C6123	PI	Inhibitor	174	COe1cccc(c1)CCN1CCN(CC1)c1e2c(c(c3n2CCCC3)C#N)ncn1
C6124	PI	Inhibitor	174	c1cc(c(cc1CCN1CCN(CC1)c1e2c(c(c3n2CCCC3)C#N)ncn1)F)F
C6125	PI	Inhibitor	174	c1ccc(cc1)CCN1CCN(CC1)c1e2c(c(c3n2CCCC3)C#N)nc(n1)I
C6126	PI	Inhibitor	174	c1ccc(cc1)CCN1CCN(CC1)c1e2c(c(c3n2CCCC3)C#N)nc(n1)c1cccc1
C6127	PI	Inhibitor	174	CC(=O)Nc1ccc(cc1)c1nc2c(c3n2c(c2c(n1)N1CCN(CC1)CCc1cccc1)CCCC3)C#N
C6128	PI	Inhibitor	174	c1cc(c(cc1CCN1CCN(CC1)c1e2c(c(c3n2CCCC3)C#N)nc(n1)c1cenc1)F)F
C6129	PI	Inhibitor	174	Cc1cccc1c1nc2c(c3n2c(c2c(n1)N1CCN(CC1)CCc1ccc(c(c1)F)F)CCCC3)C#N
C6130	PI	Noninhibitor	174	[nH]1cc(CCS(=O)(=O)c2cccc2)c2cc(C[C@@H]3CCCN3C)ccc12
C6131	PI	Inhibitor	174	c1ccc(cc1)CCN1CCN(CC1)c1e2c(c(c3n2CCCC3)C(=O)c2cccc2)ncn1
C6132	PI	Inhibitor	174	COC(=O)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1cccc1)CCCC2
C6133	PI	Inhibitor	174	Cc1c(sc(n1)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1cccc1)CCCC2)C
C6134	PI	Inhibitor	174	Cc1nc(no1)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1cccc1)CCCC2
C6135	PI	Inhibitor	174	CCNC(=O)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1ccc(c(c1)F)F)CCCC2
C6136	PI	Inhibitor	174	COe1cccc(c1OC)CNC(=O)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1ccc(c(c1)F)F)CCCC2
C6137	PI	Inhibitor	174	c1cenc(c1)CNC(=O)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1ccc(c(c1)F)F)CCCC2
C6138	PI	Inhibitor	174	c1cc(cnc1)NC(=O)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1ccc(c(c1)F)F)CCCC2
C6139	PI	Noninhibitor	174	O[C@@H]1C(O)[C@@H]2[C@H]3COC(=O)[C@@H]3[C@@H](c3cc(OC)c(O)c(OC)c3)c3cc4c(OCO4)cc23)O[C@@H]2CO[C@@H](C)O[C@H]2C1O
C6140	PI	Inhibitor	174	CO[C@@H](CCc1cccc1)c1cccc1OC[C@H](CN1CCN(CC1)c1ccc(cc1)F)O
C6141	PI	Inhibitor	174	CC(C)N(C[C@H](COc1cccc1C(=O)CCc1cccc2c1cccc2)O)C(C)C
C6142	PI	Inhibitor	174	c1ccc(cc1)CCC(=O)c1ccc(cc1)OC[C@H](CN1CCCCC1)O
C6143	PI	Inhibitor	174	c1ccc(cc1)CCC(=O)c1ccc(cc1)OC[C@H](CN1CCOCC1)O
C6144	PI	Inhibitor	174	c1ccc(cc1)CCC(=O)c1cc(ccc1OC[C@H](CN1CCCCC1)O)OCc1cccc1
C6145	PI	Noninhibitor	174	[nH]1c2cc(ccc2nc1c1ccc2[nH]c(nc2c1)c1ccc(OCC)cc1)N1CCN(C)CC1
C6146	PI	Inhibitor	174	c1ccc(cc1)CCC(=O)c1cc(ccc1OC[C@@H](CN1CCN(CC1)Cc1cccc1)O)OCc1cccc1
C6147	PI	Inhibitor	174	CC(=O)c1ccc(cc1)OC[C@H](CN1CCN(CC1)c1ccc(cc1)F)O
C6148	PI	Noninhibitor	174	CC(=O)c1ccc(cc1)OC[C@H](CN1CCOCC1)O
C6149	PI	Inhibitor	174	c1ccc(cc1)CCC(=O)c1cccc1OC[C@@H](CN1CCN(CC1)Cc1cccc1)O
C6150	PI	Inhibitor	174	c1ccc(cc1)CCC(=O)c1cccc1OC[C@H](CNCCC(c1cccc1)c1cccc1)O
C6151	PI	Inhibitor	174	CCN(CC)C[C@H](COc1cccc1C(=O)CCc1cccc1)O
C6152	PI	Inhibitor	174	c1ccc(cc1)CCC(=O)c1cccc1OC[C@@H](CN1CCCCC1)O
C6153	PI	Inhibitor	174	COe1cccc1N1CCN(CC1)C[C@@H](COc1cccc1C(=O)CCc1cccc1)O
C6154	PI	Inhibitor	174	c1ccc(cc1)CCC(=O)c1cccc1OC[C@@H](CNCC(c1cccc1)c1cccc1)O
C6155	PI	Inhibitor	174	Cc1c(c(=O)n(n1C[C@@H](CN(C(C)C)C(C)C)O)c1cccc1)C(=O)c1cccc1
C6156	PI	Inhibitor	174	Cc1cccc1N1CCN(CC1)C[C@@H](Cn1c(C)c(c(=O)n1c1cccc1)C(=O)c1cccc1)O
C6157	PI	Noninhibitor	174	CCCNC[C@H](Cn1c(c(c(=O)n1c1cccc1)C(=O)c1ccs1)C)O
C6158	PI	Noninhibitor	174	Cc1c(c(=O)n(n1C[C@H](CNC(C)C)O)c1cccc1)C(=O)c1ccs1
C6159	PI	Inhibitor	174	CCCNC[C@@H](Cn1c(c(c(=O)n1c1cccc1)C(=O)CCc1cccc1)C)O
C6160	PI	Inhibitor	174	Cc1c(c(=O)n(n1C[C@@H](CNC(C)C)O)c1cccc1)C(=O)CCc1cccc1
C6161	PI	Inhibitor	174	CCCCNC[C@H](Cn1c(c(c(=O)n1c1cccc1)C(=O)CCc1cccc1)C)O
C6162	PI	Inhibitor	174	Cc1c(c(=O)n(n1C[C@H](CNC(C)C)O)c1cccc1)C(=O)CCc1cccc1

C6163	PI	Inhibitor	174	<chem>OC[C@]1(O)O[C@H]([C@H]2C[C@H](C)[C@H](O2)[C@]2(CC)CC[C@@H](O2)[C@]2(C)CC[C@@]3(C)[C@@H](O)[C@@H](C)C(O3)[C@H](C)[C@@H](OC)[C@@H](C)C(=O)O)2)C(C)C[C@@H]1C</chem>
C6164	PI	Inhibitor	174	<chem>Cc1ccccc1N1CCN(CC1)C[C@@H](Cn1c(c(=O)n1c1ccccc1)C(=O)CCc1ccccc1)C)O</chem>
C6165	PI	Inhibitor	174	<chem>Cc1c(c(n1)C)OC[C@H](CN(C(C)C)C(C)C)O)C(=O)c1ccccc1</chem>
C6166	PI	Inhibitor	174	<chem>Cc1c(c(n1)c1ccccc1)OC[C@H](CN(C(C)C)C(C)C)O)C(=O)c1ccccc1</chem>
C6167	PI	Noninhibitor	174	<chem>CC1([C@@H](C(c2cc(ccc2O1)C#N)NC)O)C</chem>
C6168	PI	Inhibitor	174	<chem>CC1([C@@H](C(c2cc(ccc2O1)C#N)N(Cc1ccccc1)CC(=O)OC(C)(C)C)O)C</chem>
C6169	PI	Inhibitor	174	<chem>CCN(CC)CCC[C@H](C)N[C@H]1c2ccccc2N([C@H]([C@@H]1O)C)C(=O)c1ccc(cc1)C</chem>
C6170	PI	Inhibitor	174	<chem>CCN(CC)CCC[C@H](C)N[C@H]1c2ccccc2N[C@H]([C@@H]1OC(=O)c1ccc(cc1)C)C</chem>



Table S1. Reference of collected molecules

Reference	Title	Journal reference	Authors
1	The effect of multiple N-methylation on intestinal permeability of cyclic hexapeptides	Molecular pharmaceutics, 2011; 8 (2); 479-87	Ovadia, O; Greenberg, S; Chatterjee, J; Laufer, B; Opperer, F; Kessler, H; Gilon, C; Hoffman, A;
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26	ADME Evaluation in Drug Discovery. 9. Prediction of Oral Bioavailability in Humans Based on Molecular Properties and Structural Fingerprints	Pharm Res (2014) 31:1002–1014	Marlene T. Kim & Alexander Sedykh & Suman K. Chakravarti & Roustem D. Saiakhov & Hao Zhu
27	PK/DB (a freely available database for pharmacokinetic properties)	Molecular Pharmaceutics, 2011, 8, 841-851	Tian, S.;Li, Y. Y.;Wang, J. M.;Zhang, J.;Hou, T. J.
28	Experimental and computational screening models for the prediction of intestinal drug absorption	<a href="http://miro.ifsc.usp.br/pkdb/resume.php?mid=Nzc5">http://miro.ifsc.usp.br/pkdb/resume.php?mid=Nzc5</a>	
29	CODES/neural network model: A useful tool for in silico prediction of oral absorption and blood-brain barrier permeability of structurally diverse drugs	Journal of Medicinal Chemistry, 2001; 44 (12); 1927-37	Stenberg, P; Norinder, U; Luthman, K; Artursson, P
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Constitutional Crippen logP and MR	12	Sv, Sse, Spe, Sare, Sp, Si, Mv, Mse, Mpe, Mare, Mp, Mi	2D	
Detour matrix Eccentric connectivity index	2	CrippenLogP, CrippenMR	2D	Wildman, S. A., and Crippen, G. M. (1999). Prediction of Physicochemical Parameters by Atomic Contributions. <i>J Chem Inf Comput Sci</i> 39, 868-873.
Atom type electrotopological state	11	SpMax_Dt, SpDiam_Dt, SpAD_Dt, SpMAD_Dt, EE_Dt, VE1_Dt, VE2_Dt, VE3_Dt, VR1_Dt, VR2_Dt, VR3_Dt	2D	Todeschini, R. and Consonni, V. (2009). <i>Molecular descriptors for chemoinformatics</i> , (Weinheim: Wiley VCH) pg 714-726
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FMFDescriptor	1	FMF	2D	Roy K, Das R N, On some novel extended topochemical atom (ETA) parameters for effective encoding of chemical information and modeling of fundamental physicochemical properties. <i>SAR QSAR Environ Res</i> 22, 2011, 451-472, <a href="http://dx.doi.org/10.1080/1062936X.2011.569900">http://dx.doi.org/10.1080/1062936X.2011.569900</a>
Fragment complexity	1	fragC	2D	Yang, Y. and Chen, H. and Nilsson, I. and Muresan, S. and Engkvist, O., Investigation of the Relationship between Topology and Selectivity for Druglike Molecules, <i>J. Med. Chem.</i> , 2010, 53: 7709-7714
Hbond acceptor count	4	nHBAcc, nHBAcc2, nHBAcc3, nHBAcc_Lipinski	2D	Nilakantan, R. and Nunn, D.S. and Greenblatt, L. and Walker, G. and Haraki, K. and Mobilio, D., A family of ring system-based structural fragments for use in structure-activity studies: database mining and recursive partitioning., <i>Journal of chemical information and modeling</i> , 2006, 46:1069-1077
Hbond donor count	2	nHBDon, nHBDon_Lipinski	2D	
Hybridization ratio	1	HybRatio	2D	
Information content	42		2D	Todeschini, R. and Consonni, V. (2009). <i>Molecular descriptors for chemoinformatics</i> , (Weinheim: Wiley VCH) pg 408-411.
Kappa shape indices	3	Kier1, Kier2, Kier3	2D	Hall, L. H., and Kier, L. B. (1991). The molecular connectivity chi indices and kappa shape indices in structure-property modeling. In <i>Reviews of Computational Chemistry</i> , K.B. Lipkowitz, and D.B. Boyd, eds. (New York: VCH publishers), pp. 367-412.
Largest chain	1	nAtomLC	2D	
Largest Pi system	1	nAtomP	2D	
Longest aliphatic chain	1	nAtomLAC	2D	

Mannhold LogP	1	MLogP	2D	Mannhold, R. and Poda, G.I. and Ostermann, C. and Tetko, I.V., Calculation of molecular lipophilicity: State-of-the-art and comparison of log P methods on more than 96,000 compounds, J.Pharm.Sci., 2009, Abraham MH, McGowan JC. The use of characteristic volumes to measure cavity terms in reversed phase liquid chromatography. Chromatographia. 1987;23:243-6.
McGowan volume	1	McGowan_Volume	2D	
Molecular distance	19		2D	Liu, S. and Cao, C. and Li, Z., Approach to Estimation and Prediction for Normal Boiling Point (NBP) of Alkanes Based on a Novel Molecular Distance Edge (MDE) Vector, lambda, Journal of Chemical Information and Computer Sciences, 1998, 38:387-394
edge Molecular linear free energy relation	6	MLFER_A, MLFER_BH, MLFER_BO, MLFER_S, MLFER_E, MLFER_L	2D	Platts JA, Butina D, Abraham MH, Hersey A. Estimation of molecular free energy relation descriptors using a group contribution approach. J Chem Inf Comput Sci. 1999;39(5):835-45.
Path counts	22		2D	Todeschini, R. and Consonni, V. (2009). Molecular descriptors for chemoinformatics, (Weinheim: Wiley VCH) pg 574-579, pg 395-402
Petitjean number	1	PetitjeanNumber	2D	
Ring count	68		2D	
Rotatable bonds	4	nRotB, RotBFrac, nRotBt, RotBtFrac	2D	
Rule of five	1	LipinskiFailures	2D	
Topological	3	topoRadius, topoDiameter, topoShape	2D	
Topological charge	21		2D	Todeschini, R. and Consonni, V. (2009). Molecular descriptors for chemoinformatics, (Weinheim: Wiley VCH) pg 809-812
Topological distance matrix	11	SpMax_D, SpDiam_D, SpAD_D, SpMAD_D, EE_D, VE1_D, VE2_D, VE3_D, VR1_D, VR2_D, VR3_D	2D	Todeschini, R. and Consonni, V. (2009). Molecular descriptors for chemoinformatics, (Weinheim: Wiley VCH) pg 714-726
Topological polar surface area	1	TopoPSA	2D	Ertl, P. and Rohde, B. and Selzer, P., Fast Calculation of Molecular Polar Surface Area as a Sum of Fragment-Based Contributions and Its Application to the Prediction of Drug Transport Properties, J. Med. Chem., 2000, 43:3714-3717
Van der Waals volume	1	VABC	2D	
Vertex adjacency information (magnitude)	1	vAdjMat	2D	
Walk counts	20		2D	Todeschini, R. and Consonni, V. (2009). Molecular descriptors for chemoinformatics, (Weinheim: Wiley VCH) pg 875-882, pg 678-681
Weight	2	MW, AMW	2D	
Weighted path	5	WTPT-1, WTPT-2, WTPT-3, WTPT-4, WTPT-5	2D	Randic, M., On molecular identification numbers, Journal of Chemical Information and Computer Science, 1984, 24:164-175
Wiener numbers	2	WPATH, WPOL	2D	Wiener, Harry, Structural Determination of Paraffin Boiling Points, Journal of the American Chemical Society, 1947, 69:17-20
XLogP	1	XLogP	2D	Wang, R., Fu, Y., and Lai, L., A New Atom-Additive Method for Calculating Partition Coefficients, Journal of Chemical Information and Computer Sciences, 1997, 37:615-621; Wang, R., Gao, Y., and Lai, L., Calculating partition coefficient by atom-additive method, Perspectives in Drug Discovery and Design, 2000, 19:47-66

Zagreb index	1	Zagreb	2D	
Drug-likeness descriptor	9	Drug-likenessdescriptor	2D	Bickerton, G. R.; Paolini, G. V.; Besnard, J.; Muresan, S.; Hopkins, A. L., Quantifying the chemical beauty of drugs. Nat Chem 2012, 4 (2), 90-8.
Estate fingerprint	79	E-State fragments	Fingerprint	Hall LH, Kier LB. Electrotopological state indices for atom types: A novel combination of electronic, topological, and valence state information. J Chem Inf Comput Sci, 1995;35:1039-45
MACCS fingerprint	166	MACCS keys	Fingerprint	
Pubchem fingerprint	881	Pubchem fingerprint	Fingerprint	<a href="ftp://ftp.ncbi.nlm.nih.gov/pubchem/specifications/pubchem_fingerprints.txt">ftp://ftp.ncbi.nlm.nih.gov/pubchem/specifications/pubchem_fingerprints.txt</a>
Substructure	307	Presence of SMARTS Patterns for Functional Group Classification by Christian Laggner	Fingerprint	Openbabel's SMARTS_InteLigand.txt
Klekota-Roth fingerprint	4860	Presence of chemical substructures	Fingerprint	Klekota J, Roth FP. Chemical substructures that enrich for biological activity. Bioinformatics, 2008;24(21):2518-25
2D atom pairs	780	Presence of atom pairs at various topological distances	Fingerprint	

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Table S3. Analysis of variance table of the regression model

Term	Df	Sum Sq	Mean Sq	F value	Pr(>F)
CI	1	0.035491	0.035491	713.4991	5.56E-28
Diversity of Feature	1	0.001916	0.001916	38.51691	2.01E-07
Diversity of Sample	1	0.006577	0.006577	132.2188	1.48E-14
Data Set	4	0.034539	0.008635	173.5911	1.58E-25
Residuals	42	0.002089	4.97E-05		

Table S4. The adjusted  $P$ -values of pairwise contrasts for different ensemble based methods

Data set	Subset	Model	Bagging based	Boosting based	AECF
CacoP	TES	SVM-Bagging	1	0.7442	0.0002
		SVM-Boosting	0.7442	1	0.0002
		AECF	0.0005	0.0005	1
	VAS	SVM-Bagging	1	0.8948	0.0002
		SVM-Boosting	0.8948	1	0.0002
		AECF	0.0005	0.0005	1
HIA	TES	RF-Bagging	1	0.0233	0.0002
		RF-Boosting	0.0233	1	0.0002
		AECF	0.0004	0.0005	1
	VAS	RF-Bagging	1	0.123	0.0002
		RF-Boosting	0.123	1	0.0002
		AECF	0.0005	0.0005	1
OB	TES	SVM-Bagging	1	0.0098	0.0002
		SVM-Boosting	0.0098	1	0.0002
		AECF	0.0005	0.0005	1
	VAS	SVM-Bagging	1	0.0619	0.0002
		SVM-Boosting	0.0619	1	0.0002
		AECF	0.0005	0.0005	1
PS	TES	KNN-Bagging	1	0.0017	0.0002
		KNN-Boosting	0.0017	1	0.0002
		AECF	0.0005	0.0005	1
	VAS	KNN-Bagging	1	0.2264	0.0002
		KNN-Boosting	0.2264	1	0.0002
		AECF	0.0005	0.0005	1
PI	TES	SVM-Bagging	1	1	0.0002
		SVM-Boosting	1	1	0.0002
		AECF	0.0005	0.0005	1
	VAS	SVM-Bagging	1	0.1231	0.0002
		SVM-Boosting	0.1231	1	0.0002
		AECF	0.0005	0.0005	1



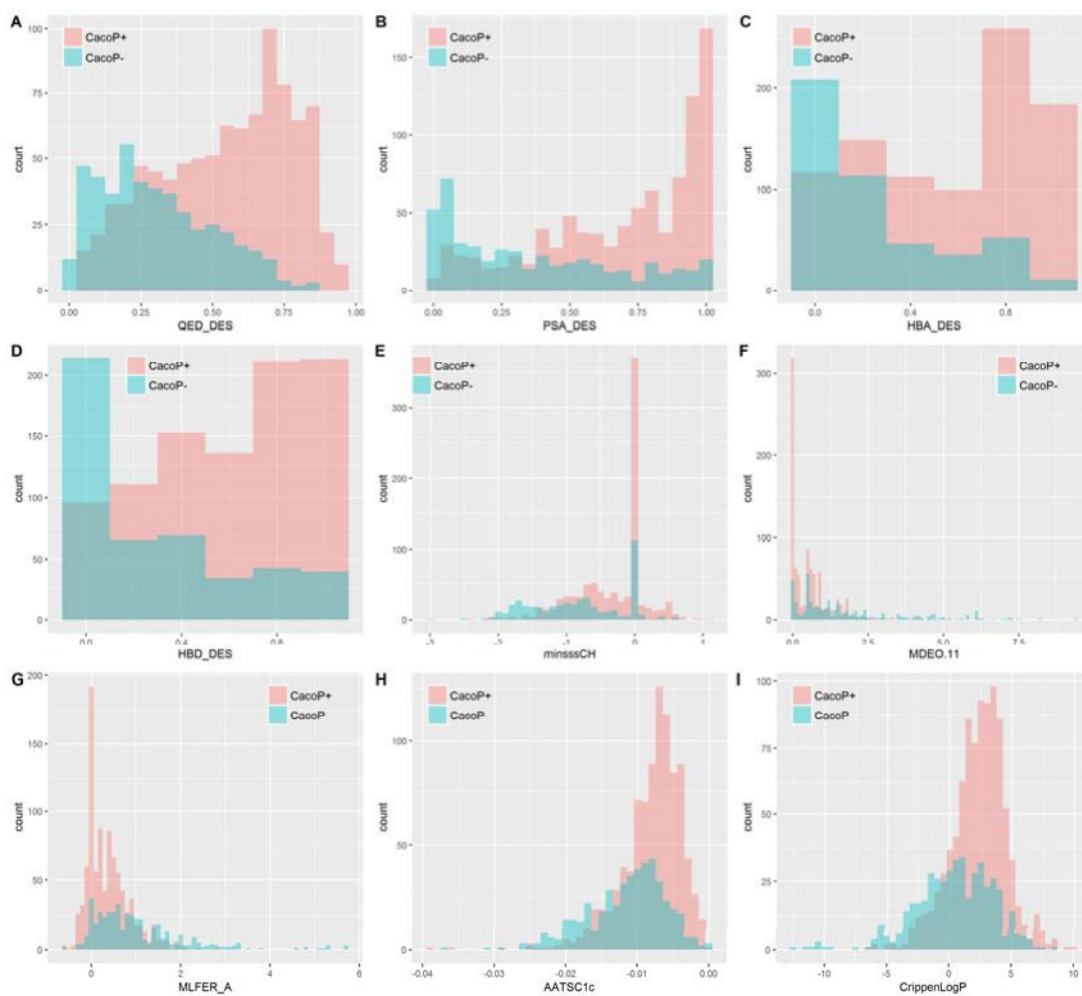


Figure S1 Distributions of top-9 molecular properties for CacoP data

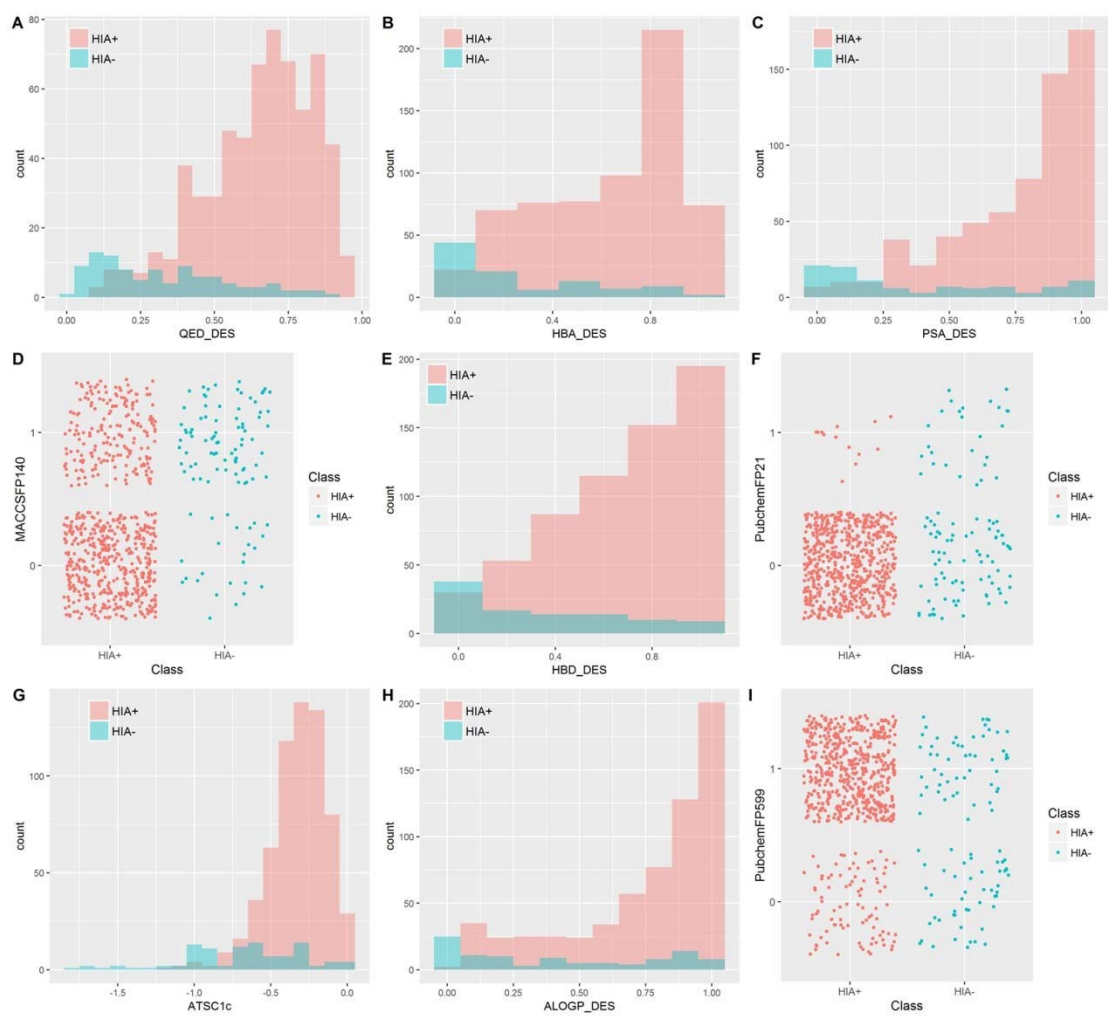


Figure S2 Distributions of top-9 molecular properties for HIA data

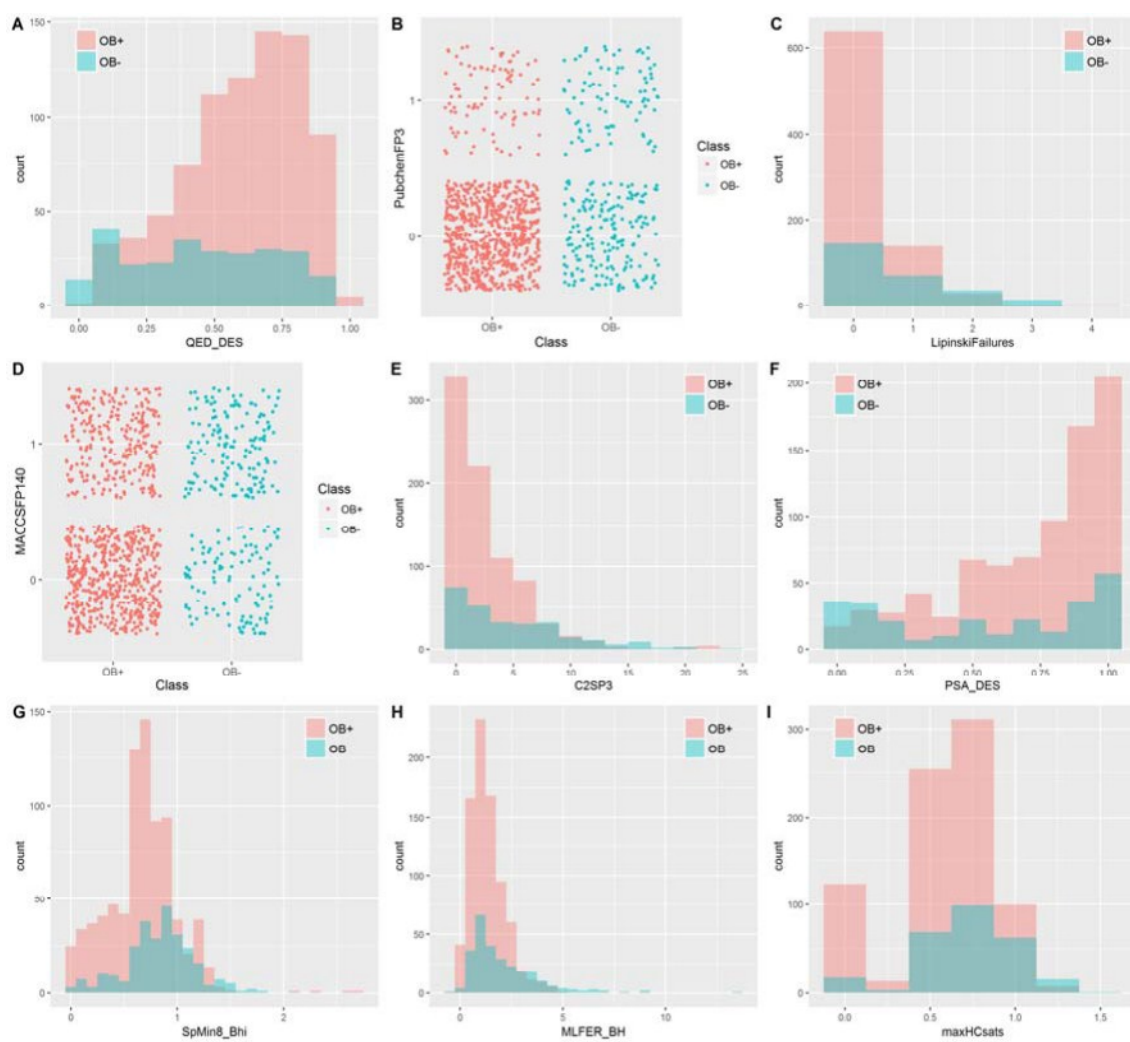


Figure S3 Distributions of top-9 molecular properties for OB data

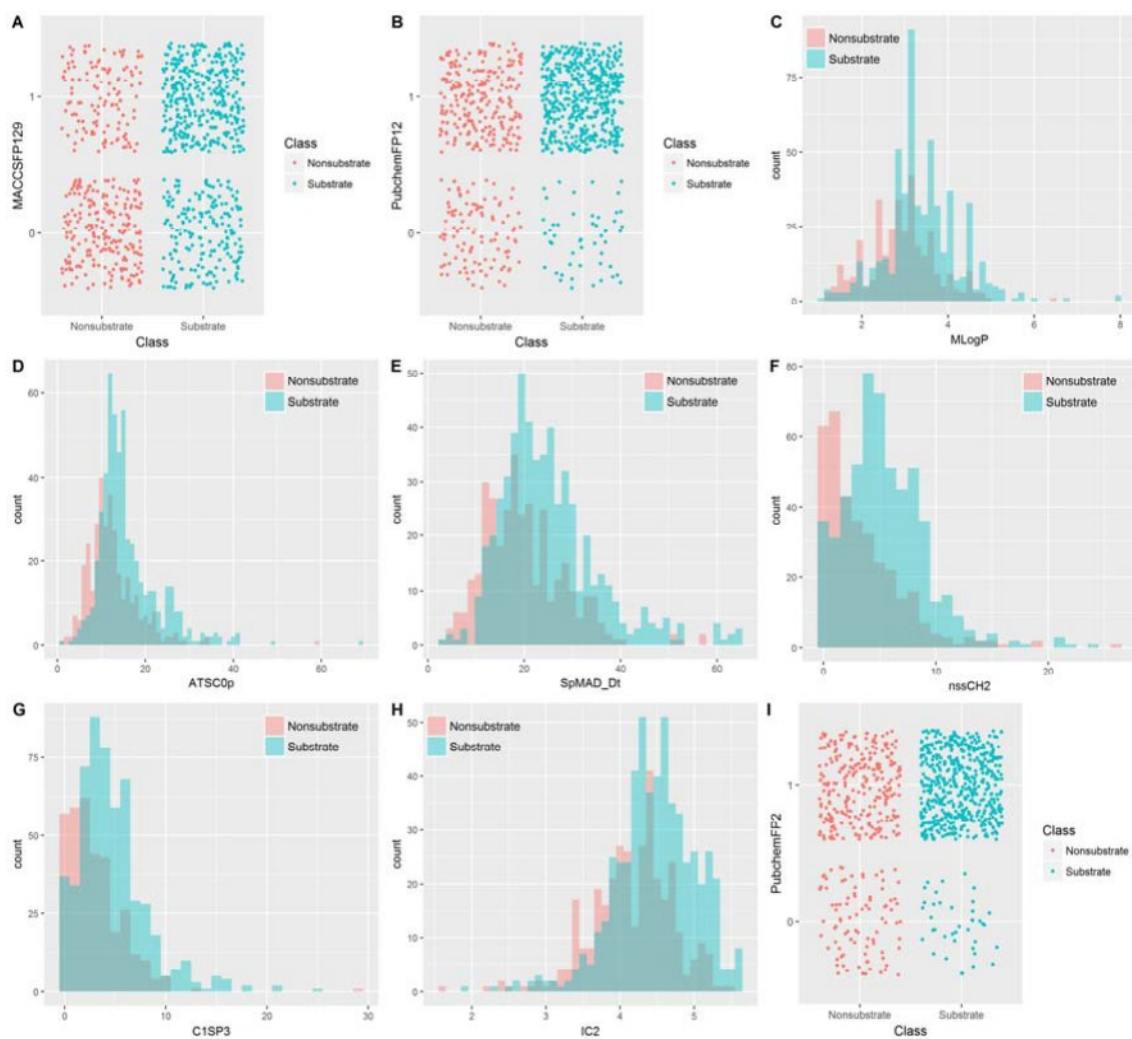


Figure S4 Distributions of top-9 molecular properties for PS data

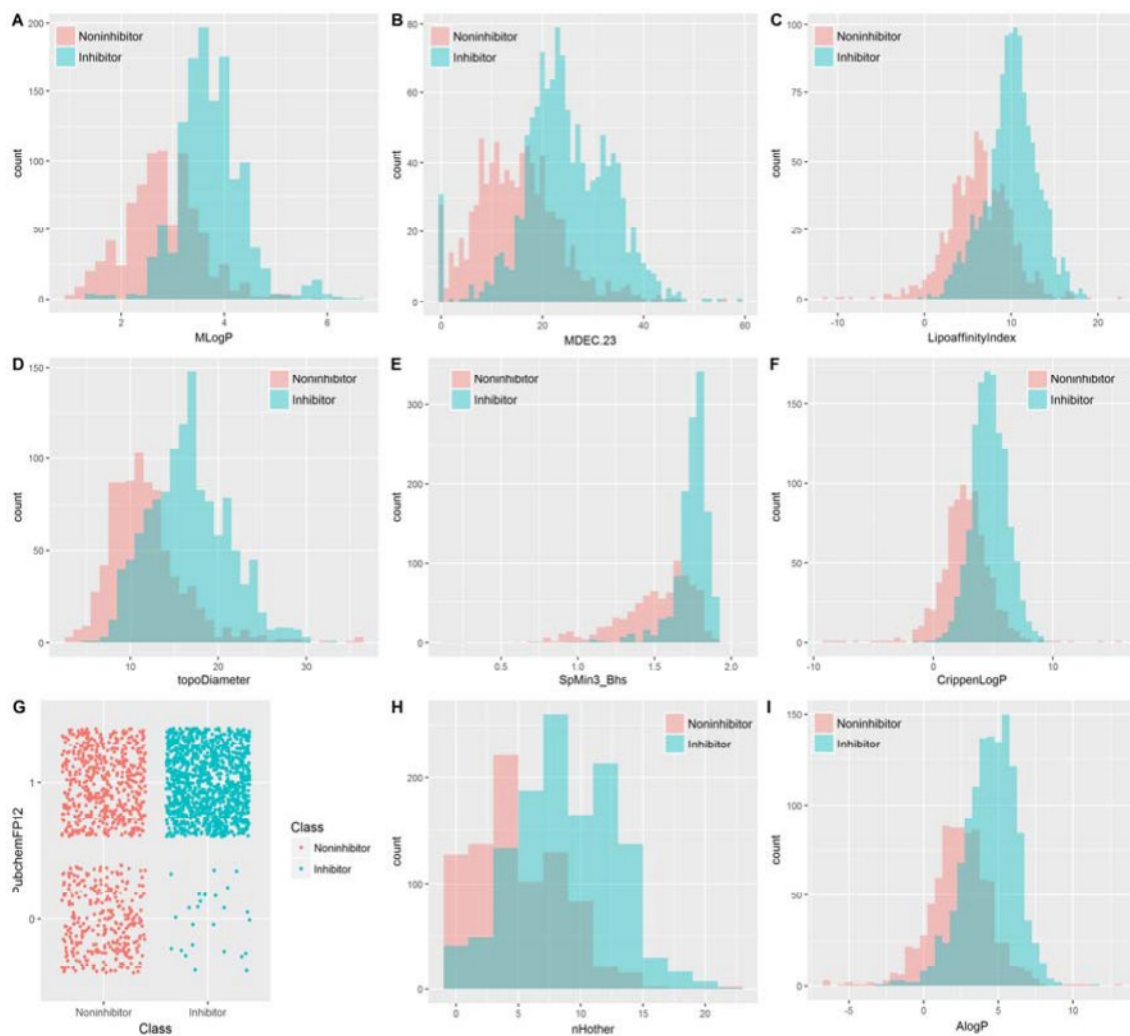


Figure S5 Distributions of top-9 molecular properties for PI data