SMILES	Class
OCC(CO)(CBr)CBr	0
[Na+].COC(=O)C1=C(C=C(I)C=C1)S(=O)(=O)[N-]C(=O)NC1=NC(OC)=NC(C)=N1	0
CC1(O)CSC(C)(O)CS1	0
COC1=C(C=CC=C1)[N+]([O-])=O	0
C1=CC(=CC=N1)C1=CC=NC=C1	0
Clc1cccc(c1)C2=NOC3CCCCC23	1
[Na+].[Na+].CC(=O)NC1=CC(=CC2=C1C(O)=C(N=NC1=CC=CC=C1)C(=C2)S([O-])(=O)=O)S([O-])(=O	0
CC(C)C1=CC=C(C)C=C1	0
O=NN1CCCCCC1	0
CC1CC(C)(C)Nc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CC1=C(NC(=N)NC(N)=N)C=CC=C1	0
CC1CCCN1c2ccc3[nH]c(=O)cc(c3c2)C(F)(F)F	1
CN\C(NCC1=CN=C(Cl)S1)=N/[N+]([O-])=O	0
CN(C)C(=N)NC(N)=N	0
CCCCc1ccc(cc1)C(=O)N2C[C@@H]3C[C@H]2[C@H]4N3C(=O)N(C4=O)c5ccc(cc5)C#N	1
CC1=CC=C(S)C=C1	0
CC#C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CCC4=C3[C@H](C[C@]12C)c5ccc(cc5)N(C)C	1
CC(C(O)=O)C1=CC=C(C(F)=C1)C1=CC=CC=C1	0
FC(F)(F)CN(Cc1cocc1)c2ccc3[nH]c(=O)cc(c3c2)C(F)(F)F	1
OC(=O)C1=C(C=CC=C1)C(=O)NC1=CC=CC2=C1C=CC=C2	0
C1COC=CC1	0
C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O	1
CC1(C)CN(Cc2cccc(F)c2)C(=O)C1Oc3ccc(C#N)c(c3)C(F)(F)F	1
N#CC(C1=CC=CC=C1)C1=CC=CC=C1	0
N1N=NN=C1C1=CC=CC=C1	0
CCC1CCNc2cc3n(C)c(=O)cc(c3cc12)C(F)(F)F	1
COC1=C(OC)C=C(C=C1)C(=CC(=O)N1CCOCC1)C1=CC=C(Cl)C=C1	1
CC(C)=CCC[C@](C)(O)[C@H]1CCC(C)=CC1	0
CCCCOC(=O)CCCCC(=O)OCCCC	0
Clc1ccc(cc1Cl)N2C(=O)[C@@H]3C4CCC(O4)[C@@H]3C2=O	1
[Na+].COC1=CC(OC)=NC(NC(=O)[N-]S(=O)(=O)C2=NC=CC=C2OCC(F)(F)F)=N1	0
COC1=CC=C(O)C=C1	0
CC12CCC(C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(c(c4)C(F)(F)F)[N+](=O)[O-]	1
[Cl-].C[N+]1(C)CCCCC1	0
CC(OC1=CC(Cl)=CC=C1)C(O)=O	0
OCC1=CC=CC=C1	0
[O-][N+](=O)c1ccc(N2C(=O)[C@@H]3C4CCC(O4)[C@@H]3C2=O)c5ccccc15	1
O[C@@H]1[C@H](CC2=CC=CC(=C2)C(O)=O)COC2=C1C=C(OCC1=NC3=C(S1)C=CC(F)=C3)C=C2	0
CCCCCCCCCOC1=CC(O)=C(C=C1)C(=O)C1=CC=CC=C1	0
C[C@]1(O)CC[C@H]2[C@@H]3[C@H](CCCc4cccc(OCCCC(=O)O)c4)CC5=CC(=O)CC[C@]5(C)[C	1
CCC(=O)C1CC(CC=C1C)C(C)C	0
CCCSC(=O)N(CCC)CCC	0
CCCCCCCCCCCCCCCCCC(=O)OCC	0
O=C1NNC(=O)C=C1	0

[Na+].[Na+].COC1=CC=CC=C1\N=N\C1=C(C=C2C=C(C=C(NC(C)=O)C2=C1O)S([O-])(=O)=O)S([O-])(	0
OC(=O)C1=CC(OC2=CC=CC=C2)=CC=C1	0
CCCCC(CN1C=NC=N1)(C#N)C1=CC=C(Cl)C=C1	0
CC1=CC(C)=C(O)C=C1	0
OC(=O)CC(O)(CC(O)=O)C(O)=O	0
CC1=CC(C)(C)Nc2ccc3-c4ccccc4O/C(=C\c5ccccc5C)/c3c12	1
CSC(=O)C1=C(N=C(C(C(=O)SC)=C1CC(C)C)C(F)(F)F)C(F)F	0
CCC(=O)N1C[C@@]2(C)O[C@@](C)(C1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F	1
CC(=O)C=CC1=C(C)CCCC1(C)C	0
CN1[C@@H]2CC[C@@H]3[C@H](CC[C@@]4(C)[C@H]3C/C(=C\c5cc(F)cc(F)c5)/[C@@H]4O)[C@	1
CCCCCCCCCCCCS	0
CON1C[C@@]2(C)O[C@@](C)(C1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F	1
CC1(C)N(CCCCO)C(=O)N(C1=O)c2ccc(C#N)c(c2)C(F)(F)F	1
OC[C@@H]1CC[C@@H](O1)N1C=NC2=C1N=CNC2=O	0
CC(C)(C)CNc1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
FC(F)(F)c1cc(ccc1C#N)N2C(=O)[C@@H]3C4CCC(O4)[C@@H]3C2=O	1
COc1cc(Oc2ccccc2C)ccc1C#N	1
OC1=CC=C2C=CC=CC2=C1\N=N\C1=CC=CC=C1	0
COc1c(ccc2oc(=O)c3c(ccc4[nH]c(=O)cc(C)c34)c12)C(=O)OC(F)(F)F	1
CCCN(CC(F)(F)F)c1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
CCOC1=CC2=C(NC(C)(C)C=C2C)C=C1	0
Cc1ccccc1Sc2ccc(cc2Cl)C#N	1
CCCCCCCCCCCCCC(=O)OC(C)C	0
C(CN1CCOCC1)OCCN1CCOCC1	0
CC(C)(O)C1=CC=C(CNC(=O)C2=CC=CN=C2OC2=CC=C(F)C=C2)C=C1	0
NCC1CCCC(CN)C1	0
NC(N)=NC1=NC(CSCCC(N)=NS(N)(=O)=O)=CS1	0
[Na+].[O-]C(=O)COC1=C(Cl)C=C(Cl)C=C1	0
Cc1c(Br)c(ccc1N2C(=O)[C@@H]3[C@H](O)CCN3C2=O)C#N	1
CC(C)=CCC\C(C)=C\COC(C)=O	0
Oc1cc2ccccc2cc1/C=N/NC(=O)c3cc4ccccc4cc3O	1
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)S(=O)(=O)c5c	1
Cc1cc(C)cc(c1)N(Cc2ccc(O)cc2)c3cc(C(=O)N4CCCC4)n(C)c3	1
Cc1cc(ccc1Br)N2C(=O)[C@@H]3C4CCC(C=C4)[C@@H]3C2=O	1
CN(C)C(C)=O	0
FC(F)(F)c1cc(OC2CCCCC2C#N)ccc1C#N	1
CCCCN(C)C(=O)CCCCCCCCC[C@@H]1CC2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC	1
OC(=O)C(Cl)Cl	0
CC1=CC(C)=C(C=C1)[N+]([O-])=O	0
CC(C)=CC1C(C(=O)OCC2=CC=CC(OC3=CC=CC=C3)=C2)C1(C)C	0
NC(=O)NO	0
CN1c2cc3nc(O)cc(c3cc2C(=CC1(C)C)C)C(F)(F)F	1
ClC(Cl)C(=O)N(CC=C)CC=C	0
CCCCN(C)C(=O)CCCCCCCC[C@@H]1CC2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C	1
N1C2=C(C=CC=C2)N=C1C1=CSC=N1	0

CCC(=O)C1=CC=C(Cl)C=C1	0
[Na+].OC[C@@H](O)[C@H]1OC(=O)C(O)=C1[O-]	0
O=C1CC2(CCCC2)CC(=O)N1CCCCN1CCN(CC1)C1=NC=CC=N1	0
C[C@@H]1CC[C@H](C)N1c2ccc3[nH]c(=O)cc(c3c2)C(F)(F)F	1
CNC(=O)\C=C(/C)OP(=O)(OC)OC	0
CCC(C)N(C)c1cc(c(cn1)C#N)C(F)(F)F	1
CCCNC(=O)NS(=O)(=O)C1=CC=C(Cl)C=C1	0
[Na+].CCCCCCCCCCCCCCCCCCOS([O-])(=O)=O	0
OCCCCO	0
CCCCCC\C=C\CCCCCCCC(O)=O	0
FC(F)(F)CN(CCCl)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
Fc1ccc(C2=NOC3CCCCC23)c(c1)C(F)(F)F	1
COC(=O)CCCC(=O)OC	0
CC1(C)CN(Cc2ccccc2F)C(=O)[C@@H]1Oc3ccc(C#N)c(c3)C(F)(F)F	1
COC1=CC=C(C=C1)N1N=C(C=C1C1=CC=C(C=C1)S(C)=O)C(F)F	0
FC(F)(F)c1cc(ncc1C#N)N2CCCCC2	1
OC(=O)CCC1=CC=CC=C1	0
CC1CC(O)CC(C)(C)C1	0
CC1(C)CCC[C@@]2(C)[C@@H]1Nc3cc4nc(O)cc(c4cc23)C(F)(F)F	1
CC1=C(CC(O)=O)C2=C(C=CC(F)=C2)\C1=C/C1=CC=C(C=C1)S(C)=O	0
CCCCOC1=CC=C(N)C=C1	0
Cl[Yb](Cl)Cl	0
COc1cccc2c(=O)oc3c(ccc4[nH]c(=O)cc(c34)C(F)(F)F)c12	1
CC(C)(OC1=CC=C(Cl)C=C1)C(O)=O	0
CC\C=C/CC1=C(C)CCC1=O	0
C[Si]1(C)N[Si](C)(C)N[Si](C)(C)N1	0
Cc1nn(c(C)c1Cc2ccc(cc2)C(=O)NC(C)(C)C)-c3ccc(C#N)c(Cl)c3	1
OC(=O)CCCCCCCC=C	0
Cl.CC1=C(N)C=CC(Cl)=C1	0
CCCCCC(=O)CC	0
CC(=O)NCCO	0
FC(F)(F)CN(CC(Cl)Cl)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
O=C1CCCC1	0
CC\C=C/CCO	0
OC1=C(C=C(C=C1)[As](O)(O)=O)[N+]([O-])=O	0
CC(C)(Cl)Cl	0
[Na+].CCC1(C(=O)NC([O-])=NC1=O)C1=CC=CC=C1	0
OC(=O)C1=CC(=CC=C1)C(O)=O	0
C=COCCOCCOCCOC=C	0
C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O1	0
CC[C@@H]1CCc2cc3c(cc(O)nc3cc2N1)C(F)(F)F	1
Cc1nn(c(C)c1CCc2ccc(F)cc2)-c3ccc(C#N)c(Cl)c3	1
CCC1(C)CCc2cc3c(cc(=O)n(C)c3cc2N1)C(F)(F)F	1
CCCC1=C(N(C(C)COC)C(=O)CCl)C(C)=CC=C1	0
COC(=O)c1csc(CN2CC(C)(C)C(Oc3ccc(C#N)c(c3)C(F)(F)F)C2=O)n1	1

CCCCC(CC)COC(C)=O	0
CC(=O)CCC1=CC=C(OC(C)=O)C=C1	0
CCCC(O)C(CC)CO	0
CC(CC1=CC=C(C=C1)C(C)(C)C)C=O	0
CCc1cc2c(cc(=O)[nH]c2cc1NCC(F)(F)F)C(F)(F)F	1
O=C1CCCCCCCCCC=CCCC1	0
CN(C)C1=NC(=O)N(C2CCCCC2)C(=O)N1C	0
BrCC(=O)OCC1=CC=CC=C1	0
COP(=O)(OC)C(O)C(Cl)(Cl)Cl	0
FC(F)(F)c1cc(=O)[nH]c2cc(NCc3ccccc3)ccc12	1
CC1=CC(NC2=CC=CC=C2)=CC=C1	0
CCC(C)C1=CC=CC(C(C)CC)=C1O	0
CCC(=O)O[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C	1
COc1cc(SCC2CC2)ccc1C#N	1
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)c5cc(Cl)ncn5	1
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)S(=O)(=O)C	1
C[C@]12C[C@H](O)[C@@]3(F)[C@@H](CCC4=CC(=O)C=C[C@]34C)[C@@H]1C[C@@H](O)[C@]	1
OC1=CC(O)=CC=C1	0
CC(C)(O)C1=CC=C(CNC(=O)C2=CC=CN=C2OC2=CC3=NON=C3C=C2)C=C1	0
CCC(C)(C)Nc1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
CCC1(C)NC(=O)NC1=O	0
CCOC(=O)C1OC1(C)C1=CC=CC=C1	0
[Cl-].C[N+](C)(C)CC1CO1	0
CCCCOC(=O)COC1=C(Cl)C=C(Cl)C=C1	0
CC1=CC[C@H]2C[C@@H]1C2(C)C	0
CCN(CC)C(=O)SCC1=CC=C(Cl)C=C1	0
OCCC1=NC=CC=C1	0
CC(C)=CCC\C(C)=C\COC=O	0
CCN(CC)C1=CC=CC=C1	0
CC(C)C[C@@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
O.O.CN(C)[C@H]1[C@@H]2[C@@H](O)[C@H]3C(=C(O)[C@]2(O)C(=O)C(C(N)=O)=C1O)C(=O)C1	0
OCCN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
C[Si](NC1CCCCC1)(NC1CCCCC1)NC1CCCCC1	0
NC1=C(Cl)C(=O)N(N=C1)C1=CC=CC=C1	0
CC(C)(C)OC(=O)N1C[C@@H]2C[C@H]1[C@H]3N2C(=O)N(C3=O)c4ccc(c5ccccc45)[N+](=O)[O-]	1
Oc1cc(c2cc3[C@H]4CCCC[C@H]4Nc3cc2n1)C(F)(F)F	1
CCN1CN(CC)CN(CC)C1	0
CC1=NC(N)=CC=C1	0
Cc1c(F)c(ccc1N2C(=O)[C@@H]3[C@H](O)CCN3C2=O)C#N	1
[K+].[O-]C(=O)CC1=C2C=CC=CC2=CC=C1	0
O=NN1CCCC1	0
CCOP(=O)(SC1=CC=CC=C1)SC1=CC=CC=C1	0
FC1=CC2=C(C=C1N1C(=O)C3=C(CCCC3)C1=O)N(CC#C)C(=O)CO2	0
COC1=CC=C(COC(C)=O)C=C1	0
Cc1nn(c(C)c1C(O)c2ccc(F)cc2)-c3ccc(C#N)c(Cl)c3	1

OC(=O)CCCCC1CCSS1	0
[O-]C(=O)C1=CC=CC=C1.CC[N+](CC)(CC(=O)NC1=C(C)C=CC=C1C)CC1=CC=CC=C1	0
Cc1nn(c(C)c1Oc2ccc(NC(=O)C(C)(C)C)cn2)-c3ccc(C#N)c(Cl)c3	1
CCCCc1ccc(cc1)C(=O)N2C[C@@H]3C[C@H]2[C@H]4N3C(=O)N(C4=O)c5ccc(C#N)c(c5)C(F)(F)F	1
Cc1ccc(CN(c2ccc(cc2)[N+](=O)[O-])c3cc(C(=O)N4CCCC4)n(C)c3)cc1	1
CCCc1cc(=O)[nH]c2ccc(cc12)N(CC(F)(F)F)CC(F)(F)F	1
CC(C)(C)N(NC(=O)C1=CC=C(Cl)C=C1)C(=O)C1=CC=CC=C1	0
O=C1CCCCCCCCCC(=O)OCCO1	0
CCCN(CC1CC1)c2cc(c(cn2)C#N)C(F)(F)F	1
C=CCOC(=O)\C=C/C(=O)OCC=C	0
OC(=O)C1=CC=CC=C1	0
Oc1ccc(Br)cc1/C=N/NC(=O)c2cc3ccccc3cc2O	1
CCOC(=O)CC(CC(=O)OCC)(OC(C)=O)C(=O)OCC	0
FC(F)(F)c1cc(ccc1C2=NOC3CCCCC23)C#N	1
CCCCCCCC1=CC=C(O)C=C1	0
CCNC(=O)N1C[C@@]2(C)O[C@@](C)(C1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)	1
FC(F)(F)CN1C(COc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F)C(F)(F)F	1
C=CC#N	0
[Na+].OC[C@H](O)[C@H]1OC(=O)C(O)=C1[O-]	0
CC1=C(O)C=CC=C1	0
COc1ccc2oc(=O)c3c(ccc4[nH]c(=O)cc(C)c34)c2c1	1
N1C=CN=C1	0
COC(CC1=CC=CC=C1)OC	0
[O-][N+](=O)c1ccc(C2=NO[C@@H]3CCCC[C@H]23)c(c1)C(F)(F)F	1
CCNC(=S)NCC	0
CC(=O)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C	1
CNC(=O)OC1=C2C=CC=CC2=CC=C1	0
CCCC(=O)C1=CC=CC=C1	0
CC1=C(CCOC2=CC=CC3=C2C=CN3CCC(O)=O)N=C(O1)C1=CC=CC=C1	0
NC1=C(C=CC(=C1)[N+]([O-])=O)C(O)=O	0
CCCCCOC(C)=O	0
CNC(C)=O	0
CCCCOCCOC(=O)COC1=C(Cl)C=C(Cl)C=C1	0
COC(OC)C=C(C)CCC=C(C)C	0
C[C@H]1[C@H](C)C(C)(C)Nc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
ClC(=O)C1=CC(=CC=C1)C(Cl)=O	0
C[C@]12C=CC3=C4CCC(=O)C=C4CC[C@H]3[C@@H]1CC[C@@H]2O	1
CC1(C)C(=O)NC(=O)NC1=O	0
C[C@](O)(CS(=O)(=O)c1ccccc1-c2ccccc2)C(=O)Nc3ccc(C#N)c(c3)C(F)(F)F	1
CC(=O)C1=C(C)C=C(C=C1C)C(C)(C)C	0
CC(=C)[C@H]1CCC(C)=CC1	0
C[C@@H]1CC[C@@H](C)N1c2ccc3[nH]c(=O)cc(c3c2)C(F)(F)F	1
CCCC\C=C\C=C/C=O	0
CN1CCC[C@H]1C1=CN=CC=C1	0
CCCCOC(=O)C1=CC=CC=C1	0

FC(F)(F)c1cc(ccc1C#N)C2=NO[C@@H]3CCC[C@H]23	1
ClC1=CC=C(SC2=CC(Cl)=C(Cl)C=C2Cl)C=C1	0
Cc1c(Cl)c(ccc1N2[C@@H]([C@@H]3[C@H](O)CCN3C2=O)C(F)(F)F)C#N	1
[Na+].CCCCCCCCOS([O-])(=O)=O	0
[Mn++].[S-]C(=S)NCCNC([S-])=S	0
[O-][N+](=O)C1=CC=CC=C1C(F)(F)F	0
CCCC(=O)OC\C=C(/C)CCC=C(C)C	0
Cl[Dy](Cl)Cl	0
CC1=CC(=O)c2ccccc2C1=O	1
CC(C)C1(C)NC(=NC1=O)C1=NC=C(C)C=C1C(O)=O	0
CS(=O)(=O)C1=CC=C(C=C1Cl)[C@@H](C[C@H]1CCC(=O)C1)C(=O)NC1=NC=CN=C1	0
COC1=CC2=C(C=C1)N(C(=O)C1=CC=C(Cl)C=C1)C(C)=C2CC(O)=O	0
CC1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
FC(F)(F)c1cc(ccc1C2=NOC3CCCCCC23)C#N	1
CC(O)=O.COCCOC1=NC=C2N(CC(=O)NC3=NC=C(Cl)C=C3)C(=CC2=C1)C(=O)NC1CCN(CC1)C(C)C	0
CCCCCCC(=O)OCC	0
C1C2=C(C=CC=C2)C2=C1C=CC=C2	0
OC(=O)CS	0
CC[C@@H]1C[C@H](C)c2cc3c(cc(O)nc3cc2N1)C(F)(F)F	1
NC1=CC=C(Cl)C=C1	0
CC1=C(N)C=C(C=C1)[N+]([O-])=O	0
CC(C)CCOC(=O)CC(C)C	0
CC1=CC(O)=C(C)C=C1	0
COP(=O)(OC)OC	0
COC1=CC(=CC=C1N)C1=CC(OC)=C(N)C=C1	0
NC1=CC=C(CC2=CC=C(N)C=C2)C=C1	0
Fc1ccc(C2=NOC3CCCCC23)c(c1)C(F)(F)F	1
CCSc1ccccc1Oc2ccc(C#N)c(c2)C(F)(F)F	1
CCC1CCc2cc3c(cc(=O)oc3cc2N1)C(F)(F)F	1
CC(C)=CCOC(C)=O	0
CC(C)(O)CC1=CC=CC=C1	0
COc1ccc(CO)cc1Oc2ccc(C#N)c(c2)C(F)(F)F	1
OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
FC(F)(F)CCN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
CC1=NN(C(=O)N1C(F)F)C1=CC(NS(C)(=O)=O)=C(Cl)C=C1Cl	0
OC1CCCC1	0
[Na+].COC1=CC=C(C=C1)\N=N\C1=C(OC)C=C(\N=N\C2=CC=C(C=C2)S([O-])(=O)=O)C(C)=C1	0
CC(C)N(CCO)C(C)C	0
OC(=O)COC1=C(Cl)C=C(Cl)C(Cl)=N1	0
CC(C)C1=CC=C(C)CC1	0
CC1(C)C(C=C(Cl)Cl)C1C(=O)OCC1=CC(OC2=CC=CC=C2)=CC=C1	0
NC(=O)NC1=CC=CC=C1	0
CC(C)(OO)C1=CC=CC=C1	0
Cc1c(Cl)c(ccc1N2[C@H]([C@@H]3[C@@H](O)CCN3C2=O)C(F)(F)F)C#N	1
CCC1[C@@H](C)CNc2cc3nc(O)cc(c3cc12)C(F)(F)F	1

CCCCCC(=O)OCCC1=CC=CC=C1	0
Nc1ccc2nc(O)cc(c2c1)C(F)(F)F	1
CC1=CC=C(C)C2=C1C=CC=C2	0
CCOCCOCCOC(=O)C=C	0
CC1=C(O)C(CO)=C(CO)C=N1	0
CCCCC(CC)COCCO	0
OC1=CC2=C(C=CC=C2)C2=CC=CC=C12	1
[Na+].C\C(=N/NC(=O)NC1=CC(F)=CC(F)=C1)C1=NC=CC=C1C([O-])=O	0
CC(O)C(O)=O	0
CC1=C(C)C(O)=CC=C1	0
CC(=O)O[C@@H]1CC2CCC1(C)C2(C)C	0
C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C	1
CC1=CC=CC(=C1)C(O)=O	0
CC(C1=CC=C(O)C=C1)(C1=CC=C(O)C=C1)C1=CC=C(O)C=C1	1
C=CCOC(=O)C1=CC=C(C(=O)OCC=C)C(=C1)C(=O)OCC=C	0
Cc1c(ccc(C#N)c1C#N)N2C(=O)[C@@H]3[C@H](O)CCN3C2=O	1
O=CCCC1=CC=CC=C1	0
[Na+].[Na+].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	1
CCCC(C)N1CC(C)(C)C(Oc2ccc(C#N)c(c2)C(F)(F)F)C1=O	1
[Mn++].[Zn++].[S-]C(=S)NCCNC([S-])=S.[S-]C(=S)NCCNC([S-])=S	0
CCCC(=O)OCCC(C)C	0
CC12CCC(C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4c(N)ccc5ncsc45	1
CCCC[C@H]1CN(CC2CCOCC2)C(=O)OC11CCN(CC1)C1(C)CCN(CC1)C(=O)C1=C(C)N=CN=C1C	0
[Na+].CC(=C)C([O-])=O	0
CC(C)N(c1ccc(cc1)[N+](=O)[O-])c2cc(C(=O)N3CCCC3)n(C)c2	1
CCCCCCC(O)=O	0
CCOC(=O)C(C)(C)OC1=CC=C(Cl)C=C1	0
BrC1=C(C=CC=C1)C1=CC=CC=C1	0
CN(C)C1=CC=CC(O)=C1	0
COc1ccccc1-c2ccc(C#N)c(c2)C(F)(F)F	1
O=C1OC(=O)C2C3CC(C=C3)C12	0
CCCCN	0
COC(=O)[C@H](CC1=CC=CC=C1)NC(=O)[C@@H](N)CC(O)=O	0
COP(N)(=O)SC	0
CCC\C=C\CO	0
Cl.Cl.NCCNC1=C2C=CC=CC2=CC=C1	0
CCCCCCCCCCCCCCCCCC(O)=O	0
CCC1CN(CC)c2cc3c(cc(=O)[nH]c3cc2O1)C(F)(F)F	1
CC1(C)N(CCCC(=O)O)C(=S)N(C1=O)c2ccc(C#N)c(c2)C(F)(F)F	1
CCCCCCCO	0
CCN(CCO)C1=CC(C)=CC=C1	0
CCC1(C(=O)NCNC1=O)C1=CC=CC=C1	0
CCCCN(CCO)CCO	0
CC(=O)C1=CC2=C(OC(C)(C)[C@H](O)[C@H]2NC(=O)C2=CC=C(F)C=C2)C=C1	0
CC1=CC(C)=C(C2=C(OC(=O)CC(C)(C)C)C3(CCCC3)OC2=O)C(C)=C1	0

OCC1=CC2=C(C(O)=C1)C(=O)C1=C(C=CC=C1O)C2=O	0
OCNC(=O)N(CO)C1N(CO)C(=O)N(CO)C1=O	0
CC1=CC(C)(C)Nc2ccc3-c4cc(F)ccc4O/C(=C\c5ccsc5)/c3c12	1
CC(COCC(C)OC(=O)C1=CC=CC=C1)OC(=O)C1=CC=CC=C1	0
C[C@@H](CCl)N(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
CCCC(=NOCC)C1=C(O)CC(CC(C)SCC)CC1=O	0
CCC1(C)CCc2cc3c(cc(O)nc3cc2N1)C(F)(F)F	1
OC(=O)CCCC[C@@H]1SC[C@@H]2NC(=O)N[C@H]12	0
C(NC1=C2N=CN=C2N=CN1)C1=CC=CC=C1	0
CC(C)[C@H](C(=O)O[C@H](C#N)C1=CC=CC(OC2=CC=CC=C2)=C1)C1=CC=C(Cl)C=C1	0
ClP(Cl)C1=CC=CC=C1	0
CC1=CC=CC(=C1O)C(C)(C)C	0
CC(=C)C1=CC(=CC=C1)C(C)(C)N=C=O	0
CCCCCCCCCCCCCC(=O)OCC(O)CO	0
CCC1=NC(C)=CN1	0
CC1=CC=C(C=C1)[N+]([O-])=O	0
CC1c2cc3c(cc(O)nc3cc2NC(C)(C)C1(C)C)C(F)(F)F	1
[Na+].[O-]C1=CC=C(C=C1)[N+]([O-])=O	0
CCCCOC(=O)[C@H](C)O	0
N1N=NC2=C1C=CC=C2	0
[Na+].[O-]C(=O)CF	0
CC(C)NC1=NC(Cl)=NC(N)=N1	0
CCOC(=O)c1c(C)[nH]c(C)c1-c2ccc(cc2)[N+](=O)[O-]	1
OCCNCCO	0
CCCCOC(=O)CC(CC(=O)OCCCC)(OC(C)=O)C(=O)OCCCC	0
NC1=NC(=S)NN1	0
CC[C@]12C=CC3=C4CCC(=O)C=C4CC[C@H]3[C@@H]1CC[C@@]2(O)C#C	1
CCCCCCCCC(O)=O	0
CCCCCCC=O	0
CCCCCCCCCCCCCN1CC(C)OC(C)C1	0
CC(C)CC(C)O	0
CCSC(=O)N(CC(C)C)CC(C)C	0
CC(C)=CCC\C(C)=C\CO	0
C1OC1C1CCC2OC2C1	0
CC(C)=CCCC(C)=CC(O)=O	0
Fc1ccc(C2=NOC3CCCC23)c(c1)C(F)(F)F	1
OC[C@H]1O[C@@H]2O[C@@H]3[C@@H](CO)O[C@H](O[C@@H]4[C@@H](CO)O[C@H](O[C@	0
CCOC(=O)COC1=C(Cl)C=C(F)C(=C1)C1=NN(C)C(OC(F)F)=C1Cl	0
CC[C@@H]1C[C@H](N(CC2=CC(=CC(=C2)C(F)(F)F)C(F)(F)F)C(C)=O)C2=C(C=CC(=C2)C(F)(F)F)N1C(	0
COC1=CC(OC)=C(C=O)C=C1OC	0
CC1=CC[C@@H]2C[C@H]1C2(C)C	0
C[C@](O)(CS(=O)(=O)c1ccccc1Cc2ccccc2)C(=O)Nc3ccc(C#N)c(c3)C(F)(F)F	1
Cn1c(=O)cc(c2cc3[C@H]4CCCC[C@H]4Nc3cc12)C(F)(F)F	1
CON(C)C(=O)NC1=CC=C(Cl)C(Cl)=C1	1
ClC1=NC(Cl)=C(Cl)C(Cl)=C1Cl	0

[NH4+].NC([O-])=O	0
O=C1CCCCCCCCCOCCCCO1	0
CC1=CC2=C3N(CC2)C(=O)[C@H](NC(=O)C2=CC=NC=C2)N=C(C2=CC=CC=C2)C3=C1	0
C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCCCCCCCCC[S+]([O-])CCCC(F)(F)C(F)(F)F)CC4CC(=O)	1
[O-][N+](=O)c1ccc(N2C(=O)[C@@H]3C4CC(C=C4)[C@@H]3C2=O)c5ccccc15	1
C[C@@H]1CNc2cc3nc(O)cc(c3cc2C1C)C(F)(F)F	1
CC(C)[C@H]1CC=C(C)C=C1	0
CCN(CC#N)C1=CC(C)=CC=C1	0
FC(F)(F)c1c(cccc1C2=NOC3CCCC23)C#N	1
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)C(=O)C5CC5	1
CC(C)C#N	0
C1CC2=C3C1=CC=CC3=CC=C2	0
CC[C@H]1Nc2cc3nc(O)cc(c3cc2CC1(C)C)C(F)(F)F	1
[O-][N+](=O)c1ccc(cc1C(F)(F)F)C2=NO[C@@H]3CCC[C@H]23	1
CCCCOCCOP(=O)(OCCOCCCC)OCCOCCCC	0
COC1=CC=CC=C1N	0
FC(F)(F)c1cc(cc(c1)C(F)(F)F)N2C(=O)[C@@H]3C4CC(C=C4)[C@@H]3C2=O	1
CC12CCC(C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c5nsnc45	1
Oc1cc(c2cc(ccc2n1)N(CC3CC3)CC(F)(F)F)C(F)(F)F	1
COP(=S)(OC1=CC(Cl)=C(Br)C=C1Cl)C1=CC=CC=C1	0
C[C@H](CCC(O)=O)[C@H]1CC[C@H]2[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C	0
OC(=O)C1=C(Cl)C=CC(Cl)=N1	0
FC(F)(F)c1cc(SCC2CC2)ccc1C#N	1
COc1c(C)c(ccc1C#N)N2C(=O)[C@@H]3[C@H](O)CCN3C2=O	1
Cn1cc(cc1C(=O)O)N(Cc2ccccc2)c3ccc(cc3)[N+](=O)[O-]	1
COC(=O)C1=C(C=CC=C1)C(=O)OC	0
CCC(C)(C)C1CCC(CC1)OC	0
CCCOC(=O)NCCCN(C)C	0
CC(C)C(OC(=O)C(C)C)C(C)(C)COC(=O)C(C)C	0
NNC1=CC=CC=C1	0
COC1=CC=C(CC=C)C=C1	0
CN(N=O)C1=CC=CC=C1	0
OC(=O)C1=C(N=CC=C1)C(O)=O	0
CC(=C)[C@@H]1CC=C(C)C(=O)C1	0
O=C(OCCCC1=CC=CC=C1)C=CC1=CC=CC=C1	0
CCC1COc2cc3[nH]c(=O)cc(c3cc2N1CC4CC4)C(F)(F)F	1
CC1=CC=CC=C1[N+]([O-])=O	0
[Mg++].[O-]C(=O)C1=CC=CC=C1.[O-]C(=O)C1=CC=CC=C1	0
COCCOCCO	0
Cc1c(Cl)c(ccc1N2C(=O)[C@@H]3[C@H](O)CCN3S2(=O)=O)C#N	1
C[C@H]1Nc2cc3nc(O)cc(c3cc2C1(C)C)C(F)(F)F	1
CC(=O)C1=CC=C(C=C1)S(=O)(=O)NC(=O)NC1CCCCC1	0
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)c5cccc(c5)S(=	1
[O-][N+](=O)C1=C(Cl)C(Cl)=CC(Cl)=C1Cl	0
CCC(C)N1CC(C)(C)C(Oc2ccc(C#N)c(c2)C(F)(F)F)C1=O	1

CC1=C(Cl)C(=O)N(C(=O)N1)C(C)(C)C	0
CCN(CC(F)(F)F)c1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
C[C@@H]1Cc2cc3c(cc(O)nc3cc2N[C@@H]1C)C(F)(F)F	1
CCN(CCC#N)C1=CC=C(C=C1)N=NC1=C(Cl)C=C(C=C1Cl)[N+]([O-])=O	0
CC(=O)OC1=CC=C(C=C)C=C1	0
NC1=CC=CC=C1[N+]([O-])=O	0
CCOP(=O)(OCC)OP(=O)(OCC)OCC	0
Cn1cc(cc1CO)N(Cc2ccccc2)c3ccc(cc3)[N+](=O)[O-]	1
[Na+].[Na+].[O-]C(=O)C1=C(C=CC=C1)C1=C2C=C(I)C(=O)C(I)=C2OC2=C(I)C([O-])=C(I)C=C12	0
CCCCCCCCCO	0
ClC1=C(Cl)C(Cl)(Cl)C(Cl)=C1Cl	0
CC1=C(O)C(=O)C=CO1	0
CCCC(=O)OCCC1=CC=CC=C1	0
CCOC(=O)C(C)OC1=CC=C(OC2=NC3=C(O2)C=C(Cl)C=C3)C=C1	0
S1C=NC2=CC=CC=C12	0
CC(C)(C)CC(C)(C)C1=CC(N2N=C3C=CC=CC3=N2)=C(O)C=C1	0
CC1=CC(C)(C)Nc2ccc3-c4cc(F)ccc4O/C(=C\c5ccccc5C)/c3c12	1
FC1=C(CCl)C(Cl)=CC=C1	0
NC1=CC=C(O)C(=C1)C(O)=O	0
[K+].[O-][N+]([O-])=O	0
[Mn+].[C-]#[O+].[C-]#[O+].[C-]#[O+].CC1C=C[C-]=C1	0
NCCCCCCN	0
CC(CCC=C(C)C)C=O	0
CCCCOC(=O)C1=C(C=CC=C1)C(=O)OCC1=CC=CC=C1	0
C[Si](C)(C)O[Si](C)(C)C	0
CCCCCCOC(=O)C1=CC=CC=C1	0
CCC1=CC(OC)=C(O)C=C1	0
OC1=CC=C(C(=O)C2=CC=CC=C2)C(O)=C1O	0
C(C1=CC=CC=C1)C1=CC=CC=C1	0
C[C@H]1Nc2cc3nc(O)cc(c3cc2[C@H]1C)C(F)(F)F	1
CC(=O)CN(CC(C)=O)N=O	0
COC1=CC(CC=C)=CC=C1OC(=O)CC1=CC=CC=C1	0
CCOC(=O)C1=CC=CC=C1	0
Cc1ccccc1Oc2ccc(cc2Cl)C#N	1
O=C(C1CCCCC1)N1CC2N(CCC3=C2C=CC=C3)C(=O)C1	0
C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCCCCC(=O)O)C[C@H]4CC(=O)CC[C@]34C)[C@@H]1	1
O=C\C=C\C1=CC=CC=C1	0
CCCCCCCCSC(=O)OC1=CC(Cl)=NN=C1C1=CC=CC=C1	0
OC(=O)CCSCCC(O)=O	0
[Cl-].CCCCN1C=C[N+](C)=C1	0
CN(C)CCCN	0
CN1C=NC(=C1SC1=NC=NC2=C1NC=N2)[N+]([O-])=O	0
OC(=O)CCCOC1=CC=C(Cl)C=C1Cl	0
[NH4+].NS([O-])(=O)=O	0
CC(N(C)c1cc(c(cn1)C#N)C(F)(F)F)c2ccccc2	1

Cn1c(=O)cc(c2cc3CCNc3cc12)C(F)(F)F	1
CN1C=NC2=C1C(=O)NC(=O)N2C	0
CCCCOCCO	0
Cl.CCC(=O)C(CC(C)N(C)C)(C1=CC=CC=C1)C1=CC=CC=C1	0
Cl.NC1=CC=C(C=C1)C1=CC=CC=C1	0
CC[N+]([O-])=O	0
CCCCNc1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
C=CC(=O)OCCC#N	0
O=C(OC1=CC=CC=C1)C1=CC(=CC=C1)C(=O)OC1=CC=CC=C1	0
CCN(c1cc(C)cc(C)c1)c2cc(C(=O)N3CCCC3)n(C)c2	1
CCC1=C(O)C(=O)C=CO1	0
OC1=CC=C(C=C1)C(C1=CC=C(O)C=C1)(C(F)(F)F)C(F)(F)F	1
CC1(C)CC2=C(O1)C(O)=CC=C2	0
CN(C)c1ccc2nc(O)cc(c2c1)C(F)(F)F	1
CCOC(=O)c1c(C)n(c(C)c1-c2ccc(cc2)[N+](=O)[O-])S(=O)(=O)c3ccccc3	1
CCOC(=O)c1cc(cn1C)N(Cc2ccccc2)c3ccc(cc3)[N+](=O)[O-]	1
OC1=C(Cl)C=CC(Cl)=C1Cl	0
COc1cc(Oc2cccc(C)c2)ccc1C#N	1
COc1ccc(cc1)-c2ccc(C#N)c(c2)C(F)(F)F	1
CC1(C)N(Cl)C(=O)N(Cl)C1=O	0
OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
CC(=O)Nc1ccc(Oc2c(C)nn(c2C)-c3ccc(C#N)c(Cl)c3)nc1	1
C=CCOC1=NC(OCC=C)=NC(OCC=C)=N1	0
CNC[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO	0
CC1=C2C=CC=CC2=CC=C1	0
COc1cc(ccc1Oc2ccccc2C)C#N	1
CC(C)CNc1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
C1=CC2=C(C=C1)C=C1C(C=CC3=C1C=CC=C3)=C2	1
C=CCSSCC=C	0
[Na+].CC1=C(C=CC(=C1)S([O-])(=O)=O)\N=N\C1=C(O)C=CC2=CC=CC=C12	0
CCCCOCCOCCOCCOCCO	0
O.O.OC1=CC(O)=C(C=C1)C1=C(O)C(=O)C2=C(O1)C=C(O)C=C2O	0
COCCO[Si](OCCOC)(OCCOC)C=C	0
CCCCCCCCCCCSCC(O)=O	0
O=C(C1=CC=CC=C1)C1=CC=CC=C1	0
OC1CCCCC1C1=CC=CC=C1	0
C[C@]1(O)CC[C@H]2[C@@H]3[C@H](CCCc4ccc(OCCCCC(=O)O)cc4)CC5=CC(=O)CC[C@]5(C)[C@	1
NC1=CC(=C(O)C=C1)[N+]([O-])=O	0
CC(C)OC(=O)C1=CC=CC=C1C(=O)OC(C)C	0
Cc1cc(ccc1Cl)N2C(=O)[C@@H]3C4CCC(O4)[C@@H]3C2=O	1
CCCC1=CC=C(N)C=C1	0
FC1=CC=C(Br)C=C1	0
CC(=O)OCC1=CC=CO1	0
CCCCCOC(=O)CCCCC	0
CC(C)(C)OC(=O)N1C[C@@H]2C[C@H]1[C@@H]3N2C(=O)N(C3=O)c4ccc(c5ccccc45)[N+](=O)[O-]	1

CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5cc(C)cc(Br)c5)c3c12	1
CNc1ncc(/C=C/2\C[C@H]3[C@@H]4CC[C@H]5N(C)C(=O)C=C[C@]5(C)[C@H]4CC[C@]3(C)[C@H]	1
CCCCCCOC(=O)CC	0
COC1=CC=C(CC=C)C=C1OC	0
O=C(OCC1=CC=CC=C1)C=CC1=CC=CC=C1	0
CC(=O)OC1=CC=C(C=C1)C(C)=O	0
[Na+].[O-]S(=O)(=O)C1=CC=CC=C1C=O	0
OC(CN1C=NC=N1)(CN1C=NC=N1)C1=C(F)C=C(F)C=C1	0
CCOC(=O)C1=C(N)C=CC=C1	0
CCCCCCCCCCOC(=O)C=C	0
CCOC(=O)COC1=C(Cl)C=C(Cl)C=C1	0
FC(F)(F)CN1[C@H](COc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F)c4ccccc4	1
OC1(CCCCC1)C(=O)C1=CC=CC=C1	0
OO.NC(N)=O	0
COc1ccc(C)cc1Oc2ccc(C#N)c(c2)C(F)(F)F	1
OC(=O)C1=CC=C(C=C1)[N+]([O-])=O	0
CC1=CC=C(OC(=O)C2=C(O)C=CC=C2)C=C1	0
CCc1c(ccc(C#N)c1C(F)(F)F)N2C(=O)[C@@H]3[C@H](O)CCN3C2=O	1
CCCC1=C(O)C=CC=C1	0
CCCCCCCCCO	0
CCC(C)(C)C1=CC(=C(O)C=C1)C(C)(C)CC	0
COc1ccc(cc1)-c2coc3cc(O)cc(O)c3c2=O	1
CC(=O)OC(C)(C)C	0
CCCCCCCCCSCCO	0
CC(C)NC(=O)N1C[C@@]2(C)O[C@@](C)(C1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)	1
CCO[Si](CCCNC(N)=O)(OCC)OCC	0
COc1cccc2OCc3c(ccc4[nH]c(=O)cc(C)c34)-c12	1
COCCOCCOC	0
Cc1cc(=O)[nH]c2ccc-3c(COc4cccc(CO)c34)c12	1
[Na+].[O-]C(=O)C(Cl)(Cl)Cl	0
[Na+].CC1=CC=C(C=C1)S([O-])(=O)=O	0
CNC(=O)O\N=C\C(C)(C)S(C)=O	0
CC(=O)OC1C2(C)CCC(C2)C1(C)C	0
CC(O)CN(CCN(CC(C)O)CC(C)O)CC(C)O	0
CC(CCO)CCC=C(C)C	0
CCOP(O)OCC	0
COC1=NC=C(F)C2=NC(=NN12)S(=O)(=O)NC1=C(F)C=CC=C1F	0
COC(=O)NS(=O)(=O)C1=CC=C(N)C=C1	0
[Zn++].CC([O-])=O.CC([O-])=O	0
CC1=CC(C)=C(O)C(C)=C1	0
CC(COC1=CC=C(OC2=CC=CC=C2)C=C1)OC1=NC=CC=C1	0
Cc1cc(c(C)n1Cc2ccccc2)-c3ccc(cc3)[N+](=O)[O-]	1
COc1cc(ccc1-c2ocnc2)N3C(=O)[C@H]4[C@@H](C3=O)C5(C)CCC4(C)O5	1
O=C(N[C@H]1CN2CCC1CC2)C1=CC2=C(OCCO2)C=C1	0
CC(C)(OC1=CC=C(C=C1)C1CC1(Cl)Cl)C(O)=O	0

CC1=CC(C)(C)Nc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CC(=O)[C@H]1[C@@H](C[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C)C	0
CC12CCC(C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(I)c4	1
Fc1ccc(cc1C(F)(F)F)C2=NOC3CCCC23	1
OC(=O)CC(C(O)=O)S(O)(=O)=O	0
CC(C)(C)OOC(C)(C)CCC(C)(C)OOC(C)(C)C	0
Fc1ccc(Oc2ccc(C#N)c(c2)C(F)(F)F)c(F)c1	1
OCCOCCOCCOCCO	0
Cc1c(Cl)c(ccc1N2[C@@H]([C@@H]3[C@@H](O)CCN3C2=O)C(F)(F)F)C#N	1
CC(C)(C)OC(=O)N1C[C@H]2C[C@@H]1[C@@H]3N2C(=O)N(C3=O)c4ccc(cc4)[N+](=O)[O-]	1
[Na+].N[C@@H](CC1=CC(I)=C(OC2=CC(I)=C(O)C=C2)C(I)=C1)C([O-])=O	0
[Na+].CC1=NN(C(=O)C1\N=N\C1=CC=CC=C1)C1=CC(=CC=C1Cl)S([O-])(=O)=O	0
COC(=O)C1=C(C=CS1)S(=O)(=O)NC(=O)NC1=NC(OC)=NC(C)=N1	0
CCC(=O)OCCC1=CC=CC=C1	0
CCN1C(C)COc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F	1
C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CCC2=O	1
C[C@@H]1CNc2cc3nc(O)cc(c3cc2[C@@H]1CCC(F)(F)F)C(F)(F)F	1
CC1(C)CC(N)CC(C)(C)N1	0
CC1(C)N(CCCNC(=O)N)C(=S)N(C1=O)c2ccc(C#N)c(c2)C(F)(F)F	1
CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5ccc(C)c(F)c5)c3c12	1
CCOC(=O)c1c(C)n(C(=O)c2ccccc2)c(C)c1-c3ccc(cc3)[N+](=O)[O-]	1
CC1=C(C)C(NC2=NC(SCC(O)=O)=NC(Cl)=C2)=CC=C1	0
CN1[C@@H]2CC[C@@H]3[C@H](CC[C@@]4(C)[C@H]3C/C(=C\c5cnc(C)nc5)/[C@@H]4O)[C@@	1
CC1=CC(=O)CCC1	0
CN1[C@@H]2CCCC[C@@H]2c3cc4c(cc(=O)n(C)c4cc13)C(F)(F)F	1
[O-][N+](=O)c1ccc(cc1)C2=NOC3CCCCC23	1
CCOC(=O)CC(=O)OCC	0
COc1c(C)c(ccc1N2C(=O)[C@@H]3[C@H](O)CCN3C2=O)C#N	1
CCCCCCCCCCCCCCCC(=O)OC[C@H](O)[C@H]1OC(=O)C(O)=C1O	0
CCOCCO	0
OC(C(=O)C1=CC=CC=C1)C1=CC=CC=C1	0
CC(N)=S	0
NC(CO)(CO)CO	0
OC(=O)C1=CC=C(Cl)C=C1	0
CSc1ccc(CN2CC(C)(C)[C@@H](Oc3ccc(C#N)c(c3)C(F)(F)F)C2=O)cc1	1
CCCOC(=O)C1=C(Cl)C(Cl)=C(Cl)C(Cl)=C1C(=O)OCCC	0
CC(C)C1=CC=C(C)C(O)=C1	0
CCCCOC(=O)C(C)O	0
CC1(C)[C@@H](C=C(Br)Br)[C@H]1C(=O)O[C@H](C#N)C1=CC=CC(OC2=CC=CC=C2)=C1	0
CCC1CC(CC)c2cc3c(cc(=O)oc3cc2N1)C(F)(F)F	1
C\C=C(/C)C(=O)OCC1=CC=CC=C1	0
CCOC(=O)C1=C(C)C=CC=C1	0
CC(C)C1(C)N=C(NC1=O)C1=NC2=C(C=CC=C2)C=C1C(O)=O	0
O=[Si]=O	0
CC(O)(CS(=O)(=O)c1ccc(F)cc1)C(=O)Nc2ccc(C#N)c(c2)C(F)(F)F	1

CCCC(=O)OCC	0
O.CC(O)(P(O)(O)=O)P(O)(O)=O	0
ClC1=CC=C(C=C1)C1=C(NC(=O)C2=C(Cl)N=CC=C2)C=CC=C1	0
C[C@@H]1[C@@H]2[C@@H](O)CCN2C(=O)N1c3ccc(C#N)c(Cl)c3C	1
COc1cc(Sc2c(C)cc(C)cc2C)ccc1C#N	1
COC1=CC=C(COC=O)C=C1	0
[K+].CC1=CC(=O)[N-]S(=O)(=O)O1	0
CCOCCOCCO	0
C[C@@H]1Cc2cc3c(cc(O)nc3cc2N1)C(F)(F)F	1
NCCCN1CCN(CCCN)CC1	0
CN1CC(C2=CC=CC=C2)C2=CC=CC(N)=C2C1	0
Cl[In](Cl)Cl	0
CC1=CC(=C(O)C(=C1)C(C)(C)C)C(C)(C)C	0
FC(F)(F)c1cccc(c1)N2C(=O)[C@@H]3C4CCC(O4)[C@@H]3C2=O	1
FC(F)(F)CN(CC(F)(F)C(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
CC(C)(C)OC(=O)N1C[C@@H]2C[C@H]1[C@@]3(C)N2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F	1
CS(O)(=O)=O.CC(C)C1=CC=C(C=C1S(C)(=O)=O)C(=O)N=C(N)N	0
ClN1C(=O)N(Cl)C(=O)N(Cl)C1=O	0
NC1=NC(=O)C2=C(N1)N=CC(CNC1=CC=C(C=C1)C(=O)N[C@@H](CCC(O)=O)C(O)=O)=N2	0
CCN(CC1=CC(=CC=C1)S(O)(=O)=O)C1=CC=CC=C1	0
CCCCCCCC\C=C/CCCCCCCC(O)=O	0
CCN(CC)C(=O)c1cc(cn1C)N(Cc2ccccc2)c3ccc(cc3)[N+](=O)[O-]	1
CCCC(=O)O[C@@H]1C[C@H]2CC[C@]1(C)C2(C)C	0
COC1=CC(=CC=C1N)[N+]([O-])=O	0
CC(=O)c1ccc(cc1)N(Cc2ccccc2)c3cc(C(=O)N4CCCC4)n(C)c3	1
COC(=O)\C=C/C(O)=O	0
O=C1N(C2CCC(=O)NC2=O)C(=O)C2=CC=CC=C12	0
O=C1OC(=O)C2=C1C=CC(OC1=CC3=C(C=C1)C(=O)OC3=O)=C2	0
CCCCCCOC(=O)CCCCC	0
FC1=CN(C2CCCO2)C(=O)NC1=O	0
CNC(=O)ON=C(CSC)C(C)(C)C	0
CCCCOP(O)(=O)OCCCC	0
CC1=CC2=C(NCCC2)C=C1	0
CN1[C@@H]2CC[C@@H]3[C@H](CC[C@@]4(C)[C@H]3C/C(=C\c5cncnc5)/[C@@H]4O)[C@@]2	1
CCc1cc2c(cc(=O)[nH]c2cc1N)C(F)(F)F	1
CCCCCCOC(=O)C1=CC=C(O)C=C1	0
CSc1ccccc1Oc2ccc(C#N)c(c2)C(F)(F)F	1
O=C1[N-]S(=O)(=O)C2=C1C=CC=C2.CC[N+](CC)(CC(=O)NC1=C(C)C=CC=C1C)CC1=CC=CC=C1	0
Oc1ccccc1-c2ccc(C#N)c(c2)C(F)(F)F	1
CC(=O)OCCOCCOCCOC(C)=O	0
CC(C)=CCCC(C)=CC=O	0
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)c5cccc(c5)C(	1
Fc1ccc(OC(=O)N2C[C@@H]3C[C@H]2[C@@H]4N3C(=O)N(C4=O)c5ccc(C#N)c6ccccc56)cc1	1
CC(C)CCCC(C)CC=O	0
CC(C)(C)OC(=O)N1C[C@@H]2C[C@H]1[C@H]3N2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F	1

CC(C)(C)C(=O)C1=CC=CC=C1	0
C1COCCN1	0
CCC1Cc2cc3c(cc(O)nc3cc2NC1(C)C)C(F)(F)F	1
ClC1=CC=CC=C1NC1=NC(Cl)=NC(Cl)=N1	0
CC(C)C(=O)N1C[C@@]2(C)O[C@@](C)(C1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F	1
ClC1=CC=C(C=C1)C(C1=CC=C(Cl)C=C1)C(Cl)(Cl)Cl	0
NC(=N)NC#N	0
CC(C)=CCCC(=C)C=C	0
CS(=O)(=O)C1=CC(=C(C=C1)C(=O)C1C(=O)CCCC1=O)[N+]([O-])=O	0
CC(=O)OCC=CC1=CC=CC=C1	0
CCCCCCNC(=O)CCCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]	1
Cc1nn(c(C)c1Cc2ccc(F)cc2)-c3ccc(cc3)C#N	1
NC1=CC=C(Br)C=C1	0
CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5ccc(Cl)c(F)c5)c3c12	1
[Na+].[N-]=[N+]=[N-]	0
CC(OC(C)=O)C1=CC=CC=C1	0
CC1(C)CN(Cc2onc(n2)-c3ccccc3)C(=O)C1Oc4ccc(C#N)c(c4)C(F)(F)F	1
COc1cc(C)ccc1Oc2ccc(C#N)c(c2)C(F)(F)F	1
COCCOCCOCCOC	0
CC\C(C)=C\CCC(C)(O)C=C	0
O=CC1=CC=CO1	0
CC(C1=CC=C(C)C(C)=C1)C1=CC=C(C)C(C)=C1	0
C[C@H](N(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F)C(F)(F)F	1
O=C1NC(=O)C(N1)(C1=CC=CC=C1)C1=CC=CC=C1	0
CC(C)C[C@@H]1[C@@H](C)CNc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CCCCC1CCC(=O)O1	0
CN(C)CCCNC(=O)C(C)=C	0
OC1=CC(O)=C(C=C1)C(=O)C1=CC=C(O)C=C1O	1
CC1=CC=CC=C1S	0
NS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
OC[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)CO	0
CN1C(=O)[C@@]2(C)O[C@](C)([C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)C1=O	1
CCOP(=S)(OCC)OC1=NN(C(C)C)C(Cl)=N1	0
CC(C)C1=CCC(C)=CC1	0
OCCCBr	0
C1N2CN3CN1CN(C2)C3	0
C[C@]12CCC3=C4CCC(=O)C=C4CC[C@H]3[C@@H]1CC[C@@H]2O	1
CCC1=CC=C(O)C=C1	0
CC1(C)N(CCCC(=O)N)C(=S)N(C1=O)c2ccc(C#N)c(c2)C(F)(F)F	1
CCN(CCN)C1=CC(C)=CC=C1	0
CC[C@H]1Nc2cc3nc(O)cc(c3cc2C[C@@H]1C)C(F)(F)F	1
Cc1nn(c(C)c1Cc2ccc(F)cc2)-c3ccc(cc3Cl)C#N	1
C=COCCOCCOC=C	0
O=C(OC1=CC=CC=C1)C1=CC=CC=C1	0
ClC1=CC=C(CN2CCS\C2=N/C#N)C=N1	0

C/C=C/1\C[C@H]2[C@@H]3CC[C@H]4N(C)C(=O)C=C[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1O	1
Cl.CN(C)CCOC(C1=CC=CC=C1)C1=CC=CC=C1C	0
CC1=CC(O)=CC(C)=C1Cl	0
[Na+].CNC([S-])=S	0
ClC1=CC=C(OS(=O)(=O)C2=CC=C(Cl)C=C2)C=C1	0
CCCCCCCCCCCCCCCCC	0
C[C@@]12CC[C@H]3C(C)(C)CCC[C@]3(C)[C@H]1CCO2	0
Cn1cc(Nc2ccc(cc2)[N+](=O)[O-])cc1C(=O)N3CCCC3	1
CO[Si](CCCNCCN)(OC)OC	0
O=C1CCCCO1	0
CC[C@@H]([C@@H](CC)C1=CC=C(O)C=C1)C1=CC=C(O)C=C1	1
COC1=C(N)C=C(C=C1)[N+]([O-])=O	0
Cc1c(C(=O)O)c(c(C)n1Cc2ccccc2)-c3ccc(cc3)[N+](=O)[O-]	1
C[C@@]12CC[C@H]3C(C)(C)CCC[C@]3(C)[C@H]1CC(=O)O2	0
CC(C)(C)C1=CC=CC(O)=C1	0
OC(=O)CCCCCCCC(O)=O	0
CCCCCCCCC	0
COc1cc(ccc1C#N)N2C(=S)N(CCCS(=O)(=O)N)C(C)(C)C2=O	1
CCOC(=O)CCC1=CC=CC=C1	0
CC1=CC(OCCOC2=CC=C(C)=C2)=CC=C1	0
CCOC(=O)OC1=C(C(=O)N[C@@]11CC[C@@H](CC1)OC)C1=C(C)C=CC(C)=C1	0
CC(C)OC(=O)C1=CC=CC=C1	0
CC(C)(C)OC(=O)N1C[C@H]2C[C@@H]1[C@@H]3N2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F	1
CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)	0
CCCCCCCCCCCCCl	0
O=C=NCCCCCCN=C=O	0
COCCO	0
OCC(O)=O	0
CC\C(=C/C(=N\O)/C(N)=O)C(C)[N+]([O-])=O	0
CC1(C)COC(=O)[C@@H]1Oc2ccc(C#N)c(c2)C(F)(F)F	1
CCCCCCCC[Si](OCC)(OCC)OCC	0
FC(F)(F)CN1[C@@H](COc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F)C(F)(F)F	1
Cc1c(-c2ccc(cc2)C#N)c(cn1Cc3cnc(Cl)c(CO)c3)C#N	1
C(NC1=C2N=CN=C2N=CN1)C1=CC=CO1	0
CCCC(CCC)C(O)=O	0
CC1CCCC1NC(=O)NC1=CC=CC=C1	0
CC(C)(C)OOC(C)(C)C	0
COc1ccccc1Sc2ccc(C#N)c(c2)C(F)(F)F	1
NCCN1CCNCC1	0
CC12CC1(C)C(=O)N(C2=O)C1=CC(Cl)=CC(Cl)=C1	1
Cc1c(ccc(C#N)c1C(F)(F)F)N2C(=O)[C@@H]3[C@H](O)CCN3C2=O	1
C[C@H]1CC[C@H]2Nc3cc4nc(O)cc(c4cc3[C@H]2C1)C(F)(F)F	1
C(CC1=CC=CC=C1)CC1=CC=CC=N1	0
CCCCC(CC)C=O	0
CCCC[Sn](Cl)(Cl)Cl	0

CCN(CC(C)=C)C1=C(C=C(C=C1[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O	0
CC[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@]2(O)C#C	1
CCCC1=CC=C(OC)C=C1	0
COC(=O)\C=C\C(\C)=C/C=C/C(/C)=C/C=C/C=C(\C)/C=C/C=C(\C)/C=C/C(O)=O	0
CC1=C(CC=O)C(C)(C)CCC1	0
CC1=CC=C(C=C1)S(N)(=O)=O	0
FC(F)(F)c1cc(ccc1C2=NOC3CCCC23)C#N	1
[Na+].CCCCN(CCCC)C([S-])=S	0
CC(C)CC(O)CC1=CC=CC=C1	0
CCCCCCCCCCOC(=O)C1=C(C=CC=C1)C(=O)OCCCCCCCC	0
CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC	0
CCC1=C(O)C=CC=C1	0
ClC1=CC(Cl)=C(Cl)C=C1	0
[Na+].OC(CCl)CS([O-])(=O)=O	0
CCOC(=O)CC1(C)OCC(C)O1	0
COC(=O)NC1=CC(OC(=O)NC2=CC=CC(C)=C2)=CC=C1	0
[Na+].CCCCCCCCCCCCOS([O-])(=O)=O	0
COP(=S)(OC)OC1=C(Cl)C=C(Br)C(Cl)=C1	0
OC1=CC=C(C=C1)C(=O)CBr	0
CCN1CCCC1=O	0
CN(C)CCOCCN(C)C	0
OC(=O)C1=NN(C(=O)C1)C1=CC=C(C=C1)S(O)(=O)=O	0
CCCCN(CCCC)CCCCCCN(CCCC)CCCC	0
O=C1CCCCCCCCCCC(=O)OCCO1	0
OC1=C(Br)C=C(Br)C=C1Br	0
C=CCC1=CC=C2OCOC2=C1	0
OCCCl	0
ON=C1CCCCC1	0
O[C@@H]1CCN2[C@@H]1C(=O)N(C2=O)c3ccc(C#N)c(Cl)c3	1
OC[C@@H]1Cc2ccccc2CN1C(=O)c3ccc(cc3)C(O)(C(F)(F)F)C(F)(F)F	1
CCC1=CC(=C(O)C=C1)C(C)(C)C	0
CN(C)CCCNCCCN(C)C	0
Cn1cc(cc1C(=O)N)N(Cc2ccccc2)c3ccc(cc3)[N+](=O)[O-]	1
CN(C)N=NC1=CC=CC=C1	0
CCCC1CCNc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CC1(C)Cc2cc3c(cc(O)nc3cc2NC1(C)C)C(F)(F)F	1
COC(=O)C(C)OC1=CC=C(OC2=CC=C(Cl)C=C2Cl)C=C1	0
ClC1=C2C(=O)OC(=O)C2=C(Cl)C(Cl)=C1Cl	0
O=NN(C1=CC=CC=C1)C1=CC=CC=C1	0
OC(=O)C1C(C(O)=O)C2(Cl)C(Cl)=C(Cl)C1(Cl)C2(Cl)Cl	0
CC1OC(C)C(C)=N1	0
CCCC1CCC(=O)CC1	0
CN(CC1=NC2=C(N)N=C(N)N=C2N=C1)C1=CC=C(C=C1)C(=O)N[C@@H](CCC(O)=O)C(O)=O	0
[K+].[O-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F	0
CC1=CC=CC(C)=C1O	0

CC1(C)COC(=O)[C@H]1Oc2ccc(C#N)c(c2)C(F)(F)F	1
CC=CC(O)=O	0
CCC1=CC=CC(O)=C1	0
CCCCCCCCC=O	0
Cl.CNC(=O)OC1=CC=CC(=C1)N=CN(C)C	0
CSC1=NN=C(C(=O)N1N)C(C)(C)C	0
CC[C@H]1[C@@H]2[C@@H](O)CCN2C(=O)N1c3ccc(C#N)c(Cl)c3C	1
OC1CCCC1c2ccc(C#N)c(c2)C(F)(F)F	1
[Na+].CC1=C(OCC([O-])=O)C=CC(Cl)=C1	0
Fc1ccc(cc1)C2=NOC3CCCCC23	1
CCn1c(=O)cc(c2cc3[C@H]4CCCC[C@H]4Nc3cc12)C(F)(F)F	1
CCCCCCCCN(C)CCCCCCCC	0
[Cl-].CCCCCCCCCC[N+](C)(CCCCCCCCCC)CCC[Si](OC)(OC)OC	0
Cc1cccc(c1)[C@@H]2COc3cc4[nH]c(=O)cc(c4cc3N2CC(F)(F)F)C(F)(F)F	1
FC(F)(F)c1cccc(c1)N2C(=O)[C@@H]3C4CC(C=C4)[C@@H]3C2=O	1
CC(CC1=CC=C(OCC(O)=O)C=C1)NCC(O)C1=CSC(=N1)C(F)(F)F	0
ClC1=C(Cl)C=CC=C1	0
CC1=C(N)C=CC=C1	0
ClCC(CCl)OP(=O)(OC(CCl)CCl)OC(CCl)CCl	1
Cl[Ni]Cl	0
CCCCCCCCCCC(CO)CCCCCCCC	0
CC[C@H]1C[C@@H](C)Nc2cc3oc(=O)cc(c3cc12)C(F)(F)F	1
Cn1cc(cc1C(=O)N2CCCCC2)N(Cc3ccccc3)c4ccc(cc4)[N+](=O)[O-]	1
CC(C)NC1=NC(NC(C)C)=NC(Cl)=N1	0
COc1ccc(cc1)C2(CO)N(C)C(=O)N(C2=O)c3ccc(C#N)c(c3)C(F)(F)F	1
COC(=O)c1c(C)n(Cc2ccccc2)c(C)c1-c3ccc(C#N)c(c3)C(F)(F)F	1
[Na+].CCCOC1=NN(C(=O)[N-]S(=O)(=O)C2=C(C=CC=C2)C(=O)OC)C(=O)N1C	0
OCC(O)C1=CC=CC=C1	0
C\C=C(/C)C(=O)OCCC1=CC=CC=C1	0
Cc1c(Cl)c(ccc1N2C[C@@H]3[C@H](O)CC[C@@H]3C2=O)C#N	1
CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5cccc(Cl)c5)c3c12	1
CNC(=O)OC1=CC=CC2=C1OC(C)(C)C2	0
[Na+].[Na+].[Na+].[O-]C(=O)C1=C(\N=N\C2=CC=C(C=C2)S([O-])(=O)=O)C(=O)N(N1)C1=CC=C(C=C...	0
CCN1N=C(CC2=CC=CC=C2)C=C1C1CCN([C@H]2C[C@@H](C[C@@H]2C2=CC=CC(F)=C2)N(C)[C@@...	0
CCCC1(C)CCc2cc3c(cc(O)nc3cc2N1)C(F)(F)F	1
FC(F)(F)C(=NOCC1OCCO1)C1=CC=C(Cl)C=C1	0
C[C@H]1Nc2cc3nc(O)cc(c3cc2CC1(C)C)C(F)(F)F	1
CC(C)C1CCNc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CCNC1=NC(N)=NC(Cl)=N1	0
C[C@@H](O)C(O)=O	0
COC(=O)C1=C(CC(C)C)C(C2=NCCS2)=C(N=C1C(F)F)C(F)(F)F	0
CC(C)C(C)(N)C#N	0
NC(=O)NC1NC(=O)NC1=O	0
Cc1nn(c(C)c1Cc2ccccc2C(=O)N)-c3ccc(C#N)c(Cl)c3	1
COC1=CC=C(N)C(=C1)[N+]([O-])=O	0

CN1C=C(C(=O)C(=C1)C1=CC(=CC=C1)C(F)(F)F)C1=CC=CC=C1	0
Oc1cc(c2cc3CCNc3cc2n1)C(F)(F)F	1
C1=CC2=CC=CC=C2C=C1	0
COc1cccc(OC)c1Oc2ccc(C#N)c(c2)C(F)(F)F	1
CC(=O)NC1=CC=C2C(CC3=C2C=CC(NC(C)=O)=C3)=C1	0
CC1=C(Cl)C=C(N)C=C1	0
CCCC1=CC(=O)NC(=S)N1	0
CCCNc1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
FC(F)(F)c1cc(=O)[nH]c2ccc-3c(OCc4ccccc34)c12	1
CCCCCOC(CC)OC(C)COC(O)CC	0
CCC1CN(CC(F)(F)F)c2cc3c(cc(=O)[nH]c3cc2O1)C(F)(F)F	1
[Na+].[O-]C(=O)C1=CN=CC=C1	0
CC(CC=O)CC(C)(C)C	0
Brc1ccc(N2C(=O)[C@@H]3C4CCC(O4)[C@@H]3C2=O)c5ccccc15	1
[NH4+].[O-]C(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
CCOC(=O)COC1=CC=C(C)C=C1	0
Fc1ccccc1Sc2ccc(C#N)c(c2)C(F)(F)F	1
OCN1C(NC(=O)NCNC(=O)NC2N(CO)C(=O)NC2=O)C(=O)NC1=O	0
FC(F)(F)C1=CC=C(Cl)C=C1	0
FC(F)(F)c1cc(O[C@@H]2CCCC[C@H]2C#N)ccc1C#N	1
CC(C)(CO)CO	0
CC(C)=CCCC(C)(OC(=O)C1=CC=CC=C1)C=C	0
Cc1c(Cl)c(ccc1N2C(=O)[C@@H]3[C@H](O)CCN3C2=O)C#N	1
OCCCCCCCCC=C	0
CC1=CC(C)(C)Nc2ccc3-c4ccccc4O/C(=C\c5ccccc5)/c3c12	1
CNC(=O)N(C)C1=NN=C(S1)C(C)(C)C	0
O[C@@H]1CCCC[C@@H]1c2ccc(C#N)c(c2)C(F)(F)F	1
CCCCCC=CCC(=O)OC	0
CC(O)C1CCCCC1	0
CN1C(=O)C2=C(C=CC=C2)C1=O	0
CCOC(=O)C1=CC=C(N)C=C1	0
FC(F)CN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
FC(F)(F)c1cc(SCC2CCC2)ccc1C#N	1
CC(C)(C)C1=CC(CCC(=O)OCC(COC(=O)CCC2=CC=C(O)C(=C2)C(C)(C)C)C(C)(C)C)(COC(=O)CCC2=CC	0
CC1=NNC(=O)N(C1)\N=C\C1=CC=CN=C1	0
[Na+].COC1=CC(OC)=NC(SC2=C(C([O-])=O)C(Cl)=CC=C2)=N1	0
CCCOC(=O)C1=CC=C(O)C=C1	0
CCOc1cc(ccc1C(=O)O)C2=NN([C@H](C2)C3CCCC3)c4ccc(C#N)c(Cl)c4	1
ClC1=C(Cl)[C@]2(Cl)[C@@H]3[C@@H]4C[C@@H](C=C4)[C@@H]3[C@@]1(Cl)C2(Cl)Cl	0
FC(F)(F)c1cc(SC2CCC2)ccc1C#N	1
Cc1c(CO)c(c(C)n1Cc2ccccc2)-c3ccc(cc3)[N+](=O)[O-]	1
C[C@](O)(COc1cccc2ccccc12)C(=O)Nc3ccc(C#N)c(c3)C(F)(F)F	1
Cc1ccccc1Oc2ccc(C#N)c(c2)C(F)(F)F	1
CCCCN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
CC(C)CC=C(C=O)C1=CC=CC=C1	0

OCC=C	0
COC1=NC(C)=NC(NC(=O)NS(=O)(=O)C2=C(Cl)C=CC=C2)=N1	0
C(N(CC1=CC=CC=C1)CC1=CC=CC=C1)C1=CC=CC=C1	0
O=C1NC2NC(=O)NC2N1	0
CC1=C(C=C(C=C1)[N+]([O-])=O)[N+]([O-])=O	0
COC(=O)C1=CC=C(C(=O)OC)C(=C1)C(=O)OC	0
CCCCC(CC)COC(=O)C1=C(C=CC=C1)C(=O)OCC(CC)CCCC	0
CC1=CC=C(C)C(=C1)S(O)(=O)=O	0
CC(C)OC(=O)N1C[C@@]2(C)O[C@@](C)(C1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)	1
CCC(C)(C)C1CCCCC1OC(C)=O	0
C[C@]12CNC[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F	1
CCCCCOC(=O)CCCCCCCC(=O)OCCCC	0
CC(C)C(C)(C)C(C)(C)C(C)(C)S	0
CCCCCCCCCCCCC=C	0
CN(C)C(=O)NC1=CC(Cl)=C(Cl)C=C1	0
COC1=CC=C(C(=O)C2=CC=CC=C2)C(O)=C1	0
OC(=O)c1ccc2C3=NN([C@@H](C4CCCC4)[C@H]3CCc2c1)c5ccc(C#N)c(Cl)c5	1
ClCC(Cl)C=C	0
[As]#[In]	0
COc1cccc2OC(C)c3c(ccc4[nH]c(=O)cc(C)c34)-c12	1
COC(=O)C=C(C)CCC=C(C)C	0
CC(O)COC1=CC=CC=C1	0
CC1=CC=NC(N)=C1	0
FC(F)CN(CC(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
CCC1CCN(C=O)c2cc3nc(O)cc(c3cc12)C(F)(F)F	1
Nc1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCCCCC[S+]([O-])CCCC(F)(F)C(F)(F)F)CC4CC(=O)CC[C	1
Clc1cc(Cl)cc(c1)N2C(=O)[C@@H]3C4CC(C=C4)[C@@H]3C2=O	1
CCCCCC#CC(=O)OC	0
Cl[C@H]1OCCO[C@@H]1Cl	0
NC1CCCCC1N	0
CCOC(=O)CCCCCCCCC=C	0
[Na+].CCCCCCCCCCCCCCOS([O-])(=O)=O	0
CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C	0
FC(F)(F)c1ccccc1-c2ccc(C#N)c(c2)C(F)(F)F	1
CC1=C2C(=O)C3=C(C(O)=C(O)C([C@@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)=C3O)C(=O	0
CC[C@H]1Nc2cc3nc(O)cc(c3cc2CC1(CC)CC)C(F)(F)F	1
CC(C)C(=O)NC1=CC(=C(C=C1)[N+]([O-])=O)C(F)(F)F	1
CCCCCOC(=O)C(C)CC	0
FC1(F)C[C@@H](C#N)N(C1)C(=O)CNC1CC2CCC(C1)N2C1=NC=CC=N1	0
CC1(C)N(CO)C(=O)NC1=O	0
FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCl	0
O[C@@H]1CCN2[C@@H]1C(=O)N(C2=O)c3ccc(C#N)c(c3)C(F)(F)F	1
NC(=O)OCC(COC(N)=O)C1=CC=CC=C1	0
COP(=O)(OC)OC=C(Cl)Cl	0

OC(=O)C1=CC(C(O)=O)=C(C=C1C(O)=O)C(O)=O	0
C1=CC2=CC3=C(C=CC=C3)C=C2C=C1	0
CCCCCCCCCCOC(C)=O	0
Cn1cc(cc1C(=O)N2CCCC2)N(Cc3ccccc3)c4ccc(c(c4)C(F)(F)F)[N+](=O)[O-]	1
CC1=C(C)C=C(O)C=C1	0
[Na+].[O-][Cl]=O	0
CN(C)[C@H]1[C@@H]2[C@@H](O)[C@H]3C(=C(O)[C@]2(O)C(=O)C(C(N)=O)=C1O)C(=O)C1=C(C	0
OS(=O)(=O)C1=CC2=C(C=CC=C2)C=C1	0
CSC1=NC=CN=C1	0
CC1(C)C2CCC(C2)C1=C	0
CCC1=CN=C(C2=NC(C)(C(C)C)C(=O)N2)C(=C1)C(O)=O	0
CN(C)C(=O)CCCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C	1
NC(N)=O	0
CC1=CC=C(C)C(O)=C1C	0
CC(=O)NC1=CC=C(C)C=C1C	0
O=C1CCCO1	0
CCOC1=C(O)C=CC(C=O)=C1	0
[O-][N+](=O)C1=CC(=CC=C1)[N+]([O-])=O	0
NCCOCCOCCN	0
CCOC(=O)CC	0
O=C1CCCCCCCCCCCCCO1	0
C1CCC(CC1)NC1CCCCC1	0
O=C1CCCCCCCCCCCCC1	0
CCCC1=CC=CC=C1	0
CC(C)[C@H](C(=O)OC(C#N)C1=CC=CC(OC2=CC=CC=C2)=C1)C1=CC=C(OC(F)F)C=C1	0
COC1=CC(OC)=CC=C1	0
OC(CCl)CCl	0
CC1=C(C=CC=C1[N+]([O-])=O)[N+]([O-])=O	0
CCCCCCCC(O)=O	0
[O-][N+](=O)c1ccc(cc1C(F)(F)F)C2=NOC3CCCC23	1
Cn1c(=O)cc(c2cc3C(=CC(C)(C)N(C)c3cc12)C)C(F)(F)F	1
CCOC(=O)CC(O)(CC(=O)OCC)C(=O)OCC	0
CC(=O)NC1=CC=C(O)C=C1	0
C[C@]12CCCC(C)(C)[C@H]3[C@H](CC[C@@H]13)C2=C	0
CCCCN(CC)C1=C(C=C(C=C1[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O	0
O[C@H]([C@@H](O)C(O)=O)C(O)=O	0
O=C1CCCCC1	0
CC1=CC(C)=C(C)C=C1C	0
CCCSP(=S)(OCC)OC1=CC=C(SC)C=C1	0
NN1C=NN=C1	0
CCC(C)N(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
CC(CCC=C(C)C)CC(O)=O	0
Cc1cc(ccc1C#N)N2C(=S)N(CCCS(=O)(=O)N)C(C)(C)C2=O	1
NC[C@H](O)C1=CC=C(O)C(O)=C1	0
Cc1ccc(cc1)-c2ccc(C#N)c(c2)C(F)(F)F	1

COc1cccc(F)c1Oc2ccc(C#N)c(c2)C(F)(F)F	1
C[C@@H]1C[C@H](C)c2cc3c(cc(O)nc3cc2N1)C(F)(F)F	1
CC(=O)CCC(O)=O	0
Fc1ccc(cc1C(F)(F)F)C2=NOC3CCCCC23	1
NC1=C(N)C=C(C=C1)[N+]([O-])=O	0
C[C@]12CC[C@H]3[C@@H](C(CCCCCCCC(=O)N)C[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@	1
CCCSc1ccc(C#N)c(OC)c1	1
COC(=O)CC(=O)OC	0
COP(=O)OC	0
CCOP(=S)(OCC)SCCSCC	0
OC(=O)C1=CC=C2C(=O)OC(=O)C2=C1	0
CCCCN(C)c1cc(c(cn1)C#N)C(F)(F)F	1
CCNCCO	0
OC1=C(Cl)C=C(Cl)C=C1Cl	0
CCCC1COC(CN2C=NC=N2)(O1)C1=C(Cl)C=C(Cl)C=C1	1
CC1=NC2=NC(=NN2C=C1)S(=O)(=O)NC1=C(F)C=CC=C1F	0
CCC[C@@H]1CCc2cc3c(cc(O)nc3cc2N1)C(F)(F)F	1
BrCC1=CC=CC(OC2=CC=CC=C2)=C1	0
CC(=O)CC(C)(C)C1CCCCC1	0
ClC1=C(Cl)C(Cl)=C(Cl)S1	0
COC1=CC(C)=C(N)C=C1	0
FC(F)(F)c1cccc(c1)N2C(=O)[C@H]3C4CCC(C4)N3C2=O	1
CC1=CC=CN=C1	0
CC(=O)OCC(COC(C)=O)OC(C)=O	0
CCCN(CC1CC1)C1=C(C=C(C=C1[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O	0
CC(C)C1=CC2=CC=CN=C2C=C1	0
CC(CCC=C(C)C)CC=O	0
CC1=CC(O)=C(Cl)C(C)=C1Cl	0
CC1=CC=CC=C1CCO	0
CCCN(CCC)N=O	0
CC1CCNc2cc3oc(=O)cc(c3cc12)C(F)(F)F	1
Cl.CCOC(=O)NNC1=NN=CC2=CC=CC=C12	0
CCCC1=CC=C(O)C=C1	0
CCCN(CCCl)C1=C(C=C(C=C1[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O	0
[Na+].[Na+].NC1=CC(N)=C(C=C1)\N=N\C1=CC=C(C=C1)C1=CC=C(C=C1)\N=N\C1=C(C=C2C=C(C(\N	0
CC(C)(C)C(O)C(=C/C1=C(Cl)C=C(Cl)C=C1)\N1C=NC=N1	1
Cc1nn(c(C)c1Oc2ccc(cc2)C(=O)NCC(C)(C)O)-c3ccc(C#N)c(Cl)c3	1
CCCN(CCC)S(=O)(=O)C1=CC=C(C=C1)C(O)=O	0
CC[C@@H]1[C@H](C)CNc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CSC1=NC(NC(C)C)=NC(NC(C)C)=N1	0
OCC(COC(=O)CCN1CC1)(COC(=O)CCN1CC1)COC(=O)CCN1CC1	0
OC(=O)C(=O)CC1=CC=CC=C1	0
OC(=O)CC1=CNC2=C1C=CC=C2	0
COCCCOC[C@H](CC1(CCCC1)C(=O)N[C@H]1CC[C@H](CC1)C(O)=O)C(=O)OC1=CC2=C(CCC2)C=C1	0
CN(C)CCCNCCC#N	0

CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCC	0
CCCCCOC(=O)CCCCCCCCC(=O)OCCCC	0
CCOP(=S)(OCC)SCSC1=C(Cl)C=CC(Cl)=C1	0
CC(C)=CCCC(C)=CCCC(C)(O)C=C	0
CC(C)(N)CO	0
OCCN(CCO)CCO.CCCCCCCCCCCCCOS(O)(=O)=O	0
NC(=O)CN(CC(F)(F)F)C1=CC(=C(C=C1)C#N)C(F)(F)F	1
CC(C)C1=CC=C(O)C=C1	0
CCCCCCC(C=O)=CC1=CC=CC=C1	0
COC[C@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
COC(=O)NC1=NC2=CC=CC=C2N1	0
CC(OC1=C(Cl)C=C(Cl)C=C1)C(O)=O	0
CC1=CC(O)=C(C)C(C)=C1	0
Clc1ccc(cc1)C2=NOC3CCCCC23	1
CC(=O)O[C@@]1(CC[C@H]2[C@@H]3C=C(Cl)C4=CC(=O)[C@@H]5C[C@@H]5[C@]4(C)[C@H]3C	1
[Na+].CCCCC(CC)CCC(CC(C)C)OS([O-])(=O)=O	0
O.O.O.[Na+].CNC([S-])=S	0
COC1=C2C=COC2=CC2=C1C=CC(=O)O2	0
CCC[Si](OC)(OC)OC	0
CC(CCO)CC(C)(C)C	0
CCCNc1ccc2nc(O)cc(c2c1)C(F)(F)F	1
CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5ccc(Br)cc5)c3c12	1
O=C1NC(=O)C2=C1C=CC=C2	0
CC1=CC(O)=CC(C)=C1	0
Cn1c(=O)cc(c2cc3CCC(C)(C)N(C)c3cc12)C(F)(F)F	1
ClC1=CC=C(C=C1)C(=O)C1=CC=C(Cl)C=C1	0
CC(C)[C@@]12C[C@@H]1C(C)C(=O)C2	0
C1C=CC2C3CC(C=C3)C12	0
CC12C[C@H](O)C(C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(I)c4	1
OC1=C(N=C2C=CC=C2=C1Br)C1C(=O)C2=C(C=CC=C2)C1=O	0
OCC1=CC=C(O1)C=O	0
CC(C)COC(=O)C1=CC=CC=C1O	0
CCCC1CCNc2cc3oc(=O)cc(c3cc12)C(F)(F)F	1
COc1c(OC(C)C)ccc2oc(=O)c3c(ccc4[nH]c(=O)cc(C)c34)c12	1
Oc1cccc2oc(cc(=O)c12)-c3ccccc3	1
CCOC(=O)N1C[C@@]2(C)O[C@@](C)(C1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)	1
OC(=O)C1=CC=CC(=C1)[N+]([O-])=O	0
CC[C@H](C)[C@H](N1SC2=CC=CC=C2C1=O)C(O)=O	0
CC1=CC(C)(C)Nc2ccc(cc12)-c3cc(F)cc(c3)C#N	1
COC1=CC(C)=CC(O)=C1	0
CCCCCC(CO)CCC	0
CCOCC(C)O	0
CC(C)C1(O)CCC(C)=CC1	0
C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]12C	1
Cc1nn(c(C)c1Cc2ccc(F)cc2)-c3ccc(C#N)c(Cl)c3	1

CCC(C)COC(=O)CC(C)C	0
Oc1cc(c2cc3C(CCNc3cc2n1)c4cc(cc(c4)C(F)(F)F)C(F)(F)F)C(F)(F)F	1
CCCCN(C)C(=O)CCCCCCCCCCC[C@@H]1CC2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)C	1
C[C@]1(O)CC[C@H]2[C@@H]3[C@H](CCCCCCCCCC(=O)O)CC4=CC(=O)CC[C@]4(C)[C@H]3CC[C	1
CCN(c1ccc(cc1)[N+](=O)[O-])c2cc(C(=O)N3CCCC3)n(C)c2	1
CC(O)=O	0
FC(F)CN(CC(F)(F)Cl)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
OC1=CC=C(C=C1)C(C1=CC=C(O)C=C1)C(Cl)(Cl)Cl	1
CC(O)CNCC(C)O	0
CCOC(=O)c1c(C)n(c(C)c1-c2ccc(cc2)[N+](=O)[O-])-c3ccccc3	1
CC=CC=CCOC(=O)C(C)C	0
COC(=O)CSC1=C(Cl)C=C(F)C(=C1)\N=C1/SC(=O)N2CCCCN12	0
CCC(C)N	0
COS(=O)(=O)OC	0
CCCCC(CC)COC(=O)CCCCC(=O)OCC1=CC=CC=C1	0
O=C(C1CCCCC1)C1=CC=CC=C1	0
COC(N)=O	0
OC[C@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](O)[C@H](O)O[C@@H]2CO)[C@H](O)[C@@H	0
CCC(C)(C1=CC=C(O)C=C1)C1=CC=C(O)C=C1	1
O=C(OCCCCOC(=O)C1=CC=CC=C1)C1=CC=CC=C1	0
COC1=C(OC)C=C(C=C1)[C@@H]1CC(=O)C2=C(O1)C=C(O[C@@H]1O[C@H](CO[C@@H]3O[C@@	0
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
NC1=CC=C(SC2=CC=C(N)C=C2)C=C1	0
CCCCCCCCCCCCO	0
COc1c(O)ccc2oc(=O)c3c(ccc4[nH]c(=O)cc(C)c34)c12	1
C[C@H]1C[C@@H]2[C@H](CC[C@@]3(C)[C@H]2CC[C@]3(OC(=O)C)C(=O)C)[C@@]4(C)CCC(=O)	1
CC(C)(C)C(=O)C(O)=O	0
C[C@]12CC[C@H]3[C@@H](C(CCCCCCCC(=O)N4CCOCC4)C[C@H]5CC(=O)CC[C@]35C)[C@@H]	1
CCN(CC)C(=O)C(C)OC1=C2C=CC=CC2=CC=C1	1
NC1=NNC=N1	0
Cl.NNC(N)=N	0
FC(F)(F)c1cc(=O)[nH]c2cc(NC3CCCCC3)ccc12	1
OC(=O)C1CCN(CC1)C1=C(NC(=O)NC(=O)C2=CC(F)=C(F)C=C2Cl)C=C(F)C=C1	0
COC1=CC=C(OC)C=C1	0
CN1C(=S)N(C(=O)C1(C)C)c2ccc(C#N)c(c2)C(F)(F)F	1
[K+].[O-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
CCCCC1=CC=C(Cl)C=C1	0
[O-][N+](=O)c1cc(ccc1Cl)N2C(=O)[C@@H]3C4CCC(O4)[C@@H]3C2=O	1
CCCN1CCOc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F	1
NC(=O)C1=CC=CC=C1O	0
CC1=NC=C(C=N1)[C@@H](CCCCCC1=NC2=C(CCCN2)C=C1)CC(O)=O	0
CC(C)C(=O)OC(C)(CCC=C(C)C)C=C	0
ClCCOP(=O)(OCCCl)OCCCl	0
CNC(=O)OC1=CC=CC(=C1)C(C)C	0
NNC(=O)C1=CC=NC=C1	0

CCCCCCC(O)CCCCCCCCCCC(O)=O	0
CC1=CC=C(Cl)C=C1	0
CCCCCCCC[C@H]1C[C@]2(C)[C@@H](O)CCC2C3CCC4=CC(=O)CCC4=C13	1
CCO[Si](CC)(OCC)OCC	0
O=c1cc(oc2ccccc12)-c3ccccc3	1
ClCCOCCCl	0
CC(=O)CCC1=C(C)CCCC1(C)C	0
CCCN(CC)CC1COC2(CCC(CC2)C(C)(C)C)O1	0
CC[C@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
NC(=O)N=NC(N)=O	0
CCCOc1ccc(/C=N/NC(=O)c2oc3ccc4ccccc4c3c2)cc1	1
CC(C)C1=CC=CC(C(C)C)=C1O	0
CC\C(=C(\CC)C1=CC=C(O)C=C1)C1=CC=C(O)C=C1	1
CN1[C@@H]2CC[C@@H]3[C@H](CC[C@@]4(C)[C@H]3C/C(=C\c5cnc(nc5)C6CC6)/[C@@H]4O)[	1
CC1=CC=C(C=C1S(O)(=O)=O)[N+]([O-])=O	0
O=S1(=O)CCCO1	0
COC1=NC(NC(C)C)=NC(NC(C)C)=N1	0
CCCSP(=S)(OCC)OC1=C(Cl)C=C(Cl)C=C1	0
[O-][N+](=O)c1ccc(cc1C(F)(F)F)C2=NO[C@H]3CCC[C@@H]23	1
CCCOC(=O)C1=CC=C(N=C1)C(=O)OCCC	0
OC1OCCOC1O	0
OCCN1CCCC1=O	0
CC(O)CCO	0
CCCCCC[C@@H](O)C\C=C/CCCCCCCC(O)=O	0
COC1=C(O)C=CC(CC=C)=C1	0
O1C2=CC=CC2C2=C1C=CC=C2	0
CCCCCCCCCC[C@H]1C[C@]2(C)[C@@H](O)CCC2C3CCC4=CC(=O)CCC4=C13	1
CCN(CC)CCO	0
CC1(C)CCc2cc3c(cc(=O)oc3cc2N1)C(F)(F)F	1
CCCCOCCOCCSC#N	0
NC1CCCCC1	0
CC[C@H]1C[C@@H](C)Nc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
COC(=O)c1c(C)n(Cc2ccccc2)c(C)c1-c3ccc(cc3)C#N	1
CCCCNS(=O)(=O)C1=CC=C(C)C=C1	0
Cn1c(=O)cc(c2cc3C(=CC(C)(C)Nc3c(C)c12)C)C(F)(F)F	1
[O-][N+](=O)c1ccc(C2=NO[C@@H]3CCCC[C@H]23)c(c1)C(F)(F)F	1
NC1=CC=CC(=C1)S(=O)(=O)C1=CC(N)=CC=C1	0
C[Si](C)(C)N[Si](C)(C)C	0
CC(Cc1ccc(O)c(O)c1)C(C)Cc2ccc(O)c(O)c2	1
CC1=CC=C(C=C1N=C=O)N=C=O	0
C[C@@H]1CC[C@H]([C@@H](O)C1)C(C)=C	0
CCOP(=S)(OCC)OC1=CC(C)=NC(=N1)N(CC)CC	0
Cn1cc(cc1C(=O)N2CCCC2)N(Cc3ccc(F)cc3)c4ccc(cc4)[N+](=O)[O-]	1
O=C1[C@@H]2C3CC(C=C3)[C@@H]2C(=O)N1c4ccc5cccnc5c4	1
NC#N	0

CCCC1CCC(=O)O1	0
CC1=CC(C)(C)Nc2c(C)c3nc(O)cc(c3cc12)C(F)(F)F	1
CC(C)OC(C)=O	0
OC1=CC=C(Cl)C=C1	0
OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
CC\C=C/CCCCCO	0
Cn1cc(cc1C(=O)N2CCCC2)N(Cc3ccccc3)c4ccc(cc4)C#N	1
CCCCCCOC(=O)CCCCC(=O)OCCCCCC	0
N(NC1=CC=CC=C1)C1=CC=CC=C1	0
CCCCC(CC)COC(=O)CS	0
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)S(=O)(=O)c5c	1
COC1=CC=C(CCC(C)=O)C=C1	0
CCOC(=O)C(O)(C1=CC=C(Cl)C=C1)C1=CC=C(Cl)C=C1	1
OCC1CCCO1	0
CC1(C)N(Br)C(=O)N(Br)C1=O	0
BrC(Br)C#N	0
ClC1=CC(Cl)=CC=C1	0
OC1=CC=CC=C1C=O	0
FC(F)(F)c1cc(O[C@H]2CCCC[C@@H]2C#N)ccc1C#N	1
FC(F)(F)CN(CC(F)(F)F)c1ccc2[nH]c(=O)ccc2c1	1
CCCCC=O	0
CC1=CC(=O)NO1	0
CCCCC1CCCCC(=O)O1	0
CCCCCCNCCCCCC	0
SCC(=O)OCCOC(=O)CS	0
CC(C)N(C)C(=O)CCCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]	1
CC(=C)C1CC=C(C)C(=O)C1	0
COc1cccc2OC(CC=C)c3c(ccc4[nH]c(=O)cc(C)c34)-c12	1
OC[C@@H](O)[C@H]1O[C@@H]2O[C@@H](O[C@@H]2[C@H]1O)C(Cl)(Cl)Cl	0
OC[C@H](O)[C@H]1OC(=O)C(O)=C1O	0
Cl.CN(C)CCOC(C1=CC=CC=C1)C1=CC=CC=C1	0
O=C(OCC=CC1=CC=CC=C1)C=CC1=CC=CC=C1	0
COC1=CC=C(C=C1)C(O)(C1CC1)C1=CN=CN=C1	0
Cn1c(=O)cc(c2cc3CCC4(C)CCCN4c3cc12)C(F)(F)F	1
CC(C)(C)C1=CC=C(S)C=C1	0
NNCCO	0
OCC1CCC(COC=C)CC1	0
CC(C)CC(C)CC(O)CC(C)C	0
CC(C)C1CCC(O)CC1	0
CCCCCC1C(CC(=O)OC)CCC1=O	0
CC(C)(C)OC(=O)N1C[C@@H]2C[C@H]1[C@H]3N2C(=O)N(C3=O)c4ccc(cc4)C#N	1
COC1=CC(OC)=NC(NC(=O)NS(=O)(=O)C2=NC=CC=C2C(=O)N(C)C)=N1	0
CC(C)(C)OOC(=O)C1=CC=CC=C1	0
NS(O)(=O)=O	0
CCCCCCCCCCCCCCCCO	0

OC1=NC(O)=NC(O)=N1	0
CN1N(C(=O)C=C1C)C1=CC=CC=C1	0
C[Sn](Cl)(Cl)Cl	0
CCCCCC1=CC=CO1	0
[Na+].[O-]S(=O)(=O)C1=CC2=C(C=C1)C(=O)C1=C(C=CC=C1)C2=O	0
N(N=NC1=CC=CC=C1)C1=CC=CC=C1	0
[Na+].OC1=C(N=NC2=CC=C(C=C2)S([O-])(=O)=O)C2=CC=CC=C2C=C1	0
[O-][N+](=O)c1ccc(C2=NOC3CCCC23)c(c1)C(F)(F)F	1
OC(=O)CCCC1=CNC2=C1C=CC=C2	0
CCN(C(C)C)c1ccc2nc(O)cc(c2c1)C(F)(F)F	1
CCCCCCOC1=C(C=CC=C1)C(O)=O	0
CCc1ccccc1Oc2ccc(C#N)c(c2)C(F)(F)F	1
OC(=O)C1=C(Cl)C=CC2=CC(Cl)=CN=C12	0
CC1(C)CN(Cc2ccc(F)cc2)C(=O)C1Oc3ccc(C#N)c(c3)C(F)(F)F	1
S=C1NCCN1	0
CCC(C)(C)C1CCC(=O)CC1	0
CCCCCCCCCCCCCCCCCO	0
Cc1ccc(cc1Cl)N2C(=O)[C@@H]3C4CCC(O4)[C@@H]3C2=O	1
CC12CCC(C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4cc(Cl)cc(Cl)c4	1
[Cl-].CCCC[N+]1(C)CCCC1	0
[O-][N+](=O)C1=CC=CC=C1	0
CCO[Si](C)(OCC)OCC	0
CC(CCl)OP(=O)(OC(C)CCl)OC(C)CCl	0
CCC(=O)OC(C)(CCC=C(C)C)C=C	0
CSCCC=O	0
CC(C)CC(=O)CC(C)C	0
CCC1CC(C)(C)Nc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CN(C)C(=O)NC1=CC=CC=C1	0
[Na+].CC(=O)NC1=C(I)C(C([O-])=O)=C(I)C(NC(C)=O)=C1I	0
CNC(=O)OC1=CC=CC=C1OC(C)C	0
CCCN(CCC)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
CCC1(CC)CCc2cc3c(cc(O)nc3cc2N1)C(F)(F)F	1
COc1cccc2oc(=O)c3c(ccc4[nH]c(=O)cc(C)c34)c12	1
C[Si](C)(O[Si](C)(C)C=C)C=C	0
CC1=CC2=CC=CN=C2C=C1	0
FC(F)(F)C1=CC=C(Cl)C(Cl)=C1	0
C[C@@H]1C[C@H]2[C@@H]3CC[C@H]4N(C)C(=O)C=C[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1O	1
C[C@H]1CNc2cc3nc(O)cc(c3cc2C1CCC(F)(F)F)C(F)(F)F	1
OS(=O)(=O)NC1CCCCC1	0
CC(C)OC(=O)NC1=CC=CC=C1	0
CCN(CC(F)(F)F)c1ccc2nc(O)cc(c2c1)C(F)(F)F	1
CCOCCOC(C)=O	0
CC(C)(C)C(=O)CCC1=CC=C(Cl)C=C1	0
CCN(CC)N=O	0
FC1=CC=C(NC(=O)C2=C(OC3=CC(=CC=C3)C(F)(F)F)N=CC=C2)C(F)=C1	0

C=COCC1CCC(COC=C)CC1	0
CC[C@@H]1[C@@H]2[C@H](O)CCN2C(=O)N1c3ccc(C#N)c(Cl)c3C	1
CC(C)=CCl	0
CCOC1=C(O)C=CC=C1	0
CCCCN(CCCCO)N=O	0
C[C@H]1[C@@H]2[C@@H](O)CCN2C(=O)N1c3ccc(C#N)c(Cl)c3C	1
Cl[Pd]Cl	0
NC1=CC(N)=C(Cl)C=C1	0
CC(C)[C@@H]1CCc2cc3c(cc(O)nc3cc2N1)C(F)(F)F	1
CC(C)(C)NC(N)=O	0
[K+].[O-]C(=O)CNC1=CC=CC=C1	0
[O-][N+](=O)C1=CC=C(Cl)C=C1	0
CC1(C)N(Cl)C(=O)N(Br)C1=O	0
CCCCCCOC(=O)C1=C(C=CC=C1)C(=O)OCCCCCC	0
C[C@]12Cc3cnoc3C=C1CC[C@@H]4[C@@H]2CC[C@@]5(C)[C@H]4CC[C@@]5(O)C#C	1
CCCC1=CC=C(C=O)C=C1	0
CC(C)C1=CC2=C(SC3=C(C=CC=C3)C2=O)C=C1	0
CC(=O)C=CC1=CC=CC=C1	0
CC(C)(CO)C(O)C(=O)NCCCO	0
FC(F)(F)CN(Cc1ccccc1)c2ccc3[nH]c(=O)cc(c3c2)C(F)(F)F	1
Cl.CC1=CC=CC=C1N	0
OC1=CC=C(C=C1)C1(OS(=O)(=O)C2=C1C=CC=C2)C1=CC=C(O)C=C1	0
OC1=CC=CC=C1C(=O)C1=CC=CC=C1	0
CC(=O)C1=CC=CC=C1	0
C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2C(=O)CO	1
CCN1CCOc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F	1
[Na+].COC1=C(OC)C(CS(=O)C2=NC3=C([N-]2)C=CC(OC(F)F)=C3)=NC=C1	0
C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O	1
CN1C(=O)N(C(=O)[C@]1(CO)c2ccccc2)c3ccc(C#N)c(c3)C(F)(F)F	1
CC1(C)NC(=O)NC1=O	0
CC(C)=CCC\C(C)=C\C\C=C(/C)C=C	0
CC(=O)\C=C\C1C(C)=CCCC1(C)C	0
[Na+].[O-]C(=O)C1=CC=CC=C1	0
CC1=CC(=CC=C1)[N+]([O-])=O	0
Fc1ccc(C2=NOC3CCCCCC23)c(c1)C(F)(F)F	1
CCOP(=S)(OCC)SCSC(C)(C)C	0
CC1=C(O)C=CC(Cl)=C1	0
S1C2=C(C=CC=C2)C2=C1C=CC=C2	0
CC(C)=CCOC(=O)C1=CC=CC=C1	0
[Na+].COS([O-])(=O)=O	0
CNCCO	0
CCCCN(CCCC)CCCC	0
OCCOC1=CC=CC=C1	0
CCCC1CCOC(C)S1	0
ClCC(Cl)CCl	0

CCCCC\C=C/C\C=C/CCCCCCCC(O)=O	0
CNC(NCCSCC1=CSC(CN(C)C)=N1)=C[N+]([O-])=O	0
COc1ccc2oc(cc(=O)c2c1)-c3ccccc3	1
OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
CC(=O)OC(C)(C)CC1=CC=CC=C1	0
CC(C)(O)C(=O)NC1=CC(=C(C=C1)[N+]([O-])=O)C(F)(F)F	1
CCCC(O)=O	0
CC[C@@H]1[C@@H]2[C@@H](O)CCN2C(=O)N1c3ccc(C#N)c(Cl)c3C	1
NNC(=O)C1=CC(=CC=C1)C(=O)NN	0
O.ClCCN(CCCl)P1(=O)NCCCO1	0
CC(C)CN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(C)c2c1	1
C[C@]12CC[C@H]3[C@@H](C(CCCCCCCC(=O)N4CCCCC4)C[C@H]5CC(=O)CC[C@]35C)[C@@H]	1
CN(C)N=O	0
Cl.NC1=CC=CC=C1	0
O.O.O.[Na+].CC1=CC=C(C=C1)S(=O)(=O)[N-]Cl	0
CCOC1=CC=C(C=C1)C(C)(C)COCC1=CC(OC2=CC=CC=C2)=CC=C1	0
ClC(Cl)=C(C1=CC=C(Cl)C=C1)C1=CC=C(Cl)C=C1	0
CCCCCCCCC(CO)CCCCCC	0
CC1(CCCCC1)C(=O)NC1=C(Cl)C(Cl)=C(O)C=C1	1
CC1=C(OCCCC(O)=O)C=CC(Cl)=C1	0
FC(F)(F)c1cc(=O)[nH]c2ccc(cc12)N3CCCC3	1
CC1(C)CC(=O)CC(C)(C)N1[O]	0
CCCN1[C@@H]2CCCC[C@@H]2c3cc4c(cc(=O)n(C)c4cc13)C(F)(F)F	1
ClC1=C(Cl)N=CC(=C1)C(Cl)(Cl)Cl	0
COC1=CC=C(C=O)C=C1OC	0
OC(=O)C1=C(C=CC=C1)C(=O)OCC1=CC=CC=C1	0
CCCCCCCCCCCCCCCC	0
C[C@]12CN(O)C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F	1
CNC(=O)OC1=CC2=C(C=C1)N(C)[C@H]1N(C)CC[C@@]21C	0
CC(C)(C)N1CCOc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F	1
C/C=C/1\C(=O)C[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C	1
COc1cc(Sc2c(C)cccc2C)ccc1C#N	1
FC(F)(F)c1cc(ccc1C#N)N2C(=O)[C@H]3[C@@H]4C[C@@H](CN4C(=O)c5ccccc5)N3C2=O	1
CNNCC1=CC=C(C=C1)C(=O)NC(C)C	0
CC1=CCC2CC1C2(C)C	0
C=CCOC(=O)CCC1CCCCC1	0
CCCCOC(=O)[C@@H](C)OC1=CC=C(OC2=CC=C(C=N2)C(F)(F)F)C=C1	0
CC(C)=CCCC(C)(OC=O)C=C	0
COC(=O)CC(C)CCC=C(C)C	0
CCCC(=O)C(CC)SC1=C(C)OC=C1	0
NC1=NC(N)=C2N=C(CNC3=CC=C(C=C3)C(=O)N[C@@H](CCC(O)=O)C(O)=O)C=NC2=N1	0
COC1=C2OC(=O)C=CC2=CC2=C1OC=C2	0
C1=CC2=C(C=C1)N=CC=C2	0
P#[In]	0
N#CC1=CC=C(C=C1)C(N1C=NC=N1)C1=CC=C(C=C1)C#N	0

SMILES	Label
COc1cc(ccc1C(=O)O)C2=NN([C@H](C2)C3CCCC3)c4ccc(C#N)c(Cl)c4	1
ClC1=CC=CC=C1C1=NN=C(N=N1)C1=C(Cl)C=CC=C1	0
CC1=C(Cl)C=CC(O)=C1	0
CCCC(CC)C1=CC=CC=C1	0
C1C=CC=C1	0
CN(C)NC(=O)CCC(O)=O	0
[Na+].[Na+].[O-][N+](=O)C1=CC=C(C=CC2=CC=C(C=C2S([O-])(=O)=O)[N+]([O-])=O)C(=C1)S([O-])(	0
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)C(=O)Nc5cccc	1
CNC(=O)OC1=CC(C)=C(C=C1)N(C)C	0
NNC(=O)OCC1=CC=CC=C1	0
CCOC(=O)CCC(C)=O	0
COC1=CC=C(\C=C\C)C=C1	0
CC(=O)OCCOC(C)=O	0
CC(C)C1=CC=C(C)C=C1O	0
[O-][N+](=O)c1ccc(cc1)N2C(=O)[C@H]3[C@@H]4C[C@@H](CN4C(=O)c5ccccc5)N3C2=O	1
CN1[C@@H]2CC[C@@H]3[C@H](CC[C@@]4(C)[C@H]3C/C(=C\c5cccc(F)c5)/[C@@H]4O)[C@@	1
OC(=O)\C=C\C(O)=O	0
CC(C)(C)OC(=O)N1CC2CC1[C@H]3N2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F	1
CCOC(=O)COC1=CC(N2N=CC(=C(C)C2=O)C(F)(F)F)=C(F)C=C1Cl	0
CCC(C)C1=NC=CN=C1OC	0
[Na+].CCCCCCCCCCCCCCCCCOS([O-])(=O)=O	0
SCCC1=CN=CC=N1	0
CCCCOC(=O)C(C)OC(=O)CCC	0
CC(C)(O)C(=O)Nc1ccc(c(c1)C(F)(F)F)[N+](=O)[O-]	1
O1C2=CC=CC=C2SC2=CC=CC=C12	0
Cc1nn(c(C)c1-c2ccc(F)cc2)-c3ccc(C#N)c(Cl)c3	1
C[Si](C)(CCCN)O[Si](C)(C)CCCN	0
[Cu]I	0
CC(=C)C(=O)OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
C[C@@H]1[C@H](C)C(C)(C)Nc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
O=C(OCCOCCOCCOC(=O)C1=CC=CC=C1)C1=CC=CC=C1	0
C1=CC=C(C=C1)B(C1=CC=CC=C1)C1=CC=CC=C1	0
CNC(=O)CSP(=S)(OC)OC	0
C\C=C(/C)C(=O)OC\C=C(/C)CCC=C(C)C	0
CCOC(=O)C(Cl)CC1=C(Cl)C=C(F)C(=C1)N1N=C(C)N(C(F)F)C1=O	0
FC(F)(F)c1cc(=O)[nH]c2cc3OC[C@H]4CCCN4c3cc12	1
Cc1nn(c(C)c1Cc2cccc(c2)C(=O)N)-c3ccc(C#N)c(Cl)c3	1
FC1=CC=CC(F)=C1C(=O)NC(=O)NC1=C(F)C(Cl)=C(F)C(Cl)=C1	0
CN(C)c1ccc(cc1)[C@H]2C[C@]3(C)[C@@H](CC[C@]3(O)CCCO)[C@@H]4CCC5=CC(=O)CCC5=C24	1
COC[C@@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
CN(C)CC1=CC(CN(C)C)=C(O)C(CN(C)C)=C1	0
CCCOCCO	0
CC1(C)NC(=O)N(C1=O)C1=CC(=C(C=C1)[N+]([O-])=O)C(F)(F)F	1
CCC1=C(N([C@@H](C)COC)C(=O)CCl)C(C)=CC=C1	0
COC(=O)C1(O)C2=C(C=CC=C2)C2=C1C=CC=C2	0

Cl.NCC1(CC2=NOC(=O)N2)CCCCC1	0
CN(c1cc(C)cc(C)c1)c2cc(C(=O)N3CCCC3)n(C)c2	1
C[C@@H]1Cc2cc3c(cc(=O)n(C)c3cc2N1)C(F)(F)F	1
CCC1=CC(=C(O)C(=C1)C(C)(C)C)C(C)(C)C	0
O.O.O.C[C@](N)(CC1=CC=C(O)C(O)=C1)C(O)=O.C[C@](N)(CC1=CC=C(O)C(O)=C1)C(O)=O	0
CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5cc(Cl)cc(Cl)c5)c3c12	1
Cn1cc(cc1C(=O)N2CCCC2)N(Cc3ccccc3)c4ccc(cc4)[N+](=O)[O-]	1
O=C1CCCCCN1	0
CC(C)N(C(C)C)C(=O)SCC(Cl)=C(Cl)Cl	0
CCCCCCCOC(=O)C1=CC=C(O)C=C1	0
CCOC(=O)COC(=O)C1=CC=CC=C1C(=O)OCC	0
[Na+].CCCCCCCCC1=CC=C(C=C1)S([O-])(=O)=O	0
CC(C)C1=CC=CC(O)=C1	0
FC(F)(F)C[C@@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5cccc(c5)C(F)(F)F)c3c12	1
CN1COCN(CC2=CN=C(Cl)S2)C1=N[N+]([O-])=O	0
CCNC1=NC(NC(C)(C)C)=NC(Cl)=N1	0
CC(C)C1CC=C(C)C=C1	0
Cl.CCCOC(=O)NCCCN(C)C	0
CC(C)(OOC(C)(C)C1=CC=CC=C1)C1=CC=CC=C1	0
CCc1cc(=O)[nH]c2ccc(cc12)N(CC(F)(F)F)CC(F)(F)F	1
C[C@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
CCCCCOC(=O)C1=CC=C(O)C=C1	0
Cc1c(C#N)c(c(C)n1Cc2cncc(CO)c2)-c3ccc(cc3)C#N	1
CCCCCCCCC[N+](C)(C)[O-]	0
CC1=CC=C(S1)C=O	0
CCOC(=O)CC1=CC=CC2=C1C=CC=C2	0
NC1=C(Cl)C(Cl)=NC(C(O)=O)=C1Cl	0
CC1(C)CN(Cc2ccccc2O)C(=O)C1Oc3ccc(C#N)c(c3)C(F)(F)F	1
CCCCCCO	0
[O-][N+](=O)C1=CC=C(Cl)C(Cl)=C1	0
FC(F)(F)CN1[C@H](COc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F)C(F)(F)F	1
O.[Na+].O=C1[N-]S(=O)(=O)C2=CC=CC=C12	0
CC(C)O[Ti](OCCN(CCO)CCO)(OCCN(CCO)CCO)OC(C)C	0
CCCCNC(=O)N1C(NC(=O)OC)=NC2=C1C=CC=C2	0
OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
OC(=O)C1=C(N=C2C=CC=CC2=C1)C(O)=O	0
OC(=O)CCCCC(O)=O	0
CCCN(C1CCN(CC1)C(=O)C1CCNCC1)[C@@H]1CCC2=C(C1)C=C(OC)C=C2	0
OC(=O)CCC(O)=O.CN(C)CCOC(C)(C1=CC=CC=C1)C1=CC=CC=N1	0
CC(C)N(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
CCCCCCC1(C)CCC(=O)O1	0
[O-][N+](=O)c1ccc(cc1C(F)(F)F)N2C(=O)[C@@H]3C4CC(C=C4)[C@@H]3C2=O	1
Cl.N[C@H]1C(O)O[C@H](CO)[C@H](O)[C@@H]1O	0
Cl.CN(C)[C@H]1[C@@H]2[C@@H](O)[C@H]3C(=C(O)[C@]2(O)C(=O)C(C(N)=O)=C1O)C(=O)C1=C	0

FC(F)(F)CN(Cc1cccs1)c2ccc3[nH]c(=O)cc(c3c2)C(F)(F)F	1
FC(F)(F)c1cccc(c1)N2C(=O)[C@@H]3C4CCC(C=C4)[C@@H]3C2=O	1
CC(C)(C)C1=CC(=C(O)C(=C1)C(C)(C)C)C(C)(C)C	0
C1CN2CCN1CC2	0
CC(C)(C)C1=CC=CC(=C1O)C(C)(C)C	0
C[C@]12CC[C@H]3[C@@H](CCC4=C3C=CC(O)=C4)[C@@H]1CCC2=O	1
FC(F)(F)CN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(Br)c2c1	1
C[Si](C)(C)O[Si](O)(O)O	0
ClC1=C(Cl)C2(Cl)C(CBr)CC1(Cl)C2(Cl)Cl	0
CC1=C(O)C=C(N)C=C1	0
OC(=O)C(Cl)(Cl)Cl	0
CSCC[C@@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)c5ncccn5	1
COc1cc(SC(C)C)ccc1C#N	1
OC(=O)C(C1=CC=C(Cl)C=C1)C1=CC=C(Cl)C=C1	0
CCOC(=O)NC1=CC(OC(=O)NC2=CC=CC=C2)=CC=C1	0
CN1C(C)=NC=C1[N+]([O-])=O	0
CNC(NCCSCC1=CC=C(CN(C)C)O1)=C[N+]([O-])=O	0
CCC(C)=NO	0
CCN(CC)C1CCCCC1	0
CC(C)CCC(=O)CCC(C)C	0
COS(C)(=O)=O	0
FC1=CC(Br)=C(C=C1)C(=O)NS(=O)(=O)\C=C\C1=CC=CS1	0
OC(=O)C1CCC(CC1)C(O)=O	0
O=C1NC2=NNC=C2C(=O)N1	0
Cc1ccccc1Sc2ccc(C#N)c(c2)C(F)(F)F	1
CC(=O)NS(=O)(=O)C1=CC=C(N)C=C1	0
OCCOCCO	0
CCN(CC)C1=CC(O)=C(C=C1)C(=O)C1=C(C=CC=C1)C(O)=O	0
OC(=O)C1=C(O)C(Cl)=CC(Cl)=C1	0
[Na+].[O-][N+](=O)C1=CC(=C(NC2=CC(=C(NC3=CC=CC=C3)C=C2)S([O-])(=O)=O)C=C1)[N+]([O-])=	0
FC[C@@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
CC(C)[C@@H]1[C@@H]2[C@H](O)CCN2C(=O)N1c3ccc(C#N)c(Cl)c3C	1
CCCCOCCOC(=O)COC1=C(Cl)C=C(Cl)C(Cl)=N1	0
CC(=C)C1CCC(C)=CC1	0
CC(C)CC(C)(O)C#C	0
Oc1cc(c2cc3CCC4(CCCC4)Nc3cc2n1)C(F)(F)F	1
CC(C)(C)C1=C(O)C=CC=C1	0
[Na+].[O-]S(=O)(=O)C(CC(=O)OC1CCCC1)C(=O)OC1CCCC1	0
CC1=CCCC(C)(C)C1\C=C\C(=O)CCC=C	0
OC1=CC=CC=C1CC=C	0
CC1=C(C=O)C(C)(C)CCC1	0
CN(C)C(Cl)=O	0
CC(C)(C)C1=CC=CC=C1	0
CN(CC1=CN=C(Cl)C=C1)C(\C)=N\C#N	0

CC1=CC(OCCCC(C)(C)C(O)=O)=C(C)C=C1	0
CCNc1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
[Na+].[Na+].[O-]S(=O)(=O)C1=CC(=C2N=C(C=CC2=C1)C1C(=O)C2=C(C=CC=C2)C1=O)S([O-])(=O)=	0
NC1=CC=C(OC2=CC=C(N)C=C2)C=C1	0
[Na+].[O-]S(=O)(=O)CC=C	0
CNCC1=CC=C(NC(=O)C2=CNC3=C2C(=O)CCC3)C=C1	0
OC1=C(C=CC=C1)C(=O)OCC1=CC=CC=C1	0
CCOP(=S)(OC(C)C)OC1=CN=C(N=C1)C(C)(C)C	0
CO[Si](C)(OC)C1=CC=CC=C1	0
C[C@@H]1CC(=O)C=C2CC[C@H](C[C@@]12C)C(C)=C	0
O.O.[Na+].[O-]C1=NC(=O)N(Cl)C(=O)N1Cl	0
CC(C)Sc1ccc(C#N)c(c1)C(F)(F)F	1
Oc1ccc(cc1)-c2ccc(C#N)c(c2)C(F)(F)F	1
C[C@@H]1CNc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
COC1=CC(Cl)=C(OC)C=C1Cl	0
CC1(C)N(CCCNS(=O)(=O)N)C(=S)N(C1=O)c2ccc(C#N)c(c2)C(F)(F)F	1
CN(C)C	0
C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@]34C)[C@@H]1CC[C@]2(O)C(=O)CO	1
CCCO	0
CC(C)COC(=O)C1=C(C=CC=C1)C(=O)OCC(C)C	0
ClC1=CC=C(C=C1)C(Cl)(Cl)Cl	0
COC1=CC2=C(C(OC)=C1OC)C1=CC=C(OC)C(=O)C=C1[C@H](CC2)NC(C)=O	0
[O-][N+](=O)c1ccc(cc1)N(Cc2ccccc2)c3cccc(c3)C(=O)N4CCCC4	1
[Cl-].C[N+](C)=CCl	0
CC(CCC#N)C#N	0
CCC(C)C1=C(O)C=CC=C1	0
CC(C)=CC1C(C(=O)OC(C#N)C2=CC=CC(OC3=CC=CC=C3)=C2)C1(C)C	0
ClC1=CC=CC(=N1)C(Cl)(Cl)Cl	0
CCC1CCC(=O)O1	0
CCCSC1=CC=C2NC(NC(=O)OC)=NC2=C1	0
OS(=O)(=O)C1=CC=C(Cl)C=C1	0
CCCOC(=O)N1C[C@@]2(C)O[C@@](C)(C1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F	1
CCN(CCC#N)C1=CC=CC=C1	0
C(=C(C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1	0
CC1=CC(C)=NC(NC2=CC=CC=C2)=N1	0
CCCCC(CC)COC(=O)CCCCCCCCC(=O)OCC(CC)CCCC	0
C=CCN=C=S	0
CC12C[C@@H](O)C(C)(O1)[C@@H]3[C@H]2C(=O)N(C3=O)c4ccc(C#N)c(I)c4	1
CCCCC\C=C/CCC=O	0
CCCCC(O)=O	0
CCCCC(CC)COC(=O)C1=CC=CC=C1C(O)=O	0
CCCCOCC1CO1	0
CC(C)CNc1cc2[nH]c(=O)cc(c2cc1C)C(F)(F)F	1
C1=CC2=C3C1=CC=CC3=CC=C2	0
OC(=O)CCCCCCCCCCC(O)=O	0

COC(=O)c1c(C)n(Cc2ccccc2)c(C)c1-c3ccc(cc3)[N+](=O)[O-]	1
[Na+].CC[C@H](C)C(=O)O[C@H]1C[C@H](O)C=C2C=C[C@H](C)[C@H](CC[C@@H](O)C[C@@H](	0
Cc1cc(=O)[nH]c2ccc(cc12)N(CC(F)(F)F)CC(F)(F)F	1
CNC(=O)O\N=C\C(C)(C)S(C)(=O)=O	0
[NH4+].[S-]C#N	0
[Na+].NC1=C(\N=N\C2=CC=CC=C2C(F)(F)F)C2=C(C=C1)C=C(C=C2O)S([O-])(=O)=O	0
COC1=C(O)C=CC(C=O)=C1	0
NCCNCCN	0
Cc1c(C#N)c(c(C)n1Cc2cccnc2)-c3ccc(cc3)C#N	1
CCCCCCCC\C=C/CCCCCCCC(=O)OC[C@@H](O)[C@H]1OC[C@H](O)[C@H]1O	0
CCOCC(O)=O	0
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)c5cccc(c5)S(=	1
CC(C)(C)C1=CC(CC2=CC(=C(O)C(=C2)C(C)(C)C)C(C)(C)C)=CC(=C1O)C(C)(C)C	0
CCC(C)(CCCC(C)C)OC(C)=O	0
OCCN(CCO)C1=CC(Cl)=CC=C1	0
CCCc1cc2c(cc(=O)[nH]c2cc1N)C(F)(F)F	1
[O-][N+](=O)\N=C1/NCCN1CC1=CN=C(Cl)C=C1	0
CC(C)=CCC\C(C)=C/CO	0
CCOP(=O)(OCC)OC1=NC(=NC(C)=C1)C(C)C	0
CCCCC(CC)COP(=O)(OC1=CC=CC=C1)OC1=CC=CC=C1	0
CC(C)(C)C(O)(CCC1=CC=C(Cl)C=C1)CN1C=NC=N1	1
CN(C)c1ccccc1/C=C/2\Oc3ccc(F)cc3-c4ccc5NC(C)(C)C=C(C)c5c24	1
FC(F)(F)c1cc(ncc1C#N)N2CCC3CCCCC3C2	1
COC(=O)C1=C(C)C=CC=C1	0
FC(F)(F)c1cc(ccc1C#N)C2=NOC3CCCCC23	1
Clc1ccc(cc1Cl)N2C(=O)[C@@H]3C4CC(C=C4)[C@@H]3C2=O	1
Cc1cc(C)cc(c1)N(Cc2ccc(CO)cc2)c3cc(C(=O)N4CCCC4)n(C)c3	1
COCC(C)O	0
NC1=C(Cl)C(=CC(Cl)=C1)C(O)=O	0
CC(C)N1C(=O)C2=C(NS1(=O)=O)C=CC=C2	0
CCCCOC(=O)C1=C(C=CC=C1)C(O)=O	0
CCC(C)N1C(=O)NC(C)=C(Br)C1=O	0
ON(CC1=CC=CC=C1)CC1=CC=CC=C1	0
CCN(CC)C(=O)CCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[	1
CC(C)COC(=O)C=CC1=CC=CC=C1	0
ClCCCCCCCl	0
CCSC(=O)N(CC)C1CCCCC1	0
CCC(C)C(=O)OCCC1=CC=CC=C1	0
ClC1=CC(Cl)=C(OC2=CC=C(OC3=NC=C(Cl)C=C3Cl)C=C2)N=C1	0
CCCCCCCCO[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O	0
Oc1cc(=O)[nH]c2ccc(cc12)N(CC(F)(F)F)CC(F)(F)F	1
CCOC(=O)c1oc(CN2CC(C)(C)C(Oc3ccc(C#N)c(c3)C(F)(F)F)C2=O)cc1	1
[Na+].CC1=CC=C(C)C(=C1)S([O-])(=O)=O	0
OC[C@H]1O[C@H](O[C@]2(CCl)O[C@H](CCl)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@H	0
OC1=C(I)C2=C(C=C1I)C1(OC(=O)C3=CC=CC=C13)C1=C(O2)C(I)=C(O)C(I)=C1	0

CCOC(=O)C1=CC=C(C)C=C1	0
CN1C(=O)N(C(=O)[C@@]1(CO)c2ccccc2)c3ccc(C#N)c(c3)C(F)(F)F	1
O=C(CC1=CC=CC=C1)C1=CC=CC=C1	0
FC(F)(F)c1cc(=O)[nH]c2cc3OCCN(CC4CC4)c3cc12	1
CCCCNP(N)(N)=S	0
C[C@H]1CC[C@@H]2[C@H](C1)c3cc4c(cc(=O)n(C)c4cc3N2C)C(F)(F)F	1
CCOC1=CC(=C(N)C=C1)[N+]([O-])=O	0
C1C=CC2=C1C=CC2	0
CCOC(=O)N(C)N=O	0
CCNS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
CCOC(=O)CN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
COC1=C(OC)C(=CC=C1)[C@H](O)C1CCN(CCC2=CC=C(F)C=C2)CC1	0
O=C(\C=C\C=C\C1=CC=C2OCOC2=C1)N1CCCCC1	0
COCC(=O)N(C(C)C(=O)OC)C1=C(C)C=CC=C1C	0
CC1=CC=C(O)C=C1	0
CN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
CC1=CC(C)=CC=C1	0
CC\C=C/CCOC(=O)C1=CC=CC=C1	0
FC(F)(F)c1cc(=O)[nH]c2cc(NC3CCC3)ccc12	1
CCCCCCOC(=O)CCC	0
CC(C)COC(=O)CCCCC(=O)OCC(C)C	0
C[C@]12CC[C@H]3[C@@H](C(CCCCCCCC(=O)N4CCCC4)C[C@H]5CC(=O)CC[C@]35C)[C@@H]1	1
O=C1NS(=O)(=O)C2=C1C=CC2	0
CCC\C=C\C=O	0
CCOC(=O)c1c(C)n(C)c(C)c1-c2ccc(cc2)[N+](=O)[O-]	1
Cc1c(C#N)c(c(C)n1Cc2ccc(Cl)nc2)-c3ccc(cc3)C#N	1
CC(=O)C1=CC2=CC=CC=C2C=C1	0
CC1=C(N)C=C(N)C=C1	0
CC12CCC(C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4c(N)ccc5nccn45	1
OC(=O)CC1=CC=CC=C1	0
[O-][N+](=O)C1=C2C=CC=CC2=CC2=CC=CC=C12	0
OCC#CCO	0
C[C@@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
OCCCC1CCCCC1	0
NC(N)=S	0
CCCCN(C)C(=O)CCCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]	1
CC\C=C/CCCCO	0
NC1=C(O)C=CC(=C1)[N+]([O-])=O	0
C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCCCC(=O)O)C[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC	1
C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	0
CC1(C)C2CCC(C)(C2)C1O	0
C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	0
NCCCOCCOCCOCCCN	0
[O-][N+](=O)c1ccc(cc1C(F)(F)F)N2C(=O)[C@@H]3C4CCC(C4)[C@@H]3C2=O	1
CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5ccc(Cl)cc5)c3c12	1

CC(C)N1C(=O)C2=C(C=CC=C2)C1=O	0
I.I.NCCN	0
FC1=CC=C(CC2CCN(CCS(=O)C3=CC=C4NC(=O)OC4=C3)CC2)C=C1	0
CCCCC1=CC=C(N)C=C1	0
CC(C)N(C(C)C)C1=CC=CC=C1	0
[Na+].[Na+].OC1=C(N=NC2=CC=C(C=C2)N=NC2=CC=C(C=C2)S([O-])(=O)=O)C(=CC2=CC(NC(=O)C3	0
[Na+].COC1=NN(C(=O)[N-]S(=O)(=O)C2=C(OC(F)(F)F)C=CC=C2)C(=O)N1C	0
CCCCCCCCCCCCCC(O)=O	0
O=C1OC2=C(C=CC=C2)C=C1	0
OC1CCCCC1	0
CCCCCCCCCCCCCCO	0
FC(F)(F)c1cccc(c1)N2C(=O)[C@@H]3C4CCCC(CC4)[C@@H]3C2=O	1
CC(C)(CS(O)(=O)=O)NC(=O)C=C	0
CC[C@@H]1C[C@H](CC)c2cc3c(cc(O)nc3cc2N1)C(F)(F)F	1
CCCCC(CC)CN1C(=O)C2C3CC(C=C3)C2C1=O	1
CC(C)(C)C1=CC=C(N)C=C1	0
COP(=O)(NC(C)=O)SC	0
CC(C)COC(=O)C1=CC=CC=C1	0
OC(=O)COC1=CC=C(Cl)C=C1	0
COC(=O)C1=C(C=CC=C1)C(O)=O	0
OC1=C(O)C=CC=C1	0
OCC1=CC=CC(OC2=CC=CC=C2)=C1	0
C[Si](CN1C=NC=N1)(C1=CC=C(F)C=C1)C1=CC=C(F)C=C1	1
CCCCC1=CC=C(O)C=C1	0
CC1=CC(=O)NC(=S)N1	0
CC(C)(C)CN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
CCCC(=O)C(C)=O	0
[O-][N+](=O)c1ccc(cc1)N2C(=O)[C@@H]3C4CC(C=C4)[C@@H]3C2=O	1
[Na+].COC1=CC(OC)=NC(OC2=CC=CC(OC3=NC(OC)=CC(OC)=N3)=C2C([O-])=O)=N1	0
N#CCCCCC#N	0
C[C@H]1Nc2cc3n(C)c(=O)cc(c3cc2C1(C)C)C(F)(F)F	1
C[C@@H]1CC[C@H](CO)N1c2ccc3[nH]c(=O)cc(c3c2)C(F)(F)F	1
CC1CC(C)(C)C2=C(C=C(C)C(=C2)C(C)=O)C1(C)C	0
[Na+].CC1=CC=C(C(C)=C1)S([O-])(=O)=O	0
CCC(=O)OC(C)C1=CC=CC=C1	0
CC(O)CN	0
CN1CCOc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F	1
CSc1cc(ccc1C#N)N2C(=O)[C@H]3[C@@H](C2=O)C4(C)CCC3(C)O4	1
CCCCCCOCCO	0
OC(=O)C1=NC(Cl)=CC=C1	0
C[As](C)(O)=O	0
CCCCCCCCCC	0
Cc1cc(ccc1Br)N2C(=O)[C@@H]3C4C=CC([C@H](O)[C@@H]4O)[C@@H]3C2=O	1
CNC(=O)c1ccc(Cc2c(C)nn(c2C)-c3ccc(C#N)c(Cl)c3)cc1	1
C[C@@H]1CC[C@H]2C(C)(C)[C@H]3C[C@@]12CC(C(C)=O)=C3C	0

NC(=O)C1=CC=C(N)C=C1	0
FC(F)(F)c1cccc(c1)N2C(=O)[C@@H]3C4C=CC([C@H]5C[C@@H]45)[C@@H]3C2=O	1
CCC(C)(C)C(=O)OC1=C(C(=O)OC11CCCCC1)C1=CC(Cl)=CC(Cl)=C1	0
OCCN(CCO)CCO	0
COc1cc(/C=N/NC(=O)c2oc3ccc4ccccc4c3c2)cc(OC)c1O	1
OC1=C(CC2=CC=CC=C2)C=C(Cl)C=C1	1
CCCCCCCCOC(=O)C1=C(C=CC=C1)C(=O)OCCCCCCCC	0
CCCN(CCC)c1cc(c(cn1)C#N)C(F)(F)F	1
Oc1ccc(cc1)-c2coc3cc(O)cc(O)c3c2=O	1
OC[C@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
Cl.Cl.C1CNCCN1	0
C[C@@H](O)C1=NC(=CC=N1)N1[C@@H](C)CN(C[C@H]1C)C1=NC(C)=NC(C)=N1	0
OC1=C(C=CC2=C1C=CC=C2)C(=O)OC1=CC=CC=C1	0
[Na+].[O-]C(=O)CCl	0
COc1c(Cl)c(ccc1C#N)N2C(=O)[C@@H]3[C@H](O)CCN3C2=O	1
C[C@]12CC[C@H]3[C@@H](CCC4=C3C=CC(O)=C4)[C@@H]1CC[C@H]2O	1
CCOC(OCC)\C=C\CC\C=C/CC	0
CCCCCCCCCCC=CC#N	0
CC1CC(C)(C)Nc2c(C)c3n(C)c(=O)cc(c3cc12)C(F)(F)F	1
ClC1=CC=C(C=C1)N=C=O	0
Cc1cc(C)cc(c1)C(=O)N2Cc3ccccc3C[C@H]2CO	1
CCCC1=CC(OC)=C(O)C=C1	0
CC(C)(O)C#N	0
[Na+].[Na+].OC1=CC2=C(C=C(C=C2)S([O-])(=O)=O)C=C1S([O-])(=O)=O	0
Cl.CC1=NC=C(CO)C(CO)=C1O	0
NC1=C(Cl)C(F)=NC(OCC(O)=O)=C1Cl	0
CCCCC(CC)COC(=O)C1=CC=C(C(=O)OCC(CC)CCCC)C(=C1)C(=O)OCC(CC)CCCC	0
BrC1=CC(Br)=C(Br)C=C1	0
C(NC1=NC=NC2=C1N=CN2C1CCCCO1)C1=CC=CC=C1	0
CC(C)(C)CNc1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
Cc1ccc(cc1)C(=O)CC(Nc2ccc(cc2)[N+](=O)[O-])c3cccc(F)c3	1
[Li+].[O-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
CC(=O)OC(C)(C)C1CCC(C)=CC1	0
C[C@](O)(CS(=O)(=O)c1cccc2ccccc12)C(=O)Nc3ccc(C#N)c(c3)C(F)(F)F	1
OC(=O)\C=C\C(O)=O.CC1=C(C=CO1)C(=O)NC1=CC=C(C=C1)C(=O)N1CCC(F)(F)\C(=C/C(=O)N2CCC	0
CCCC\C=C/CCCCCCCCC=O	0
CC1CC(=O)CC(C)(C)C1	0
CCNC1=CC=CC=C1	0
Clc1ccc(cc1Cl)N2C(=O)[C@@H]3C4CCC(C=C4)[C@@H]3C2=O	1
[Na+].CC1=NN(C(=O)C1N=NC1=CC=CC=C1)C1=CC=C(C=C1)S([O-])(=O)=O	0
CC\C=C/CC\C=C\CO	0
OC[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO	0
NC1=CC(=C(NCCO)C=C1)[N+]([O-])=O	0
COc1ccc(cc1)C2=NOC3CCCC23	1
CC(C)(C)C1=CC=C(OC(=O)C2=C(O)C=CC=C2)C=C1	0

CC1(C)N(CCCS(=O)(=O)N)C(=S)N(C1=O)c2ccc(C#N)c(c2)C(F)(F)F	1
CCCCCCC(=O)C1=CC=CC=C1	0
CCOC1=CC=CC=C1OCC	0
CC1=C(C=O)C=CC=C1	0
CN1[C@@H]2CC[C@@H]3[C@H](CC[C@@]4(C)[C@H]3C/C(=C\c5ccncc5)/[C@@H]4O)[C@@]2(	1
CCCSc1ccc(C#N)c(c1)C(F)(F)F	1
CC1=CC=C(O1)C(O)=O	0
COC(=O)NC(=S)NC1=C(NC(=S)NC(=O)OC)C=CC=C1	0
NC(=O)CF	0
OC1=CC(C[C@H]2COC(=O)[C@@H]2CC2=CC(O)=CC=C2)=CC=C1	0
CN(C)C(C)(C)CO	0
CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5ccc(C)cc5)c3c12	1
CC(C)(C1=CC=CC=C1)C1=CC=C(NC2=CC=C(C=C2)C(C)(C)C2=CC=CC=C2)C=C1	0
CN1CCCC1	0
CC(N)=O	0
CC1(C)Nc2cc3nc(O)cc(c3cc2C=C1)C(F)(F)F	1
CC(C)CCOC(=O)C1=CC=CC=C1	0
N#Cc1ccc(cc1)C2=NOC3CCCCC23	1
CCCCCCC1CCCC(=O)O1	0
CC1(C)COP(OC2=CC=CC=C2)OC1	0
CN(C)C(=O)c1ccc(Cc2c(C)nn(c2C)-c3ccc(C#N)c(Cl)c3)cc1	1
FC(F)(F)CN1[C@@H](COc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F)c4ccccc4	1
[O-][N+](=O)c1ccc(N2C(=O)[C@H]3[C@@H]4C[C@@H](CN4C(=O)Oc5ccc(F)cc5)N3C2=O)c6cccc	1
Oc1cc(c2cc3[C@H]4CCCC[C@H]4CNc3cc2n1)C(F)(F)F	1
CCCSP(=O)(OCC)SCCC	0
CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5ccccc5)c3c12	1
CN([C@H]1CC[C@@]2(CCCO2)C[C@@H]1N1CCCC1)C(=O)CC1=CC=CC2=C1C=CO2	0
CC1(C)CN(Cc2ccccc2)C(=O)[C@@H]1Oc3ccc(C#N)c(c3)C(F)(F)F	1
CCOP(=S)(OCC)OC(Cl)C(Cl)(Cl)Cl	0
COC[C@@H]1C[C@H]2[C@@H]3CC[C@H]4N(C)C(=O)C=C[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1O	1
CCCCC(CC)COC(=O)\C=C/C(=O)OCC(CC)CCCC	0
CCC1CN(C)c2cc3c(cc(=O)[nH]c3cc2O1)C(F)(F)F	1
CCCCCCCC#N	0
CC(C)(C)C1CCC(O)CC1	0
CC1=C(C=C(C#N)C(=O)N1)C1=CC=NC=C1	0
CC1=C(C=CC=C1COC(=O)[C@H]1[C@@H](\C=C(/Cl)C(F)(F)F)C1(C)C)C1=CC=CC=C1	0
OC(=O)C1=CC2=C(C=CC=C2)C=C1O	0
CCCCC(CC)C(O)C#C	0
[O-][N+](=O)c1ccc(C2=NOC3CCCCCC23)c(c1)C(F)(F)F	1
CCCCSc1ccc(C#N)c(c1)C(F)(F)F	1
CC1=C(C)C(=C(C(=C1C)[N+]([O-])=O)C(C)(C)C)[N+]([O-])=O	0
CC1(C)CC(CC(C)(CN=C=O)C1)N=C=O	0
CC1CCC2(O1)C(C)=CCCC2(C)C	0
NC1=CC=C(C=C1)S(=O)(=O)C1=CC=C(N)C=C1	0
CCC1=CC(C(O)=O)=C(N=C1)C(O)=O	0

CCCCOC(=O)CCC(=O)OCCCC	0
CC1=CC2=C(C=C1C(=C)C1=CC=C(C=C1)C(O)=O)C(C)(C)CCC2(C)C	0
N#CC1=CSC=N1	0
CC(C)CC(C)(O)C#CC(C)(O)CC(C)C	0
COC(=O)c1c(C)n(Cc2ccccc2)c(C)c1-c3ccccc3	1
CCCN(CCC)C1=C(C=C(C=C1[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O	0
CCCN(CCC)C(=O)SCC	0
Cn1c(=O)cc(c2cc3c(N[C@@H]4CCCC[C@]34C)cc12)C(F)(F)F	1
OC[C@H](O)[C@H](O)[C@@H](O)[C@H](O)CO	0
COC(=O)C1CCC(CC1)C(=O)OC	0
C[C@@H](OC1=CC=C(OC2=NC=C(Cl)C=C2F)C=C1)C(=O)OCC#C	0
Cc1ccccc1-c2ccc(C#N)c(c2)C(F)(F)F	1
COc1ccccc1C2=NOC3CCCCC23	1
CCC(=O)OCC1=CC=C(OC)C=C1	0
NC(=O)C1=CC=CN=C1	0
CCCO[Si](OCCC)(OCCC)OCCC	0
O=C1[C@@H]2C3CC(C=C3)[C@@H]2C(=O)N1c4ccc5ccccc5c4	1
FC(F)(F)CN1CCOc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F	1
[NH4+].[O-]N(N=O)C1=CC=CC=C1	0
[K+].CCCCC(CC)C([O-])=O	0
CCSC(=O)N1CCCCC1	0
CC(=O)O[Hg]C1=CC=CC=C1	1
NCC1=CC(CN)=CC=C1	0
OP(=O)(OC1=CC=CC=C1)OC1=CC=CC=C1	0
CCC(=O)C=CC1=CC=C(OC)C=C1	0
CC(C)=C1CCC(C)=CC1	0
CC1=CN([C@H]2C[C@H](N=[N+]=[N-])[C@@H](CO)O2)C(=O)NC1=O	0
O=C(OCCCCCCOC(=O)C1=CC=CC=C1)C1=CC=CC=C1	0
COC1=C(N)C=C(NC(C)=O)C=C1	0
Cl.N[C@@H](CCC(O)=O)C(O)=O	0
CCCCOCCOCCOCCO	0
CC1=CC(=C(O)C=C1)C(C)(C)C	0
NC1=CC(Cl)=C(N)C(Cl)=C1	0
CCN1C=C(C(O)=O)C(=O)C2=C1N=C(C)C=C2	0
CCC(Br)(CC)C(=O)NC(N)=O	0
OC1=C(Cl)C=C(Cl)C=C1	0
FC(F)(F)c1cc(=O)[nH]c2cc3OCC4CCCCN4c3cc12	1
OP(O)(=O)C1=CC=CC=C1	0
OCCOCCOCCO	0
FC(F)(F)c1cc(ccc1Cl)N2C(=O)[C@@H]3C4CCC(O4)[C@@H]3C2=O	1
CC(=O)O[Cr](O)OC(C)=O.CC(=O)O[Cr](O)OC(C)=O.CC(=O)O[Cr](OC(C)=O)OC(C)=O	0
Cn1cc(cc1C(=O)N2CCCC2)N(Cc3ccccc3)c4ccc(cc4)C(F)(F)F	1
CC1CCN(CC1)c2cc(c(cn2)C#N)C(F)(F)F	1
COC1=CC=C(C=C1)C(Cl)=C(C1=CC=C(OC)C=C1)C1=CC=C(OC)C=C1	0
CC1=CC=C(C=C1C)[N+]([O-])=O	0

CCCCOC(=O)C(C)CC	0
NC1=CN=CC=C1	0
CN(C)C1=CC=C(C)C=C1	0
Oc1cc(c2cc3CCCNc3cc2n1)C(F)(F)F	1
C[C@@H]1CC[C@H]2C(C)(C)C3C[C@@]12CC=C3C	0
CN(N=O)C(N)=O	0
CNC(=O)[C@H]1O[C@H]([C@H](O)[C@@H]1N)N1C=NC2=C1N=CN=C2NCC1=CC(Cl)=CC=C1OCC1	0
CCCCOCCOCCOCC1=CC2=C(OCO2)C=C1CCC	0
CC1CC(C)(C)Nc2c(C)c3nc(O)cc(c3cc12)C(F)(F)F	1
CC(C)[C@@H](NC1=C(Cl)C=C(C=C1)C(F)(F)F)C(=O)OC(C#N)C1=CC(OC2=CC=CC=C2)=CC=C1	0
CCCCCCCOC(=O)CCC	0
CCCNC(=O)CCCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C	1
CC\C=C/CCOC(=O)C(C)C	0
CCCCCCC1CCC(=O)O1	0
CCCCCC(C)O	0
[O-][N+](=O)c1ccc(C2=NO[C@H]3CCCC[C@@H]23)c(c1)C(F)(F)F	1
C[C@](O)(CS(=O)(=O)c1ccc(C#N)c2ccccc12)C(=O)Nc3ccc(C#N)c(c3)C(F)(F)F	1
CC1C(C)(C)C2=C(C(=O)CCC2)C1(C)C	0
NC(=O)NC1=CC=C(Cl)C=C1	0
Cc1nn(c(C)c1Cc2ccc(cc2)C(=O)N)-c3ccc(C#N)c(Cl)c3	1
CC(C)(C)C1=CC=C(CCC=O)C=C1	0
COC1=C(Cl)C(Cl)=C(Cl)C(Cl)=C1Cl	0
CCC1(CC)CCNc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
C1CC=CCCC=CCCC=C1	0
CCOC(=O)C1=CC=C(O)C=C1	0
OCC(CO)(CO)[N+]([O-])=O	0
NC1=CC=C(C=C1)S(N)(=O)=O	0
CC[C@H]1Nc2cc3nc(O)cc(c3cc2C[C@H]1C)C(F)(F)F	1
CC1CN(CC(F)(F)F)c2cc3c(cc(=O)[nH]c3cc2O1)C(F)(F)F	1
CC(=O)OC1CCCC1C(C)(C)C	0
BrC1=CC=C(OC2=CC=C(Br)C=C2)C=C1	0
O.O.O.O.[Na+].[O-]C1=C(C=CC=C1)C1=CC=CC=C1	0
CCS(=O)(=O)N1C[C@@]2(C)O[C@@](C)(C1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(	1
Cc1nn(c(C)c1Cc2ccc(F)cc2)-c3ccc(C#N)c(c3)C(F)(F)F	1
OC(=O)CCC(O)=O	0
CCCCCCCCCCCCN(C)C	0
BrCC1=CC=C(Br)C=C1	0
CCCCCC(C)=O	0
C1CNCCN1	0
CC(C\N=C\C1=CC=CC=C1O)\N=C\C1=CC=CC=C1O	0
CC(C)(C)N	0
Cn1c(=O)cc(c2cc3C(=CC(C)(C)Nc3cc12)C)C(F)(F)F	1
OC1=C(CC2=C(O)C=CC=C2)C=CC=C1	0
COC1=NC(C)=NC(NC(=O)NS(=O)(=O)C2=C(OCCCl)C=CC=C2)=N1	0
FC(F)c1cc(=O)[nH]c2ccc(cc12)N(CC(F)(F)F)CC(F)(F)F	1

O(P(OC1=CC=CC=C1)OC1=CC=CC=C1)C1=CC=CC=C1	0
C[C@H]1Cc2cc3c(cc(O)nc3cc2N[C@@H]1C)C(F)(F)F	1
CN(N=O)C(=O)N[C@H]1[C@@H](O)O[C@H](CO)[C@@H](O)[C@@H]1O	0
C[C@](O)(COc1ccc(cc1)C#N)C(=O)Nc2ccc(C#N)c(c2)C(F)(F)F	1
ClC1=NC(Cl)=NC(Cl)=N1	0
CC(N(O)C(N)=O)C1=CC2=C(S1)C=CC=C2	0
CCCOC(=O)C1=CC(O)=C(O)C(O)=C1	0
CCCC1=C(OCCCOC2=CC=C(OCC(O)=O)C=C2)C=CC(C(C)=O)=C1O	0
CCCC(C)C1=C(O)C=CC=C1	0
OC(=O)C1=CC=CN=C1	0
CCC(=O)OCCOC1=CC=CC=C1	0
CC(=O)C1=NC=CS1	0
O=C(OCC1=CC=CC=C1)C(=O)OCC1=CC=CC=C1	0
CN(\C=N\C1=C(C)C=C(C)C=C1)\C=N\C1=C(C)C=C(C)C=C1	0
NC1=CC(Cl)=CC(Cl)=C1	0
CCOC(=O)CC(=O)C1=CC=CC=C1	0
OC1=C(C=CC=C1)[N+]([O-])=O	0
CC(C)C1=C(O)C=CC=C1	0
CC1=C(SCCO1)C(=O)NC1=CC=CC=C1	0
NC1=CC=C(C=C1)C1=CC=C(F)C=C1	0
CN1[C@H]2[C@H](CCCC2(C)C)c3cc4c(cc(=O)n(C)c4cc13)C(F)(F)F	1
CC1=CC=CC(C)=C1NC(=O)CN1CCCC1=O	0
COC(=O)[C@@H]1CC2=CC(=O)CC[C@]2(C)[C@@]34O[C@@H]3C[C@@]5(C)[C@@H](CC[C@@]	1
CC1=CC(C)(C)Nc2ccc3-c4cccc(F)c4O/C(=C\c5ccccc5)/c3c12	1
CCCCCCCCCCC(=O)N(C)CC(O)=O	0
CC(=O)O[C@@H]1C[C@H]2CC[C@]1(C)C2(C)C	0
Cn1cc(cc1C(=O)N2CCCC2)N(Cc3ccccc3)c4ccccc4[N+](=O)[O-]	1
CC(C)(C)C1CCC(=O)CC1	0
CC1=CC(C)(C)Nc2cc3nc(O)cc(C)c3cc12	1
CN(C)C1=CC=CC=C1	0
Cc1c(ccc(C#N)c1C(F)(F)F)N2C(=S)N(CCCS(=O)(=O)N)C(C)(C)C2=O	1
CCOC(=O)C1=C(OC)C=CC=C1	0
C[C@@H]1CCc2cc3c(cc(O)nc3cc2N1)C(F)(F)F	1
CCCCCCCCCCCCN1CCCC1=O	0
ClCC=O	0
CC(C)C1(C)N=C(NC1=O)C1=NC=CC=C1C(O)=O	0
COCC1=NN=C(N1C1=C(Cl)C(Cl)=CC2=C1NC(=O)C(=O)N2)C1=C[N+]([O-])=CC=C1	0
[Na+].[Fe+3].[O-]C(=O)CN(CCN(CC([O-])=O)CC([O-])=O)CC([O-])=O	0
CC(=O)OCC1=CC=CC=C1	0
CS(=O)(=O)C1=CC=C(Cl)C=C1	0
C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCCCCCCC[S+]([O-])CCCC(F)(F)C(F)(F)F)CC4CC(=O)CC	1
N1C=NC=N1	0
CCCC(=O)C1=CC(O)=C(O)C=C1O	0
COc1ccccc1Sc2ccc(C#N)c(OC)c2	1
NS(=O)(=O)C1=CC2=C(NCNS2(=O)=O)C=C1Cl	0

O=NN1CCOCC1	0
OP(O)(=O)CCCl	0
CCC1COC(=O)O1	0
Fc1ccc(cc1Cl)N2C(=O)[C@@H]3C4CC(C=C4)[C@@H]3C2=O	1
CC12CCC(O1)[C@@H]3[C@H]2C(=O)N(C3=O)c4cccc(c4)C(F)(F)F	1
C1=CC=C(C=C1)N=NC1=CC=CC=C1	0
C[C@H](CCl)N(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
Cl.CN(C)[C@H]1[C@@H]2C[C@@H]3CC4=C(C(O)=CC=C4N(C)C)C(=O)C3=C(O)[C@]2(O)C(=O)C(C	0
CCCCCCCCC(=O)OCC	0
CC(C)C1=CC(=CC=C1)C(C)C	0
CC(C)(C)C1=CC=C(O)C=C1	0
CC1(C)N(Br)C(=O)N(Cl)C1=O	0
Cl.NC(=N)NC(=O)C1=NC(Cl)=C(N)N=C1N	0
CN(C)C1=C(C)N(C)N(C1=O)C1=CC=CC=C1	0
C[C@]12CC[C@H]3[C@@H](CCC4=CC(O)=CC=C34)[C@@H]1CC[C@@]2(O)C#C	1
CC12CCC(C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F	1
CC1=CC=C(C=C)C=C1	0
CCCCCCCC(=O)N(C)C	0
C[C@H]1CNc2cc3nc(O)cc(c3cc2C1C)C(F)(F)F	1
Fc1ccc(cc1C(F)(F)F)C2=NOC3CCCCCC23	1
CN(C)C(=O)NC1=CC=C(Cl)C=C1	0
FC(F)(F)c1cc(=O)[nH]c2ccc(NCC(F)C(F)(F)F)cc12	1
N[C@@H](CC1=CC(I)=C(OC2=CC(I)=C(O)C(I)=C2)C(I)=C1)C(O)=O	0
FC(F)(F)c1cccc(c1)N2C(=O)[C@@H]3C4CCC(C4)[C@@H]3C2=O	1
CCCCNC(=O)NS(=O)(=O)C1=CC=C(N)C=C1	0
C1CCC2C(C1)ON=C2c3ccccc3	1
Cn1cc(cc1C(=O)N2C[C@H](O)[C@@H](O)C2)N(Cc3ccccc3)c4ccc(cc4)[N+](=O)[O-]	1
CCOC(C)OCC\C=C/CC	0
COc1ccccc1C(=O)/C=C/c2ccccc2[N+](=O)[O-]	1
COC1=CC=C(C=O)C=C1	0
CC(C)N(c1cc(C)cc(C)c1)c2cc(C(=O)N3CCCC3)n(C)c2	1
CC(OC1=C(Cl)C=CC(Cl)=C1)C(O)=O	0
C1CCC2=C(C1)C=CC=C2	0
Fc1ccccc1C2=NOC3CCCC23	1
NC1=C(Cl)C(Cl)=C(Cl)C(Cl)=C1Cl	0
C[C@@H](N(C)c1cc(c(cn1)C#N)C(F)(F)F)c2ccccc2	1
CCCCN(CCC(=O)OCC)C(C)=O	0
C1CCC2(CCCCO2)OC1	0
CCCCCCCCCCCN	0
OC(=O)CCCCCCCC(O)=O	0
CN1C(=O)N(C(=O)C1(C)c2ccc3[nH]ccc3c2)c4ccc(C#N)c(c4)C(F)(F)F	1
CC(C)(O)C(=O)C1=CC=CC=C1	0
CCCCN(C)C(=O)CCCCCCCC[C@@H]1CC2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[	1
NC1=CC2=C3N(CCC3=C1)C(=O)[C@H](NC(=O)C1=CC=CN=C1)N=C2C1=CC=CC=C1	0
CC(C)=CCC\C(C)=C/COC(C)=O	0

NC1=CC(Cl)=C(Cl)C=C1	0
COC1=CC(CCC(C)=O)=CC=C1O	0
CCCCCCCOC(C)=O	0
CCOC1=NC(F)=CC2=NC(=NN12)S(=O)(=O)NC1=C(Cl)C=CC=C1Cl	0
CCON=C(CC)C1=C(O)CC(CC1=O)C1=C(C)C=C(C)C=C1C	0
COC(=O)C1=CC=C(O)C=C1	0
Cn1cc(cc1C(=O)N2CCc3ccccc23)N(Cc4ccccc4)c5ccc(cc5)[N+](=O)[O-]	1
CCCCCOC(=O)C(C)OC1=CC=C(OC2=CC=C(C=N2)C(F)(F)F)C=C1	0
CNC(=O)CCCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@H	1
[Na+].ClN1C(=O)[N-]C(=O)N(Cl)C1=O	0
[Na+].CC(C)C1=CC=CC(C(C)C)=C1NC(=O)[N-]S(=O)(=O)C1=CC(=CO1)C(C)(C)O	0
[Na+].[O-]N=O	0
CCCCP(CCCC)CCCC	0
CC1CCC(C(=O)C1)C(C)(C)S	0
Cc1c(Cl)c(ccc1N2C[C@@H]3[C@H](O)CCN3C2=O)C#N	1
CCCCSP(=O)(SCCCC)SCCCC	0
Cc1cccc(C)c1Oc2ccc(C#N)c(c2)C(F)(F)F	1
N1C2=CC=CC=C2SC2=C1C=CC=C2	0
CC1=CC=C(C=C1)S(O)(=O)=O.CCN(C(C)C)C(=O)C1=CC(OC[C@H](C)NC2=CC=NC=C2)=CC(C)=C1	0
CCCCOCCOC(C)=O	0
CC1CC=C(C)C(C=CC(C)=O)C1(C)C	0
CCOP(=O)(SC(C)CC)N1CCSC1=O	0
CCC1CCN(C)c2cc3oc(=O)cc(c3cc12)C(F)(F)F	1
COC(=O)C1=CC=CC=C1S(=O)(=O)NC(=O)N(C)C1=NC(OC)=NC(C)=N1	0
CCC(C)C(O)=O	0
CCC(=C(C1=CC=C(O)C=C1)C1=CC=C(OCCN(C)C)C=C1)C1=CC=CC=C1	1
CCCC(=O)OCCC(C)CCC=C(C)C	0
NN.OS(O)(=O)=O	0
C1=CC2=C3C(C=CC4=CC=CC(C=C2)=C34)=C1	0
Oc1cc(c2cc3[C@H]4CCCC[C@@H]4CNc3cc2n1)C(F)(F)F	1
CC(C)NC(=O)N1CC(=O)N(C1=O)C1=CC(Cl)=CC(Cl)=C1	0
CNc1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	0
CCCCCOC(=O)CCC	0
CCCCCCCCCCCC(=O)OC	0
FC(F)(F)c1cc(=O)[nH]c2cc(NC3CCCC3)ccc12	1
OC(=O)CCCC(O)=O	0
FC(F)(F)c1cc(=O)[nH]c2ccc(NC3CCCC3)cc12	1
CCOC(=O)C1OC1C1=CC=CC=C1	0
NCCO.OC(=O)C1=C(Cl)C=CC(Cl)=N1	0
Cl.CC(C)NCC(O)C1=CC(O)=C(O)C=C1	0
CC(=C)C(=O)OCCNC(C)(C)C	0
OCC1CCC2C3CC(CC3CO)C12	0
FC1(F)C(F)(F)C(F)(F)C2(F)C(F)(C1(F)F)C(F)(F)C(F)(F)C1(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C21F	0
CCC(C)OC(=O)N1CCCCC1CCO	0

CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5cccc(Br)c5)c3c12	1
CNS(=O)(=O)CCCN1C(=S)N(C(=O)C1(C)C)c2ccc(C#N)c(c2)C(F)(F)F	1
COC(=O)C1=CC=C(OC)C=C1	0
CC12CCC(CC1)C(C)(C)O2	0
CCO[Si](CCCN)(OCC)OCC	0
OC(C1=CC=C(F)C=C1)(C1=CN=CN=C1)C1=CC=CC=C1Cl	0
CC1=CC=C(C=C1)C(C)(C)C	0
OC1=C(C=C(Cl)C=C1)C1CCCC1	0
CCNC1=NC(NC(C)(C)C#N)=NC(Cl)=N1	0
CC(C)=CCCC(C)(OC(C)=O)C=C	0
[K+].[O-][Cl](=O)=O	0
CC=C1CC2CC1C=C2	0
Cn1cc(cc1C(=O)N2CCCC2)N(Cc3ccc(CO)cc3)c4ccc(cc4)[N+](=O)[O-]	1
Cc1cc(=O)[nH]c2ccc3c(c(=O)oc4cccc(C(=O)OC(C)(C)C)c34)c12	1
CC(C)CCC(C)=O	0
N#CC1=CN=CC=C1	0
CC(=O)CC(C1=CC=CC=C1)C1=C(O)C2=CC=CC=C2OC1=O	0
OCC1CO1	0
CCOP(=S)(OCC)SCCl	0
CC1=CC(O)=C(C=C1)C(C)(C)C	0
CC(=O)OC(C1=CC=CC=C1)C(Cl)(Cl)Cl	0
COP(C)(=O)OC	0
FC(F)(F)c1cc(=O)[nH]c2cc(NCC(F)(F)C(F)(F)F)ccc12	1
C[C@]12CCCC[C@H]1Nc3cc4nc(O)cc(c4cc23)C(F)(F)F	1
ClC(Cl)C1=CC=CC=C1	0
Cl.Cl.NC1=CC=C(O)C(N)=C1	0
CC(C)N1C(=O)[C@@]2(C)O[C@](C)([C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)C1=	1
CCCC(=O)OC(C)(C)CC1=CC=CC=C1	0
CC\C=C/CCOC(=O)C(\C)=C\C	0
CC1=C(C(=O)N2CC[C@H](O)[C@@H]12)c3ccc(C#N)c(Cl)c3C	1
CCC(=O)OC(C)(C)C1CCC(C)=CC1	0
CN(N=O)C1=CC=C(C=C1)[N+]([O-])=O	0
CC1=CC(N)=CC=C1	0
CC1CC(OC(C)=O)OC(C)O1	0
ClC1=CC=C(Cl)=C1C#N	0
[Na+].CCCCC1=NC2=C(N=CC=C2)N1CC1=CC=C(C=C1)C1=CC=CC=C1C1=NN=N[N-]1	0
CC1(C)CN(Cc2ccncc2)C(=O)C1Oc3ccc(C#N)c(c3)C(F)(F)F	1
C1CCC(CC1)C1CCCCC1	0
CC1(C)N(CCCS(=O)(=O)O)C(=S)N(C1=O)c2ccc(C#N)c(c2)C(F)(F)F	1
CCCCCCCCCCCC(=O)OCC	0
OC(=O)CCC([O-])=O.CO[C@@H]1COCC[C@@H]1[NH2+][C@@H]1CC[C@](C1)(C(C)C)C(=O)N1CC	0
CCOP(=O)(OCC)OCC	0
[Na]I	0
CC(C)(C#N)C1=CC(=CC(CN2C=NC=N2)=C1)C(C)(C)C#N	0
CCC(CO)(COCC=C)COCC=C	0

CC1=C(C)C(C)(C)Nc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CC(CC1=CC=C(C=C1)C(C)C)C=O	0
COC1=CC=C(C)C=C1N	0
FC(OC(F)(F)F)C(F)(F)OC1=C(Cl)C=C(NC(=O)NC(=O)C2=C(F)C=CC=C2F)C=C1	0
CCCN(CCC)C1=C(C=C(C=C1[N+]([O-])=O)C(C)C)[N+]([O-])=O	0
CC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C	1
COc1cc(=O)[nH]c2ccc(cc12)N(CC(F)(F)F)CC(F)(F)F	1
C1=CC=C(C=C1)C1=CC=CC=C1	0
FC1=CC=C(C=O)C=C1	0
NC1=NC(=O)N(C=C1)[C@@H]1O[C@H](CO)[C@@H](O)[C@@H]1O	0
CC(C)OC(=O)COC1=C(Cl)C=C(Cl)C=C1	0
OC1CCCCCCCCCC1	0
CN1C2C=CC([C@@H]3[C@H]2C(=O)N(C3=O)c4ccc(c5ccccc45)[N+](=O)[O-])C1=O	1
OC[C@H]1O[C@@H]2[C@@H](OC3=NC(=N)C=CN23)[C@@H]1O	0
N[C@@H](CC1=CNC2=CC=CC=C12)C(O)=O	0
CCCCCCOC(=O)CCCCCCCC(=O)OCCCCCC	0
Cl.CC(CCC1=CC=CC=C1)NCC(O)C1=CC(C(N)=O)=C(O)C=C1	0
Oc1cccc2c(=O)oc3c(ccc4[nH]c(=O)cc(c34)C(F)(F)F)c12	1
CCCCCOC(=O)COC1=C(Cl)C=C(F)C(=C1)N1C(=O)C2=C(CCCC2)C1=O	0
CCOC(=S)SSC(=S)OCC	0
COC(=O)C1=C(CS(=O)(=O)NC(=O)NC2=NC(OC)=CC(OC)=N2)C=CC=C1	0
CC1=CC(N2N=C3C=CC=CC3=N2)=C(O)C=C1	0
Cl[C@H]1[C@H](Cl)[C@@H](Cl)[C@H](Cl)[C@@H](Cl)[C@@H]1Cl	0
CC(C)(C)C=C	0
CCC(=O)OCCC(C)CCC=C(C)C	0
[Na+].[Na+].CCCCC1=NC2=C(C=C1)[C@@H]([C@H]([C@@H]2C1=CC=C(OC)C=C1C[C@H](C)C([O-	0
CN1C2=C(NC=N2)C(=O)N(C)C1=O	0
Cc1nn(c(C)c1Cc2ccc(cc2)C(=O)N3CCOCC3)-c4ccc(C#N)c(Cl)c4	1
CC1(C)NC(=O)N(C1=O)c2ccc(c(c2)C(F)(F)F)[N+](=O)[O-]	1
CCCCCC(O)=O	0
C1CCC2C(C1)ON=C2c3cccc4ccccc34	1
C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O	1
CC(C)C(=O)OC1=C(C)OC=CC1=O	0
CCCCCCCCCCCCCC(Br)C(O)=O	0
CCCCCCCC\C=C/CCCCCCCC(=O)OCC	0
CN(C)C(=O)CCCCCC[C@@H]1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C	1
CC1CCNc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CC1(C)CCNc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CN(C)C1=CC=C(C=O)C=C1	0
CC(O)CO	0
C[Si]1(O[Si](C)(O[Si](C)(O[Si](C)(O1)C=C)C=C)C=C)C=C	0
CCC(CC)NC1=CC(C)=C(C)C=C1	0
CC1(C)CNC(=O)C1Oc2ccc(C#N)c(c2)C(F)(F)F	1
CC(CCOC=O)CCC=C(C)C	0
CC1=CC=C2OCC(=O)COC2=C1	0

CC1=CC(=CC(C)=C1N)C1=CC(C)=C(N)C(C)=C1	0
CN(C)C(=O)CC(C)=O	0
CC1=C(Cl)C=CC=C1Cl	0
CCCCCCC1=C(O)C=C(O)C=C1	1
C[C@]1(O)CC[C@H]2[C@@H]3[C@H](CCCc4ccc(OCCC(=O)O)cc4)CC5=CC(=O)CC[C@]5(C)[C@H]	1
CC1=CC2=C(C=C1)C(=O)OC2=O	0
CCCCCCCCCCCCCC	0
Fc1cccc(c1)C2=NOC3CCCCC23	1
CC(C)CCCC(C)(C)O	0
C=CCOC(=O)C1=C(C=CC=C1)C(=O)OCC=C	0
CN1CC[C@@H](C1)N(Cc2ccccc2C(F)(F)F)c3ccc(C#N)c(Cl)c3	1
CC1CC(CC(C)(C)C1)OC(=O)C1=C(O)C=CC=C1	0
ClCCOCCOCCCl	0
CCNC1=CC(C)=CC=C1	0
COC1=C(Cl)C=C(Cl)=C1C(O)=O	0
CC1CC(C)(C)Nc2cc3n(C)c(=O)cc(c3cc12)C(F)(F)F	1
Cl.CCN(CC)CCOC(=O)C1=CC=C(N)C=C1	0
[Na+].[Na+].[Na+].S=C1[N-]C(=S)[N-]C(=S)[N-]1	0
CCNC1=NC(NC(C)C)=NC(Cl)=N1	0
CC1(C)O[C@@H]2CO[C@@]3(COS(N)(=O)=O)OC(C)(C)O[C@H]3[C@@H]2O1	0
C[C@](O)(CS(=O)(=O)c1ccc(F)cc1)C(=O)Nc2ccc(C#N)c(c2)C(F)(F)F	1
C[C@H]1CC[C@H]2Nc3cc4n(C)c(=O)cc(c4cc3[C@H]2C1)C(F)(F)F	1
CNC	0
[Cl-].Cl\C=C/C[N+]12CN3CN(CN(C3)C1)C2	0
COc1cc(Oc2ccc(C)cc2)ccc1C#N	1
CC(C)(C)OC(=O)N1C[C@@H]2C[C@H]1[C@@H]3N2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F	1
[Na+].CC(C)COC(=O)CC(C(=O)OCC(C)C)S([O-])(=O)=O	0
[O-][N+](=O)c1ccc(N2C(=O)[C@@H]3C4CCCC(C=C4)[C@@H]3C2=O)c5ccccc15	1
ClC(Cl)C(=O)N1CCOC11CCCCC1	0
CN(C)CCCN(C)CCCN(C)C	0
CC(=O)OCCCCCCCCC=C	0
BrCCBr	0
Cl.ClCC1=NC=CC=C1	0
OCC=CC1=CC=CC=C1	0
FC(F)(F)c1cc(=O)oc2cc3NCCC(c3cc12)C(F)(F)C(F)(F)F	1
NCC1=CC=CC=C1	0
NC1=NC2=CC=CC=C2N1	0
CCNC(=O)CCCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@	1
CCCCN(C)C(=O)CCCCCCC[C@@H]1CC2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@	1
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)S(=O)(=O)c5c	1
CCCCC(CC)COC(=O)C1=CC=C(C=C1)N(C)C	0
OCCC1=CC=NC=C1	0
OC1=C(C=CC=C1)C(=O)OC1=CC=CC=C1	0
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)C(=O)Nc5ccc(	1
OS(=O)(=O)C1=CC=CC=C1	0

CCCCS(Cl)(=O)=O	0
CO[Si](CCCN1C(=O)N(CCC[Si](OC)(OC)OC)C(=O)N(CCC[Si](OC)(OC)OC)C1=O)(OC)OC	0
CCC1(C)CCc2cc3c(cc(=O)n(C)c3cc2N1C)C(F)(F)F	1
CC(=O)C1=CC=CC=C1O	0
ClC1=CC=C(Cl)C=C1	0
ClC1=CC=C(C=N1)C(Cl)(Cl)Cl	0
CN1[C@@H](CCC1=O)C1=CN=CC=C1	0
COc1ccccc1Oc2ccc(C#N)c(c2)C(F)(F)F	1
CSC1=CC=C(Cl)C=C1	0
[O-][N+](=O)c1ccc(cc1C(F)(F)F)C2=NOC3CCCCCC23	1
CC(CCCC(C)(C)O)CC=O	0
OC1=C2C(CC3=CC=C(O)=C3C2=O)=CC=C1	0
CCC1CCc2cc3c(cc(=O)[nH]c3cc2N1)C(F)(F)F	1
C[C@@H]1CN([C@@H](C)CN1C(=O)Nc2ccc(nc2)C(F)(F)F)c3ccc(C#N)c(c3)C(F)(F)F	1
CC(=O)Nc1ccc(Oc2c(C)nn(c2C)-c3ccc(C#N)c(Cl)c3)cn1	1
Cl.NC1=NC(=O)N(C=C1)[C@@H]1O[C@H](CO)[C@@H](O)[C@@H]1O	0
OC1=C(C=CC=C1)C#N	0
CCCCCCCCCC	0
CCCCCCCCOC(=O)C1=CC=C(O)C=C1	0
CC(=O)C(\C)=C\C1C(C)=CCCC1(C)C	0
[K+].[O-]C1=NC(=O)N(Cl)C(=O)N1Cl	0
O=C1CCC(CC1)C1CCCCC1	0
CC(C)C1CC(C)(C)Nc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CNC(=O)ON=C(SC)C(=O)N(C)C	0
CC(=O)C(O)=O	0
CNC(=O)OC1=CC=CC2=C1OC(C)(C)O2	0
CC1(C)N(CCS(=O)(=O)N)C(=S)N(C1=O)c2ccc(C#N)c(c2)C(F)(F)F	1
CS(=O)(=O)OCCCCOS(C)(=O)=O	0
OC(=O)C1=C(C=CC=C1)C(C1=CC=C(O)C=C1)C1=CC=C(O)C=C1	0
NC1=CC=C(C=C1)[As](O)(O)=O	0
OC(=O)C1=CC=CC=C1N1C=C(C(O)=O)C(=O)C2=C1C=C(Cl)C(NC1=C(F)C=C(F)C=C1Cl)=C2	0
CCCCCCCCCCCO	0
COC(=O)C1=C(OC)C=CC=C1	0
CC(C)Nc1ccc2nc(O)cc(c2c1)C(F)(F)F	1
CCC1CCNc2cc3oc(=O)cc(c3cc12)C(F)(F)F	1
CC(=O)C1=CC(=CC2=C1CCC2(C)C)C(C)(C)C	0
CC\C=C/CCOC(C)=O	0
C[C@@H](N(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F)C(F)(F)F	1
[Na+].C\C([O-])=C1/C(=O)OC(C)=CC1=O	0
CC(C)NCC(O)COC1=CC=C(CC(N)=O)C=C1	0
BrCC(Br)C1CCC(Br)C(Br)C1	1
OC(=O)CN1C(=O)N(CC2=CC=C(Br)C=C2F)C(=O)C2=C1C=C(Cl)C=C2	0
O=C(OCCC1=CC=CC=C1)C1=CC=CC=C1	0
CCCCC(CC)COP(=O)OCC(CC)CCCC	0
CC(C)C1=CC(C(C)C)=C(O)C=C1	0

CCCNc1cc2[nH]c(=O)cc(c2cc1C)C(F)(F)F	1
CCOC(N)=O	0
CC1=CC(C)=C(C(=O)P(=O)(C(=O)C2=C(C)C=C(C)C=C2C)C2=CC=CC=C2)C(C)=C1	0
CCCCCCCCCCCCN1CCOCC1	0
CC1=CC(NC(=O)C(O)=O)=CC(C)=C1OC1=CC=C(O)C2=C1CCC2	0
CCCCCCC#CC(=O)OC	0
CCCCCCCCC1=CC=C(O)C=C1	0
CC(N(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F)C(=O)C	1
CCN(CC)c1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
O[C@@H]1CCN2[C@@H]1C(=O)N(C2=O)c3ccc(C#N)c(Cl)c3F	1
CC(COC(C)=O)OC(C)=O	0
CN(C)c1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
CC12CCC(C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)n5nccc45	1
CC(=O)S[C@@H]1CC2=CC(=O)CC[C@]2(C)[C@H]3CC[C@@]4(C)[C@@H](CC[C@@]45CCC(=O)O	1
CO[C@@H]1[C@@H](CC[C@]2(CO2)[C@H]1[C@@]1(C)O[C@@H]1CC=C(C)C)OC(=O)NC(=O)CCl	0
ClN1C(=O)NC(=O)N(Cl)C1=O	0
OCNC(=O)NCO	0
NC1=CC=C(C=C1)C(O)=O	0
[O-][N+](=O)C1=CC2=C(NC=N2)C=C1	0
CCOC(=O)NC(=S)NC1=C(NC(=S)NC(=O)OCC)C=CC=C1	0
CS\C(C)=N\OC(=O)N(C)SN(C)C(=O)O\N=C(/C)SC	0
CN1N=CC(C(=O)C2=C(C)C(C3=NOCC3)=C(C=C2)S(C)(=O)=O)=C1O	0
OS(O)(=O)=O.O=C1C[C@@H]2OCC=C3CN4CC[C@@]56[C@@H]4C[C@@H]3[C@@H]2[C@@H]5	0
CC(C)(C)C1CCCCC1=O	0
CC1=CCC2C(C1)C2(C)C	0
CCOc1ccc2oc(=O)c3c(ccc4[nH]c(=O)cc(C)c34)c2c1OC	1
CC(C)C(=O)OCC=CC1=CC=CC=C1	0
CC(=O)C1=CC2=C(CCCC2)C=C1	0
CN(C)C=O	0
CC(=O)OCCC1CCCCC1	0
CCCCCCCCCCCC(O)=O	0
CC(C)C(C(=O)OC(C#N)C1=CC=CC(OC2=CC=CC=C2)=C1)C1=CC=C(Cl)C=C1	0
FC(F)(F)c1cc(ccc1C#N)C2=NOC3CCCC23	1
CC(C)(O)C(=O)Nc1ccc(c(c1O)C(F)(F)F)[N+](=O)[O-]	1
CCOC1=CC=C(O)C=C1	0
COC(O)C=C(C)OP(O)(OC)OC	0
CCOC(=O)CCC(=O)OCC	0
O=C(OCC1CCC2OC2C1)C1CCC2OC2C1	0
CC(CC=O)C1=CC=CC=C1	0
CC(OC1=C(C)C=C(Cl)C=C1)C(O)=O	0
FC(F)(F)c1cc(=O)[nH]c2cc3OCCNc3cc12	1
CN1[C@@H]2CC[C@@H]3[C@H](CC[C@@]4(C)[C@H]3C/C(=C\c5cccnc5)/[C@@H]4O)[C@@]2(	1
O[C@@H]1CCN2[C@@H]1C(=O)N(C2=O)c3ccc(C#N)c(F)c3F	1
CCCCCC\C=C/CCCCCCCC(O)=O	0
CCC(CC1=C(I)C=C(I)C(N)=C1I)C(O)=O	0

CCCCNC(N)=O	0
CC(C)C(=O)Nc1ccc(c(c1)C(F)(F)F)[N+](=O)[O-]	1
CC(C)(C1=CC=CC=C1)C1=CC=C(O)C=C1	1
FC(F)(F)CN(C(=O)C(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
OC[C@@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
O1C2=CC=CC=C2OC2=C1C=CC=C2	0
CCOC(=O)c1c(C)n(CC2CCCCC2)c(C)c1-c3ccc(cc3)[N+](=O)[O-]	1
CC[C@@H]1[C@H](C)CNc2cc3oc(=O)cc(c3cc12)C(F)(F)F	1
CC(CCC(O)=O)(\N=N\C(C)(CCC(O)=O)C#N)C#N	0
Cn1c(=O)cc(c2cc3CCC(C)(C)Nc3cc12)C(F)(F)F	1
CC1(C)CN(Cc2nc3ccccc3s2)C(=O)C1Oc4ccc(C#N)c(c4)C(F)(F)F	1
CC(C)(C1CCC(O)CC1)C1CCC(O)CC1	0
CC(=O)OCCCC1=CC=CC=C1	0
CC(=O)c1c(C)n(Cc2ccccc2)c(C)c1-c3ccc(cc3)[N+](=O)[O-]	1
O[C@@H]1CCN2[C@@H]1C(=O)N(C2=O)c3ccc(C#N)c4cccnc34	1
Cc1ccc(O)c(Oc2ccc(C#N)c(c2)C(F)(F)F)c1	1
OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
CC1=CC=C(N)C=C1	0
COC1=CC=C(NC(=O)CC(C)=O)C=C1	0
OC(=O)CC1=C2C=CC=CC2=CC=C1	0
CC(C)C1=CC2=C(C=C1)C=C(C=C2)C(C)C	0
CC(C)COCNC(=O)C=C	0
[Na+].[O-]C1=CC=CC=C1	0
O=C(OCCC1=CC=CC=C1)C=CC1=CC=CC=C1	0
CC1COC(=O)O1	0
CC(=O)NC1=NN=C(S1)S(N)(=O)=O	0
O=NN1CCCCCCC1	0
CC1=CC(=O)CC(C)(C)C1	0
FC(F)(F)c1cc(ccc1C#N)C2=NOC3CCCCCC23	1
NC(=O)C1=NC=CN=C1	0
[Na+].FC1=CC=C(C(=O)[N-]S(=O)(=O)\C=C\C2=CC=CC=C2)C(Cl)=C1	0
OC1=C2C=CC3=CC=CC4=CC=C(C=C1)C2=C34	0
NCCOCCO	0
CC[C@@H]1Cc2cc3c(cc(O)nc3cc2N[C@@H]1C)C(F)(F)F	1
CCC1Nc2cc3oc(=O)cc(c3cc2CC1C)C(F)(F)F	1
CCNP(=S)(OC)O\C(C)=C\C(=O)OC(C)C	0
ClP(=O)(OC1=CC=CC=C1)OC1=CC=CC=C1	0
[Na+].[Na+].[O-]S(=O)(=O)OOS([O-])(=O)=O	0
[O-][N+](=O)c1ccc(C2=NO[C@H]3CCCCC[C@@H]23)c(c1)C(F)(F)F	1
Oc1cccc2OCc3c(ccc4[nH]c(=O)cc(c34)C(F)(F)F)-c12	1
CCC12COCN1COC2	0
FC[C@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
CCCN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
[Na+].CCCCCCCCCOS([O-])(=O)=O	0
CCCC1=C(OCCCC2=NN=NN2)C=CC(C(C)=O)=C1O	0

Cl.Cl.OC(=O)COCCN1CCN(CC1)C(C1=CC=CC=C1)C1=CC=C(Cl)C=C1	0
[Cl-].CCCC[N+]1=CC=CC=C1	0
CC1=CC(O)=C(Cl)C=C1C	0
CC1=NN(CO)C(C)=C1	0
CC(CCC(O)=O)(C1=CC=C(O)C=C1)C1=CC=C(O)C=C1	0
CCc1cc2c(cc(=O)[nH]c2cc1NC)C(F)(F)F	1
CCC1CCN(C)c2cc3n(C)c(=O)cc(c3cc12)C(F)(F)F	1
CO[Si](OC)(OC)C1=CC=CC=C1	0
CC1=CC(=CC=C1NC(=O)C1=CC=CC(I)=C1C(=O)NC(C)(C)CS(C)(=O)=O)C(F)(C(F)(F)F)C(F)(F)F	0
COCC(C)N	0
CCC1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
COC(CC(C)CCCC(C)(C)O)OC	0
CC(=O)OC1=C(C=CC=C1)C(O)=O	0
ClC1=C(Cl)C(=O)SS1	0
Cl\C=C\Cl	0
CC1(C)SC(C)(C)SC(C)(C)S1	0
CCCCc1ccc(cc1)C(=O)N2C[C@@H]3C[C@H]2[C@H]4N3C(=O)N(C4=O)c5ccc(cc5)[N+](=O)[O-]	1
CC1(C)[C@@H]2C[C@H]1C(=C)CC2	0
Oc1cc(c2cc3[C@H]4CCC[C@H]4CNc3cc2n1)C(F)(F)F	1
NC1=CC=CC2=C(N)C=CC=C12	0
Cl[Nd](Cl)Cl	0
CCC(C)(C)C1CCC(O)CC1	0
CCN(C)C(=O)CCCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[	1
CCCCCCCC=O	0
Clc1cc(ccc1I)N2C(=O)[C@@H]3C4CCC(O4)[C@@H]3C2=O	1
COC1=CC=C(OC)C(OC)=C1	0
FC(F)(F)c1cc(=O)[nH]c2cc3OCCN(Cc4ccccc4)c3cc12	1
OC(=O)CC1=CC(I)=C(OC2=CC(I)=C(O)C(I)=C2)C(I)=C1	0
O=C(OCCOCCOC(=O)C1=CC=CC=C1)C1=CC=CC=C1	0
CC1(C)CCC[C@H]2[C@@H]1Nc3cc4nc(O)cc(c4cc23)C(F)(F)F	1
CCOC(=O)C1CC(=O)C(=C(O)C2CC2)C(=O)C1	0
CC(C)=CC(O)=O	0
Cl.NC1CCCCC1	0
Cc1cc(ccc1N2C(=O)[C@@H]3[C@H](O)CCN3C2=O)C#N	1
CCNC1=NC(NCC)=NC(Cl)=N1	0
CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5ccc(Cl)c(Cl)c5)c3c12	1
CC(=O)C1=CC=CC=N1	0
CCCCCCCCCCCCCO	0
COC1=CC2=C(C(=O)N(COC3=CC(=O)N4C=CC=C(OCCN5CCCC5)C4=N3)S2(=O)=O)C(=C1)C(C)C	0
CC(O)CN(CC(C)O)CC(C)O	0
CC[C@H]1Cc2cc3c(cc(O)nc3cc2N[C@@H]1C)C(F)(F)F	1
CSC(C)(C)C=NO	0
O[C@@H]1CCN2[C@@H]1C(=O)N(C2=O)c3ccc(C#N)c4ccccc34	1
CCCC(=O)OCC1=CC=CC=C1	0
C=CCNCC=C	0

CCc1cc(ccc1N2C(=O)[C@@H]3[C@H](O)CCN3C2=O)C#N	1
COc1ccccc1/C=C/2\Oc3ccc(F)cc3-c4ccc5NC(C)(C)C=C(C)c5c24	1
CCCCCC(C=O)=CC1=CC=CC=C1	0
CN1[C@@H]2CCCC[C@]2(C)c3cc4c(cc(=O)n(C)c4cc13)C(F)(F)F	1
CN(C)N	0
C[C@]12O[C@](C)([C@H]3[C@@H]1C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)C(=O)N(CC5CC5)C2=	1
CCCCOC(=O)CCCCCCCCC=C	0
CC(C)OP(C)(=O)OC(C)C	0
C1=CC2=C(C=C1)C=NC=C2	0
CC(C)(C)C1=CC=C(C=C)C=C1	0
CCOP(=S)(OCC)OC1=CC=C(Cl)C=C1Cl	0
NC1=CC=C(C=C1)C1=CC=C(N)C=C1	0
OCC1=CC=CO1	0
C\C=C\C=C\C(O)=O	0
CCC(=NOC\C=C\Cl)C1=C(O)CC(CC1=O)C1CCOCC1	0
CC1COc2cc3[nH]c(=O)cc(c3cc2N1)C(F)(F)F	1
CC(CCO)CCC1=CC=CC=C1	0
C[C@]12CC[C@H]3[C@@H](CC=C4C[C@@H](O)CC[C@]34C)[C@@H]1CC[C@@H]2O	1
C[C@H]1C[C@@H](O)CC(C)(C)C1	0
[Na+].[Na+].OC1=C(\N=N\C2=CC=CC=C2)C2=C(C=C(C=C2C=C1)S([O-])(=O)=O)S([O-])(=O)=O	0
COC1=CC(=C(O)C(=C1)C(C)(C)C)C(C)(C)C	0
CCN(CC)c1ccc2nc(O)cc(c2c1)C(F)(F)F	1
Cc1cc(C)cc(Nc2cc(C(=O)N3CCCC3)n(C)c2)c1	1
CCCCCCCCCC(=O)OC	0
CC(CN)CCCN	0
Cc1cc(ccc1Br)N2C(=O)[C@@H]3C4CC(C=C4)[C@@H]3C2=O	1
CN1C(=O)N(C(=O)C1(CO)c2ccccc2)c3ccc(C#N)c(c3)C(F)(F)F	1
C[C@H]1[C@@H]2[C@H](O)CCN2C(=O)N1c3ccc(C#N)c(Cl)c3C	1
CC[C@H]1[C@@H]2[C@H](O)CCN2C(=O)N1c3ccc(C#N)c(Cl)c3C	1
Cc1c(Cl)c(ccc1N2[C@H]([C@@H]3[C@H](O)CCN3C2=O)C(F)(F)F)C#N	1
O[C@@H]1CCN2[C@@H]1C(=O)N(C2=O)c3ccc(C#N)c(c3)-c4ccccc4	1
Cc1c(Cl)c(ccc1C#N)N2C(=O)[C@@H]3[C@H](O)CCN3C2=O	1
COc1c(ccc(C#N)c1C(F)(F)F)N2C(=O)[C@@H]3[C@H](O)CCN3C2=O	1
[O-][N+](=O)c1ccc(N2C(=O)[C@@H]3C4CCC(C=C4)[C@@H]3C2=O)c5ccccc15	1
[O-][N+](=O)c1ccc(N2C(=O)[C@@H]3C4C=CC([C@H]5C[C@@H]45)[C@@H]3C2=O)c6ccccc16	1
Cc1c(C)c(ccc1C#N)N2C(=O)[C@@H]3[C@H](O)CCN3C2=O	1
COc1cc(ccc1C#N)N2C(=O)[C@@H]3[C@H](O)CCN3C2=O	1
CCC1COc2cc3[nH]c(=O)cc(c3cc2N1CC)C(F)(F)F	1
CC1COc2cc3[nH]c(=O)cc(c3cc2N1CC4CC4)C(F)(F)F	1
COc1ncc(/C=C/2\C[C@H]3[C@@H]4CC[C@H]5N(C)C(=O)C=C[C@]5(C)[C@H]4CC[C@]3(C)[C@H]	1
CC1(C)CCC(=CC2=CC=C(Cl)C=C2)C1(O)CN1C=NC=N1	1
CN1[C@@H]2CC[C@H]3[C@@H]4CC[C@H](O)[C@@]4(C)CC[C@@H]3[C@@]2(C)C=CC1=O	1
CN1C(=O)N(C(=O)C1(CO)c2ccc(O)cc2)c3ccc(C#N)c(c3)C(F)(F)F	1
CN1[C@@H]2CC[C@@H]3[C@H](CC[C@@]4(C)[C@H]3C/C(=C\c5ccccc5)/[C@@H]4O)[C@@]2(	1
C[C@]12CC(=O)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@]34C)[C@@H]1CC[C@]2(O)C(=O)CO	1

C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@]2(O)C#C	1
C[C@]1(O)CCC2C3CCC4=CC(=O)CC[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]12C	1
C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@H]2O	1
C[C@H](O)[C@@H](Nc1ccc(C#N)c(Cl)c1C)c2oc(nn2)-c3ccc(cc3)C#N	1
CN1C(=O)N(C(=O)C1(C)c2ccc3[nH]cnc3c2)c4ccc(C#N)c(c4)C(F)(F)F	1
CN1[C@@H]2CC[C@@H]3[C@H](CC[C@]4(C)[C@@H](O)[C@H](Cc5cccc(F)c5)C[C@@H]34)[C@	1
Cc1c(C#N)c(Cl)nc2c3C(CC(=O)Nc3sc12)c4ccccc4Cl	1
CC[C@@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
CC(C)[C@@H]1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
CC(=O)Nc1ccc(OC[C@](C)(O)C(=O)Nc2ccc(c(c2)C(F)(F)F)[N+](=O)[O-])cc1	1
Cc1ccc(cc1)S(=O)(=O)N[C@](C)(CS(=O)(=O)c2ccc(F)cc2)C(=O)Nc3ccc(C#N)c(c3)C(F)(F)F	1
C[C@](O)(CBr)C(=O)Nc1ccc(c(c1)C(F)(F)F)[N+](=O)[O-]	1
C[C@@H]1CC[C@H](CCl)N1c2ccc3[nH]c(=O)cc(c3c2)C(F)(F)F	1
CCOC(=O)c1c(C)n(CCc2ccccc2)c(C)c1-c3ccc(cc3)[N+](=O)[O-]	1
CC[C@H]1[C@H](C)CNc2cc3oc(=O)cc(c3cc12)C(F)(F)F	1
FC(F)(F)c1cc(=O)oc2cc3NCCCc3cc12	1
CCC1CC(C)c2cc3c(cc(=O)oc3cc2N1)C(F)(F)F	1
Cc1c(C#N)c(c(C)n1Cc2ccccc2)-c3ccc(cc3)C#N	1
CC(C)c1cc(=O)[nH]c2ccc(cc12)N(CC(F)(F)F)CC(F)(F)F	1
FC(F)(F)CN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(Cl)c2c1	1
FC(F)(F)CN1C(CC#N)COc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F	1
FC(F)C1COc2cc3[nH]c(=O)cc(c3cc2N1CC(F)(F)F)C(F)(F)F	1
FC(F)(F)CN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
CC#C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CCC4=C3[C@H](C[C@]12C)C1=CC=C(C=C1)N(C)	1
CN(C)S(=O)(=O)CCCN1C(=S)N(C(=O)C1(C)C)c2ccc(C#N)c(c2)C(F)(F)F	1
CC1(C)N(CCCS(=O)(=O)N)C(=S)N(C1=O)c2ccc(C#N)c(Cl)c2	1
Cc1nn(c(C)c1Cc2ccc(cc2)C(=O)NCC(C)(C)O)-c3ccc(C#N)c(Cl)c3	1
Cc1nn(c(C)c1Oc2ccc(F)cc2)-c3ccc(C#N)c(Cl)c3	1
Cc1nn(c(C)c1Cc2ccc(cc2)C(=O)NCCO)-c3ccc(C#N)c(Cl)c3	1
C[C@@H]1CC[C@H]([C@H](O)C(F)(F)F)N1c2ccc3[nH]c(=O)cc(c3c2)C(F)(F)F	1
CCCCN(CCCC)c1ccc2nc(O)cc(c2c1)C(F)(F)F	1
Cc1cc(=O)[nH]c2ccc3c4cc(F)ccc4oc(=O)c3c12	1
CC1CN(C)c2cc3c(cc(=O)[nH]c3cc2O1)C(F)(F)F	1
CCC1CCN(C)c2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CC(C)CC1CCNc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CC1(C)CNc2cc3nc(O)cc(c3cc12)C(F)(F)F	1
CC(C)CNc1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
C[C@@H]1CC[C@H]([C@H](O)C(F)(F)F)N1c2ccc3[nH]c(=O)cc(c3c2)C(F)(F)F	1
CC[C@H]1Cc2cc3c(cc(O)nc3cc2N[C@@H]1CC)C(F)(F)F	1
CCC[C@H]1Cc2cc3c(cc(O)nc3cc2N[C@@H]1CC)C(F)(F)F	1
CC[C@@H]1Cc2cc3c(cc(O)nc3cc2N[C@@H]1CC)C(F)(F)F	1
COC1Oc2cccc(OC)c2-c3ccc4[nH]c(=O)cc(C)c4c13	1
COc1cccc2OC(O)c3c(ccc4[nH]c(=O)cc(C)c34)-c12	1
CCC(C)c1cc2c(cc(=O)[nH]c2cc1N)C(F)(F)F	1
COc1cccc2OCc3c(ccc4[nH]c(=O)cc(c34)C(F)(F)F)-c12	1

COc1cccc2COc3c(ccc4[nH]c(=O)cc(c34)C(F)(F)F)-c12	1
COc1c(O)ccc2OCc3c(ccc4[nH]c(=O)cc(C)c34)-c12	1
CN(Cc1ccccc1)C(=O)CCCCCCCC2C[C@H]3CC(=O)CC[C@]3(C)[C@H]4CC[C@]5(C)[C@@H](O)CC[	1
C[C@]12CC[C@H]3[C@@H](CCC4=CC(O)=CC=C34)[C@@H]1CC[C@@H]2O	1
C[C@]1(O)CC[C@H]2[C@@H]3[C@H](CCCCc4cccc(OCCCC(=O)O)c4)CC5=CC(=O)CC[C@]5(C)[C@	1
C[C@]1(O)CC[C@H]2[C@@H]3[C@H](CCCCc4cccc(OCCCCC(=O)O)c4)CC5=CC(=O)CC[C@]5(C)[	1
C[C@]1(O)CC[C@H]2[C@@H]3[C@H](CCCc4ccc(OCCCC(=O)O)cc4)CC5=CC(=O)CC[C@]5(C)[C@H	1
CCCCCCN(CCCCCC)C(=O)CCCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)	1
CCCN(C)C(=O)CCCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4	1
CN(C)C(=O)CCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@	1
CC(=O)S[C@@H]1CC2=CC(=O)CC[C@]2(C)[C@H]2CC[C@@]3(C)[C@@H](CC[C@@]33CCC(=O)O:	1
CC(=O)O[C@@]1(CC[C@H]2[C@@H]3C=C(Cl)C4=CC(=O)[C@@H]5C[C@@H]5[C@]4(C)[C@H]3C	1
C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCCCCC(CCCC(F)(F)C(F)(F)F)C(=O)O)C[C@H]4CC(=O)C	1
FC(F)(F)C1CCNc2cc3oc(=O)cc(c3cc12)C(F)(F)F	1
Cc1c(C#N)c(c(C)n1Cc2cnc(Cl)c(CO)c2)-c3ccc(cc3)C#N	1
CC(C)(C)CCN(CC(F)(F)F)c1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
Oc1cc(c2cc(ccc2n1)N(CC3CC3)CC4CC4)C(F)(F)F	1
CC(C)CN1CCOc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F	1
FC(F)(F)CNc1ccc2[nH]c(=O)cc(c2c1)C(F)(F)F	1
Cc1c(C#N)c(cn1Cc2cnc(Cl)c(CO)c2)-c3ccc(cc3)C#N	1
C[C@]1(O)CC[C@H]2[C@@H]3[C@H](CCCCc4ccc(OCCCCC(=O)O)cc4)CC5=CC(=O)CC[C@]5(C)[C	1
CCN(CC)C(=O)CCCCCCCC1C[C@H]2CC(=O)CC[C@]2(C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4	1
C[C@]12CC[C@H]3[C@@H]([C@H](CCCCC[S+]([O-])CCCC(F)(F)C(F)(F)F)CC4CC(=O)CC[C@]34	1
C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCCC[S+]([O-])CCCC(F)(F)C(F)(F)F)CC4CC(=O)CC[C@]	1
COC(=O)CN1CC(C)(C)C(Oc2ccc(C#N)c(c2)C(F)(F)F)C1=O	1
CC\C(=C(/C1=CC=CC=C1)C1=CC=C(OCCN(C)C)C=C1)C1=CC=CC=C1	1
CCC1CCNc2cc3[nH]c(=O)cc(c3cc12)C(F)(F)F	1
Cc1nn(c(C)c1Oc2ccc(cc2)C(=O)N3CCOCC3)-c4ccc(C#N)c(Cl)c4	1
C[C@H]1Nc2cc3n(C)c(=O)cc(c3cc2[C@H]1C)C(F)(F)F	1
FC(F)(F)CNc1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
CC1(C)CCc2cc3c(cc(O)nc3cc2N1)C(F)(F)F	1
OC1=C(OC2=CC=C(Cl)C=C2Cl)C=CC(Cl)=C1	1
CC1=CC(C)(C)Nc2ccc3-c4ccccc4OC(c5ccc(Cl)c(C)c5)c3c12	1
CC1=CC(C)(C)Nc2ccc(cc12)-c3cccc(c3)C#N	1
CC1=CC(C)(C)Nc2ccc3-c4cc(F)ccc4O/C(=C\c5ncccc5C)/c3c12	1
CC1=CC(C)(C)Nc2ccc3-c4cc(F)ccc4O/C(=C\c5ccccc5)/c3c12	1
CC1=CC(C)(C)Nc2ccc3-c4ccccc4O/C(=C\c5cc(F)ccc5F)/c3c12	1
CCn1c(=O)cc(c2cc3C(=CC(C)(C)Nc3cc12)C)C(F)(F)F	1
CC1=CC(C)(C)Nc2ccc3-c4ccccc4O/C(=C\c5cccc(F)c5)/c3c12	1
CC1=CC(C)(C)Nc2ccc3-c4ccccc4O/C(=C\c5ccc(F)c(F)c5)/c3c12	1
Cn1cc(cc1C(=O)N2CCCC2)N(Cc3ccc(O)cc3)c4ccc(cc4)[N+](=O)[O-]	1
COC(=O)c1ccc(cc1)N(Cc2ccccc2)c3cc(C(=O)N4CCCC4)n(C)c3	1
CCCCN(CCCC)C(=O)c1cc(cn1C)N(Cc2ccccc2)c3ccc(cc3)[N+](=O)[O-]	1
CN(c1ccc(cc1)[N+](=O)[O-])c2cc(C(=O)N3CCCC3)n(C)c2	1
C[C@]12CN(C[C@](C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(F)F)C(=O)c5ccccc	1

CC(C)[N+]1([O-])C(=O)[C@@]2(C)O[C@](C)([C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(C#N)c(c4)C(F)(	1
CCCN(CCOC1=C(Cl)C=C(Cl)C=C1Cl)C(=O)N1C=CN=C1	1
CCCN1C[C@@]2(C)O[C@@](C)(C1)[C@H]3[C@@H]2C(=O)N(C3=O)c4cccc(c4)C(F)(F)F	1
[O-][N+](=O)c1ccc(cc1C(F)(F)F)N2C(=O)[C@@H]3[C@@H]4CC[C@@H](C4)[C@@H]3C2=O	1
CC12CCC(C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4cccc(c4)C(F)(F)F	1
CC1(C)CN(Cc2noc(n2)-c3ccccc3)C(=O)C1Oc4ccc(C#N)c(c4)C(F)(F)F	1
CC1(C)CN(Cc2ccccc2)C(=O)C1Oc3ccc(C#N)c(c3)C(F)F	1
CC1(C)CN(Cc2ccccc2F)C(=O)C1Oc3ccc(C#N)c(c3)C(F)(F)F	1
CC1(C)CN(Cc2cccc(O)c2)C(=O)C1Oc3ccc(C#N)c(c3)C(F)(F)F	1
CSc1ccc(CN2CC(C)(C)C(Oc3ccc(C#N)c(c3)C(F)(F)F)C2=O)cc1	1
CS(=O)(=O)C1=CC=C(C=C1Cl)[C@@H](CC1CCCC1)C(=O)NC1=NC=CN=C1	1
CC1(C)N(CCCCS(=O)(=O)N)C(=S)N(C1=O)c2ccc(C#N)c(c2)C(F)(F)F	1
CC1Cc2cc3c(cc(O)nc3cc2NC1(C)C)C(F)(F)F	1
CN1CCc2cc3c(cc(=O)n(C)c3cc12)C(F)(F)F	1
C[C@](O)(COc1ccc(C#N)c2ccccc12)C(=O)Nc3ccc(C#N)c(c3)C(F)(F)F	1
[O-][N+](=O)c1ccc(N2C(=O)[C@H]3[C@H]4CC[C@H](C4)N3C2=O)c5ccccc15	1
C[C@H]1N(C)c2cc3n(C)c(=O)cc(c3cc2C1(C)C)C(F)(F)F	1
Fc1ccc(OC(=O)N2C[C@@H]3C[C@H]2[C@H]4N3C(=O)N(C4=O)c5ccc(C#N)c(c5)C(F)(F)F)cc1	1
CC(C)Nc1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F	1
CC(C)(Nc1ccc2c(cc(=O)[nH]c2c1)C(F)(F)F)C=C	1
[O-][N+](=O)c1ccc(cc1)N(Cc2ccccc2)c3ccc(cc3)C(=O)N4CCCC4	1
CCCN1CC(C)(C)C(Oc2ccc(C#N)c(c2)C(F)(F)F)C1=O	1
CCCCN1CC(C)(C)C(Oc2ccc(C#N)c(c2)C(F)(F)F)C1=O	1
CC1(C)COC(=O)C1Oc2ccc(C#N)c(c2)C(F)(F)F	1
FC(F)(F)c1cc(ccc1C#N)C2=NO[C@H]3CCC[C@@H]23	1
COc1cccc(OC)c1-c2ccc(C#N)c(c2)C(F)(F)F	1
COc1cccc(c1)-c2ccc(C#N)c(c2)C(F)(F)F	1
CCOc1ccccc1Oc2ccc(C#N)c(c2)C(F)(F)F	1
CCCCSc1ccc(C#N)c(OC)c1	1
CCCc1ccccc1Oc2ccc(C#N)c(c2)C(F)(F)F	1
Oc1ccccc1Oc2ccc(C#N)c(c2)C(F)(F)F	1
COc1cc(ccc1C#N)-c2ccccc2O	1
Cc1cc(C)c(Oc2ccc(C#N)c(c2)C(F)(F)F)c(C)c1	1
OC(=O)CC(O)(CC(O)=O)C(O)=O.CCN(CC)CCOC1=CC=C(C=C1)C(=C(Cl)C1=CC=CC=C1)C1=CC=CC=C1	1
CC(C)(C1=CC=C(O)C=C1)C1=CC=C(O)C=C1	1
Fc1ccc(cc1C(F)(F)F)C2=NOC3CCCCCC23	1
Clc1ccccc1C2=NOC3CCCCC23	1
Cc1ccccc1Oc2ccc(C#N)c(Cl)c2	1
CC1=CC(C)(C)Nc2ccc3-c4cc(F)ccc4O/C(=C\c5ccncc5C)/c3c12	1
CC1=CC(C)(C)Nc2ccc3-c4cc(F)ccc4O/C(=C\c5occc5)/c3c12	1
[O-][N+](=O)c1ccc(cc1C(F)(F)F)C2=NOC3CCCCCC23	1
CC12CCC(C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4ccc(c5c(Br)cccc45)[N+](=O)[O-]	1
CC12CCC(C)(O1)[C@H]3[C@@H]2C(=O)N(C3=O)c4cnc(C#N)c(Cl)c4	1
COc1cccc(CN2CC(C)(C)C(Oc3ccc(C#N)c(c3)C(F)(F)F)C2=O)c1	1
CC1(C)CN(Cc2ccc(O)cc2)C(=O)C1Oc3ccc(C#N)c(c3)C(F)(F)F	1

CC12CCCN1c3cc4nc(O)cc(c4cc3CC2)C(F)(F)F	1
CC(C)(C)OC(=O)N1C[C@@H]2C[C@H]1[C@@H]3N2C(=O)N(C3=O)c4ccc(cc4)C#N	1
COc1cccc(c1)C2=NOC3CCCCC23	1
FC(F)(F)c1cc(ccc1C2=NOC3CCCC23)C#N	1
O[C@@H]1CCN2[C@@H]1C(=O)N(C2=O)c3ccc(cc3)C#N	1
Cc1cc2c(cc(=O)[nH]c2cc1N)C(F)(F)F	1
CCCCC[C@H]1C[C@]2(C)[C@@H](O)CCC2C3CCC4=CC(=O)CCC4=C13	1
CCCCCCCCCCCC[C@H]1C[C@]2(C)[C@@H](O)CCC2C3CCC4=CC(=O)CCC4=C13	1
CCCCCCCCCCCCC(=O)/C=C/CCCOC[C@H](O)COCC#C	1
C/C=C\1/C(=O)C[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C	1
Cc1cccc(c1)[C@H]2COc3cc4[nH]c(=O)cc(c4cc3N2CC(F)(F)F)C(F)(F)F	1
CC[C@H]1C[C@]2(C)[C@@H](O)CCC2C3CCC4=CC(=O)CCC4=C13	1
OC1=C(CC=C)C=C(C=C1)S(=O)(=O)C1=CC(CC=C)=C(O)C=C1	1
CC(C)OP(=S)(OC(C)C)SCCNS(=O)(=O)C1=CC=CC=C1	1
CC(C)=CC1C(C(=O)OC2CC(=O)C(CC#C)=C2C)C1(C)C	1
FC(F)C(F)(F)OCC(CN1C=NC=N1)C1=C(Cl)C=C(Cl)C=C1	1
OC(C1=CC=C(Cl)C=C1)(C1=CC=C(Cl)C=C1)C(Cl)(Cl)Cl	1
C[C@H](CCCC(C)(C)O)[C@H]1CC[C@H]2/C(=C/C=C\3/C[C@@H](O)C[C@H](O)C3=C)/CCC[C@]12	1
CCOP(=S)(OCC)SCSP(=S)(OCC)OCC	1
[Na+].[Na+].[O-]S(=O)(=O)C1=CC=C2N\C(C(=O)C2=C1)=C1\NC2=CC=C(C=C2C1=O)S([O-])(=O)=O	0
[Na+].[Na+].CC1=NN(C(=O)C1\N=N\C1=CC=C(C=C1)S([O-])(=O)=O)C1=CC(Cl)=C(C=C1Cl)S([O-])(=	0
[Na+].[O-]C(=O)C1=CC=C2N(CC3=NOC(=C3)C3=CC=C(Cl)S3)C(=NC2=C1)C(=O)NC1CCN(CC1)C1CC	0
[Na+].CCN(CC1=CC=(CC=C1)S([O-])(=O)=O)C1=CC=C(C=C1)C(C1=CC=CC=C1)=C1C=CC(C=C1)=[N+]	0
C[C@@H](OC1=CC=C(CNC(=O)C2=CC=CN=C2OC2=CC=C3OCOC3=C2)C(F)=C1)C(O)=O	0
CC(=O)NC1=CC=C(CC(O)=O)C=C1	0
CC[C@@]12CCCN3CCC4=C([C@H]13)N(C1=C4C=CC=C1)[C@](O)(C2)C(=O)OC	0
CC1(CO)CN(NC1=O)C1=CC=CC=C1	0
CC1=C(C)C(NC2=C(C=CC=C2)C(O)=O)=CC=C1	0
CCC(C)NC1=C(C=C(C=C1[N+]([O-])=O)C(C)(C)C)[N+]([O-])=O	0
CCC(CC)NC1=C(C(C)=C(C)C=C1[N+]([O-])=O)[N+]([O-])=O	0
CCCCC1(COC(=O)CCC(O)=O)C(=O)N(N(C1=O)C1=CC=CC=C1)C1=CC=CC=C1	0
CCCOC1=C(C=C(C=C1)S(=O)(=O)N1CCN(CC)CC1)C1=NC2=C(CC)N(CC3=CC=CC=N3)N=C2C(=O)N1	0
CCOC(=O)C(C)OC1=CC=C(OC2=CN=C3C=C(Cl)C=CC3=N2)C=C1	0
Cl.CCC1=CN=C(CCOC2=CC=C(CC3SC(=O)NC3=O)C=C2)C=C1	0
Cl.ClCC1=CC=CN=C1	0
Cl.N(C=CC=CC=NC1=CC=CC=C1)C1=CC=CC=C1	0
CN(C)C(=O)NC1=CC=CC(=C1)C(F)(F)F	0
CN(C)C1=CC=NC=C1	0
CNC1=C(Cl)C(=O)N(N=C1)C1=CC=CC(=C1)C(F)(F)F	0
COC1=CC(NC(=O)CC(C)=O)=C(OC)C=C1Cl	0
COC1=CC2=C(NC=C2CCNC(C)=O)C=C1	0
CS(O)(=O)=O.CCOC1=CC=CC(=C1)[C@]1(CC[C@H](C)CC1)N1CCN(CC1)C1=CC=CC=C1	0
FC(F)(F)C(=O)NC1=CC2=C(C=C1)C1=CC=CC=C1C2	0
FC1=CC=CC(F)=C1C(=O)NC(=O)NC1=CC=C(Cl)C=C1	0
N(C1=CC=CC=C1)C1=CC=CC=C1	0

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N1C=CC2=C1C=CC=C2                                                                                    0
O=C(CCCCCCCCC1=CN=CC=C1)N1CCC(CC1)C=C(C1=CC=CC=C1)C1=CC=CC=C1                                         0
O=C(N[C@H]1CN2CCC1CC2)C1=CC2=C(OC=C2)C=N1                                                             0
OC(=O)C1=CC=CC(=N1)C(O)=O                                                                             0
OCCN(CCO)C1=CC=CC=C1                                                                                  0
CC(C)(O)C1=COC(=C1)S(=O)(=O)NC(=O)NC1=C2CCCC2=CC2=C1CCC2                                              0
CCCCCCC(C)OC(=O)COC1=NC(F)=C(Cl)C(N)=C1Cl                                                             0
CCOC1=CC(OP(=S)(OC)OC)=NC(CC)=N1                                                                      0
ClCN1N=NC2=C(C=CC=C2)C1=O                                                                             0
COCC1=CN=C(C2=NC(C)(C(C)C)C(=O)N2)C(=C1)C(O)=O                                                        0
COP(=S)(OC)OC1=NC(Cl)=C(Cl)C=C1Cl                                                                     0
[Na+].[Na+].CC1=CC(C)=C(C=C1N=NC1=CC(=C2C=CC=CC2=C1O)S([O-])(=O)=O)S([O-])(=O)=O                      0
[Na+].[Na+].CCOC1=CC=C(C=C1)N=NC1=CC=C(C=CC2=CC=C(C=C2S([O-])(=O)=O)N=NC2=CC=C(OC                      0
[Na+].[Na+].COC1=C(C=C(C)C(=C1)S([O-])(=O)=O)\N=N\C1=C2C=CC=CC2=CC=C1O)S([O-])(=O)=C                  0
[Na+].[Na+].OC1=C(\N=N\C2=CC=C(C=C2)S([O-])(=O)=O)C2=C(C=C1)C=C(C=C2)S([O-])(=O)=O                    0
[Na+].CC1=CC=C(N=NC2=C(O)C=CC(N=NC3=CC=C(C=C3)S([O-])(=O)=O)=C2O)C(C)=C1                              0
[O-][N+](=O)C1=CC2=CC=CC=C2C(=C1)[N+]([O-])=O                                                         0
CC1=C(N)C(N)=CC=C1                                                                                    0
CC1=CC(=CC=C1N)C1=CC=C(N)C(C)=C1                                                                      0
CC1=CC=CC(=C1[N+]([O-])=O)[N+]([O-])=O                                                                0
CC1=NOC(NS(=O)(=O)C2=CC=C(N)C=C2)=C1C                                                                 0
CCC1(CCC(=O)NC1=O)C1=CC=C(N)C=C1                                                                      0
CCCCCC1=CC=C(N)C=C1                                                                                   0
CCOP(=S)(OC1=CC=C(C=C1)[N+]([O-])=O)C1=CC=CC=C1                                                       0
CCOP(=S)(OCC)OC1=NOC(=C1)C1=CC=CC=C1                                                                  0
CN(C)C(=O)OC1=C(C)C(C)=NC(=N1)N(C)C                                                                   0
COC(=O)C1=C(N)C=CC=C1                                                                                 0
COC1=CN=C(OC)N2N=C(NS(=O)(=O)C3=C(C=CC=C3OCC(F)F)C(F)(F)F)N=C12                                       0
CS(=O)(=O)NC(=O)C1=CC(OC2=CC=C(C=C2Cl)C(F)(F)F)=CC=C1[N+]([O-])=O                                     0
NC1=CC(N)=CC=C1                                                                                       0
NC1=CC=C(C=C1)[N+]([O-])=O                                                                            0
NC1=CC=C(N)C=C1                                                                                       0
NC1=CC=C(N)C2=C1C(=O)C1=CC=CC=C1C2=O                                                                  0
NC1=CC=C2C(=O)C3=C(C=CC=C3)C(=O)C2=C1                                                                 0
NC1=CC2=C(C=CC=C2)C=C1                                                                                0
[Na+].O=C1NC(C(=O)[N-]1)(C1=CC=CC=C1)C1=CC=CC=C1                                                      0
CC(C)(OC1=CC=C(CCNC(=O)C2=CC=C(Cl)C=C2)C=C1)C(O)=O                                                    0
CC(C)N(CC1=CC=CC=C1)C(=O)C(C)(C)C                                                                     0
CC1=CC=CC(C)=C1N                                                                                      0
CCC1=CC=CC(C)=C1N                                                                                     0
CCC1=CC=CC(CC)=C1N                                                                                    0
CCN(CC)C(=O)C1=CC=CC(C)=C1                                                                            0
CN(C)CC1=CC=CC=C1O                                                                                    0
CN1C(C2=CC=C(Cl)C=C2)S(=O)(=O)CCC1=O                                                                  0
COC1=CC=CC(C(=O)NN(C(=O)C2=CC(C)=CC(C)=C2)C(C)(C)C)=C1C                                               0
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COP(=S)(OC)SCN1C(=O)C2=C(C=CC=C2)C1=O	0
O.Cl.Cl.CCCN[C@H]1CCC2=C(C1)SC(N)=N2	0
[Na+].COC1=CC=C(\C=C\S(=O)(=O)[N-]C(=O)C2=CC=C(C)C=C2Cl)C=C1	0
CC1=NC=CN1	0
CN1C(COC(N)=O)=NC=C1[N+]([O-])=O	0
CS(=O)(=O)C1=C(C=CC(=C1)C(F)(F)F)C(=O)C1=C(ON=C1)C1CC1	0
C(CC1=CC2=C(OCO2)C=C1)N1CCC[C@H](C1)OC(C1=CC=CC=C1)C1=CC=CC=C1	0
CN(C)C(=O)C(C1=CC=CC=C1)C1=CC=CC=C1	0
O[C@@H]1[C@@H](COC2=CC(O)=CC=C12)N1CCC(O)(CC1)C1=CC=C(F)C=C1	0
N[C@@H](CC1=CC(I)=C(OC2=CC(I)=C(O)C=C2)C(I)=C1)C(O)=O	0
[Na+].[Na+].OC1=C(O)C(=CC(=C1)S([O-])(=O)=O)S([O-])(=O)=O	0
[Na+].[O-]S(=O)(=O)C1=CC=CC2=C1C=CC=C2	0
[Na+].CC(=O)CC(C1=CC=CC=C1)C1=C([O-])C2=CC=CC=C2OC1=O	0
[Na+].CC1=CC=CC=C1S([O-])(=O)=O	0
Br.CN1[C@H]2C[C@@H](C[C@@H]1[C@H]1O[C@@H]21)OC(=O)[C@H](CO)C1=CC=CC=C1	0
BrC1=CC=C(OC(=O)N2CCN3CCC2CC3)C=C1	0
C(COC1=CC=CC=C1)OC1=CC=CC=C1	0
C1=CC=C(C=C1)P(C1=CC=CC=C1)C1=CC=CC=C1	0
C1=CC2=C(C=C1)C1=C3C2=CC=CC3=CC=C1	0
CC(=C)C(=O)OCC1=CC=CC=C1	0
CC(=O)C1=CC=C(O)C=C1	0
CC(=O)CCC1=CC2=C(OCO2)C=C1	0
CC(C)(C)C1=CC(CCC(=O)NN)=CC(=C1O)C(C)(C)C	0
CC(C)(C)C1=CC=C(C=C1)C(O)=O	0
CC(C)(C)C1=CC=C(C=C1)C1=CC=C(C=C1)C(C)(C)C	0
CC(C)(O)C(=O)C1=CC=C(OCCO)C=C1	0
CC(C)=CC1C(C(=O)OCC2=COC(CC3=CC=CC=C3)=C2)C1(C)C	0
CC(C)C(OC(=O)C1=CC=CC=C1)C(C)(C)COC(=O)C1=CC=CC=C1	0
CC(C)C1=CC(=CC(=C1)C(C)C)C(C)C	0
CC(C)C1=CC(Cl)=C(C)C=C1O	0
CC(C)CC(=O)OC1=CC=C(C)C=C1	0
CC(C)CC(=O)OCC1=CC=CC=C1	0
CC1(C)C(C=C(Cl)Cl)C1C(=O)OC(C#N)C1=CC=C(F)C(OC2=CC=CC=C2)=C1	0
CC1(C)C(C=C(Cl)Cl)C1C(=O)OC(C#N)C1=CC=CC(OC2=CC=CC=C2)=C1	0
CC1=C(F)C(F)=C(COC(=O)C2C(\C=C(/Cl)C(F)(F)F)C2(C)C)C(F)=C1F	0
CC1=CC(C)=C(C(O)=O)C(C)=C1	0
CC1=CC(C)=C(C)C=C1	0
CC1=CC(O)=CC=C1	0
CC1=CC=C(C=C1)C1=CC=CC=C1	0
CC1=CC=C(C=C1)S(=O)(=O)NC(=O)NN1CCCCCC1	0
CCC(=O)OCC1=CC=CC=C1	0
CCC(C)C1=CC=C(O)C=C1	0
CCC(C)OC(=O)C1=CC=C(O)C=C1	0
CCC1=CC2=C(C=C1)C(=O)C1=C(C=CC=C1)C2=O	0
CCCCC(CC)COC(=O)\C=C\C1=CC=C(OC)C=C1	0

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CCCCC(CC)COC(=O)C1=CC=C(C=C1)C(=O)OCC(CC)CCCC                        0
CCCCC(CC)COC(=O)C1=CC=C(O)C=C1                                       0
CCCCC(CC)COC(=O)C1=CC=CC=C1                                          0
CCCCC1=CC=CC=C1                                                      0
CCCCCC1=CC=C(Cl)C=C1                                                 0
CCCCCCCCCCCC1=CC=CC=C1                                               0
CCCCNS(=O)(=O)C1=CC=CC=C1                                            0
CCCCOC(=O)COC(=O)C1=CC=CC=C1C(=O)OCCCC                               0
CCCCOCCOC(=O)C1=CC=CC=C1C(=O)OCCOCCCC                                0
CCOC(=O)C1=CC=CC=C1C(=O)OCC                                          0
CCOC(=O)C1=NOC(C1)(C1=CC=CC=C1)C1=CC=CC=C1                           0
CCOP(=O)(NC(C)C)OC1=CC=C(SC)C(C)=C1                                  0
CCOP(=S)(OCC)OC1=C(Cl)C=C(Br)C(Cl)=C1                                0
ClC1=CC(Cl)=C(Cl)C=C1Cl                                              0
ClC1=CC=C(C=C1)S(=O)(=O)C1=CC=CC=C1                                  0
ClC1=CC=CC(Cl)=C1Cl                                                  0
CN(C)[C@H]1[C@@H]2C[C@H]3C(=C(O)[C@]2(O)C(=O)C(C(N)=O)=C1O)C(=O)C1=C(C=CC=C1O)[    0
COC(=O)C1=C(C=CC=C1)S(=O)(=O)NC(=O)NC1=NC(C)=NC(OC)=N1               0
COC(=O)C1=C(Cl)C(Cl)=C(C(=O)OC)C(Cl)=C1Cl                           0
COC(=O)C1=C(O)C(C)=C(O)C=C1C                                         0
COC(=O)C1=CC(=CC=C1)C(=O)OC                                          0
COC(=O)C1=CC=C(C=C1)C(=O)OC                                          0
COC(C(O)=O)C1=CC=CC=C1                                               0
COC1=CC(C)=CC=C1O                                                    0
COC1=CC(C=CC)=CC=C1O                                                 0
COC1=CC=CC(OC)=C1C(O)=O                                              0
COC1=CC=CC=C1OC                                                      0
COC1=CC2=C(C=CC(=O)O2)C(OC)=C1                                       0
COC1=CC2=CC=C(C=C2C=C1)[C@H](C)C(O)=O                                0
COP(N)(=S)OC1=C(C=CC=C1)C(=O)OC(C)C                                  0
CS(=O)(=O)C1=C(COCC(F)(F)F)C(Cl)=C(C=C1)C(=O)C1C(=O)CCCC1=O          0
O(C1=CC=CC=C1)C1=CC=CC=C1                                            0
O.CC1=CC=C(C=C1)S(O)(=O)=O                                           0
O=C(C1CCC1)C1=CC=CC=C1                                               0
O=C(OCC1=CC=CC=C1)C1=CC=CC=C1                                        0
O=CCC1=CC=CC=C1                                                      0
O=P(OC1=CC=CC=C1)OC1=CC=CC=C1                                        0
O1C=CC2=C1C=CC=C2                                                    0
OC(=O)\C=C\C1=CC=CC=C1                                               0
OC(=O)C1=C(Cl)C(Cl)=CC=C1Cl                                          0
OC(=O)C1=CC(Br)=C(O)C(Br)=C1                                         0
OC(=O)C1=CC=C(O)C=C1                                                 0
OC(=O)C1=CC=CO1                                                      0
OC(=O)CC1=C(Cl)C=CC(Cl)=C1Cl                                         0
OC(=O)COC1=C(Cl)C=C(Cl)C(Cl)=C1                                      0
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OC(=O)COC1=C(Cl)C=C(Cl)C=C1	0
OC(=O)COC1=CC2=C(C=CC=C2)C=C1	0
OC1=C(C=CC=C1)C1=CC=CC=C1	0
OC1=CC(Cl)=CC=C1Cl	0
OC1=CC(O)=C(O)C2=C1C(=O)C1=C(C=CC=C1)C2=O	0
OC1=CC=CC=C1Cl	0
SC1=CC=CC=C1	0
CCCCCCCCOC(=O)C1=CC=C(C(=O)OCCCCCCCC)C(=C1)C(=O)OCCCCCCCC	0
ClC(Cl)(Cl)C1=CC=CC=C1	0
OCCC1=CC=CC=C1	0
[Cl-].CCCC[N+](C)(CCCC)CCCC	0
[Na+].CC(C)(CO)[C@@H](O)C(=O)NCCC([O-])=O	0
C1CCCNCC1	0
CCCCN(CC)C(=O)SCCC	0
CCCCN(CCCC)N=O	0
CN(C1CCCCC1)C1CCCCC1	0
CN1CCCC1=O	0
O=C1CCCN1	0
[Br-].CCC[N+](CCC)(CCC)CCC	0
[Cl-].C[N+](C)(CC=C)CC=C	0
CC1=CN([C@@H]2O[C@H](CO)C=C2)C(=O)NC1=O	0
Cl.CC(=O)O[C@H](CC([O-])=O)C[N+](C)(C)C	0
CN\C(NCC1CCOC1)=N\[N+]([O-])=O	0
NC1=NC(=O)N(C=C1)[C@H]1CS[C@@H](CO)O1	0
NCCCN1CCOCC1	0
O=C1NC(=O)C2CC=CCC12	0
O=C1NC(=S)NC=C1	0
C=CC(=O)NCNC(=O)C=C	0
CC(C)(C)C1=NNC(=S)N(N)C1=O	0
CCN(CCO)CCO	0
CN1C=CNC1=S	0
CN1CCOCC1	0
COP(=O)(OC)O\C(C)=C\C(=O)N(C)C	0
OCCN1CCNCC1	0
CC1(C)CC(N)CC(C)(CN)C1	0
CCC(C)C1SC(C)C(C)=N1	0
CCNC1=NC(SC)=NC(NC(C)C)=N1	0
CN(C)CCO	0
CNC(=O)ON=C(C)SC	0
CNC(=O)ON=CC(C)(C)SC	0
CNC(=S)NC	0
CC(=O)OC(C)(C)CCCC(=C)C=C	0
COC(=O)[C@]1(C)CCC[C@]2(C)[C@H]3CCC(=CC3=CC[C@@H]12)C(C)C	0
[Na+].CCCC(CCC)C([O-])=O	0
[Na+].CCCCC(CC)COS([O-])(=O)=O	0

C[C@H](CCO)CCCC(C)=C	0
CC(C)(C)C1CCCCC1O	0
CC1(C)[C@@H]2CC[C@@]1(C)[C@H](O)C2	0
CC1(C)[C@@H]2CC[C@@]1(C)C(=O)C2	0
CC1=CC(=O)[C@H]2C[C@@H]1C2(C)C	0
CCC(C)CCCC(C)(C)O	0
CCCCC(CC)C(=O)OCCOCCOCCOC(=O)C(CC)CCCC	0
CCCCC(CC)C(Cl)=O	0
CCCCC(CC)CO	0
CCCCC(CC)COC(=O)C=C	0
CCCCC(CC)COC(=O)CCCCC(=O)OCC(CC)CCCC	0
CCCCC(CC)COC(=O)CCCCCCCC(=O)OCC(CC)CCCC	0
CCCCC1CCC(O)CC1	0
CCCCCCC1CCOC1=O	0
CCCCCCCCCCCCCCCCCC(=O)OCC(CC)CCCC	0
O=C1CCCCC1C1CCCCC1	0
[Na+].CCCCCCCCCCCCOS([O-])(=O)=O	0
[Na+].CCCCCCCCCCOS([O-])(=O)=O	0
C[C@H](CCO)CCC=C(C)C	0
CC(=O)C1C(=O)OC(C)=CC1=O	0
CC(=O)CC(C)(C)O	0
CC(C)=CCCC(C)(O)C=C	0
CC(C)CC(=O)OC(C)(CCC=C(C)C)C=C	0
CC(C)CC(C)=NO	0
CC(C)CCCC(O)=O	0
CC(C)CCOC(C)=O	0
CC(O)CC(C)(C)O	0
CC\C=C/C\C=C/C\C=C/CCCCCCCC(O)=O	0
CC\C=C\CCCCCCCCCOC(C)=O	0
CC1CCC(=O)C1=O	0
CCC(C)(O)CCC=C(C)C	0
CCCC(C)C(=O)OCC	0
CCCC1CCCC(=O)O1	0
CCCCCC(O)C=C	0
CCCCCC\C=C\C=O	0
CCCCCC1=CC=CC(=O)O1	0
CCCCCC1CCC(=O)O1	0
CCCCCCC(C)O	0
CCCCCCCC(=O)OC	0
CCCCCCCC(=O)OCCCCCC	0
CCCCCCCC\C=C\CCCOC(C)=O	0
CCCCCCCC1CCC(=O)O1	0
CCCCCCCCBr	0
CCCCCCCCCC(C)=O	0
CCCCCCCCCC(O)=O	0

CCCCCCCCCCCCC(=O)OCC(O)CO	0
CCCCCCCCCCCCBr	0
CCCCCCCCCCCCCC(=O)OCC	0
CCCCCCCCCCCCOC(C)=O	0
CCCCCCCCOC(C)=O	0
CCCCCOC(=O)CC(CC(=O)OCCCCCC)(OC(=O)CCC)C(=O)OCCCCCC	0
OC(=O)CC(C(CC(O)=O)C(O)=O)C(O)=O	0
Cl.N#CC1=CC=C(C=C1)C1CCCC2=CN=CN12	0
CC(C)NC1=CC=C(NC(C)C)C2=C1C(=O)C1=CC=CC=C1C2=O	0
CC(C)OC1=CC(NC(=O)C2=C(C=CC=C2)C(F)(F)F)=CC=C1	0
CC(C)OC1=CC=CC(NC(=O)C2=C(C)C=CC=C2)=C1	0
NC(=O)N1C2=CC=CC=C2C=CC2=C1C=CC=C2	0
NC1=CC(=CNC1=O)C1=CC=NC=C1	0
CC1=CC2=C(OC(CN(CC3=CC=CC=C3)C(=O)NC3=C(F)C=C(F)C=C3F)=C2C2=CC=C(Cl)C=C2)C=C1	0
CCOP(=S)(OCC)OC1=NC(Cl)=C(Cl)C=C1Cl	0
[Na+].[O-]C1=C(C=CC=C1)[N+]([O-])=O	0
CC(C)OC(=O)C1=CC(=CC(=C1)C(=O)OC(C)C)[N+]([O-])=O	0
CC1=CC=CC(=C1C)[N+]([O-])=O	0
Cl.COC1=CC=C(N)C=C1	0
CN(C)C=NC1=CC=C(Cl)C=C1C	0
NC1=CC=C(C(N)=C1)S(O)(=O)=O	0
NC1=CC=C(Cl)C=C1Cl	0
CN(C)CC1=CC(=C(O)C(=C1)C(C)(C)C)C(C)(C)C	0
NC1=C(C=C(Br)C2=C1C(=O)C1=C(C=CC=C1)C2=O)S(O)(=O)=O	0
CN1C(C(=O)NC2=NC=C(C)S2)=C(O)C2=C(C=CC=C2)S1(=O)=O	0
CCC(C(=O)NC(N)=O)C1=CC=CC=C1	0
Cl.CCOC(=O)COC1=CC2=C(CCC(C2)NCC(O)C2=CC(Cl)=CC=C2)C=C1	0
[K+].OC(=O)C1=C(C=CC=C1)C([O-])=O	0
[Na+].[O-]S(=O)(=O)C1=CC2=C(C=CC=C2)C=C1	0
CC(=O)OC1=CC=C(C)C=C1	0
CC(C)=C[C@@H]1[C@@H](C(=O)OCC2=COC(CC3=CC=CC=C3)=C2)C1(C)C	0
CC(C)C(=O)C1=CC=CC=C1	0
CC1=C(Cl)C=CC=C1	0
CC1=C(OCC(O)=O)C=CC(Cl)=C1	0
CC1=CC(=C(C)C=C1O)C1(OS(=O)(=O)C2=C1C=CC=C2)C1=C(C)C=C(O)C(C)=C1	0
CCC(=O)OC1=CC=C(C=C1)C(\CC)=C(/CC)C1=CC=C(OC(=O)CC)C=C1	0
CCCCC(CC)COC(=O)COC1=C(C)C=C(Cl)C=C1	0
CCCCCOC(=O)C1=C(C=CC=C1)C(=O)OCCCCC	0
COC(=O)C1=C(O)C=CC=C1	0
COC(OC)C(C)C1=CC=CC=C1	0
COC1=C(C=C(C(=O)C2=CC=CC=C2)C(O)=C1)S(O)(=O)=O	0
COC1=C(OC(=O)C(C)C)C=CC(C=O)=C1	0
COC1=CC(C)=CC=C1C(C)C	0
FC1=C(F)C(F)=C(Br)C(F)=C1F	0
OC(=O)C1=C(O)C=CC=C1	0

OC(=O)C1=CC=C(C=C1)C(O)=O	0
OC[C@H]1O[C@@H](OC2=CC=C(O)C=C2)[C@H](O)[C@@H](O)[C@@H]1O	0
OC1=C(Cl)C=C(Cl)C(Cl)=C1	0
OC1=CC=CC=C1	0
ONC(=O)C1(CCCC1)N(CCC(O)=O)S(=O)(=O)C1=CC=C(OC2=CC=C(F)C=C2)C=C1	0
OP(O)(=O)OC1=CC=CC=C1	0
C1=CC2=C(C=C1)C1=C(C=CC=C1)C=C2	0
C=CN1CCCC1=O	0
C[C@@H]1[C@@H]2NC[C@@H](C)C[C@H]2O[C@]11CC[C@H]2[C@@H]3CC=C4C[C@@H](O)C	0
C=CCN(CC=C)CC=C	0
CCCCCCCCN(C)C	0
OS(=O)(=O)CCCN1CCOCC1	0
CCNC(=O)NC(=O)C(=N\OC)\C#N	0
FC1=CNC(=O)NC1=O	0
NC1=NC(NC2CC2)=NC(N)=N1	0
CC(=C)C(N)=O	0
CC1=CC(O)CC(C)(C)C1	0
CC1C=C(C)CCC1C=O	0
ClC12C3(Cl)C4(Cl)C5(Cl)C(Cl)(C1(Cl)C4(Cl)Cl)C2(Cl)C(Cl)(Cl)C35Cl	0
CC(CCOC(C)=O)CC(C)(C)C	0
CCCCCCCCCC=O	0
CCCCCCCCCCO	0
CCCCCCCCCCOC(C)=O	0
CCOC(=O)CC(C)C	0
ClC(Cl)=C(Cl)C(Cl)=C(Cl)Cl	0
OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
[Mn++].CC([O-])=O.CC([O-])=O	0
[Na+].F[B-](F)(F)F	0
[NH4+].CCOP([O-])(=O)C(N)=O	0
[O-][N+](=O)OCC(CO[N+]([O-])=O)(CO[N+]([O-])=O)CO[N+]([O-])=O	0
Br[Ca]Br	0
C[SiH](O[Si](C)(C)C)O[Si](C)(C)C	0
C1CCC(CC1)SSC1CCCCC1	0
CC(=C)C(=O)OCCOCCOC(=O)C(C)=C	0
CC(=O)O[Al](O)OC(C)=O	0
CC(=O)OC[C@H]1O[C@@](COC(C)=O)(O[C@H]2O[C@H](COC(C)=O)[C@@H](OC(C)=O)[C@H](O	0
CC(C)=CC(C)=O	0
CC(C)=CCC\C(C)=C/C#N	0
CC(C)OCCO	0
CC(CCOC(=O)C(C)=C)OC(=O)C(C)=C	0
CC(Cl)(Cl)C(O)=O	0
CC[Si](OC(C)=O)(OC(C)=O)OC(C)=O	0
CC\C=C/CCOC(=O)CC	0
CC\C=C\CCO	0
CCCC(=O)OC	0

CCCC\C=C\CCCCO	0
CCCC=C(CC)C=O	0
CCCC=NO	0
CCCCC[Si](OCC)(OCC)OCC	0
CCCCCC(=O)OCC	0
CCCCCC(=O)OCC\C=C/CC	0
CCCCOCCOCCO	0
CCCCOP(=O)(OCCCC)OCCCC	0
CCOC(=O)CC(SP(=O)(OC)OC)C(=O)OCC	0
CCOC(OCC)OCC	0
CCOC1=NC(=NS1)C(Cl)(Cl)Cl	0
CCOS(=O)(=O)OCC	0
Cl[C@H]1[C@H](Cl)[C@@H](Cl)[C@@H](Cl)[C@H](Cl)[C@H]1Cl	0
CN=C=S	0
CO[Si](C)(C)OC	0
COC(=O)CCC(=O)OC	0
COC(=O)CCSCCC(=O)OC	0
COCCOC(=O)CC#N	0
COCCOCCOCCO	0
CS(C)=O	0
NCCO	0
O[C@@H]1COC(O)[C@H](O)[C@H]1O	0
OB(O)O	0
OC(=O)C(Br)Br	0
OC(=O)CF	0
OC[C@H]1O[C@@](CO)(O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@	0
OCC(O)CCl	0
OCC(O)CO	0
OCCO	0
OCCOC(=O)C=C	0
OP(O)(O)=O	0
CC(=C)C(=O)OCCCCOC(=O)C(C)=C	0
CC(C)=CCCC(C)=CC#N	0
CC1CCC(=O)O1	0
CCCC(C)=O	0
CCCCOC(O)CC	0
CCOP(=S)(OCC)SCSCC	0
ClCCOP(OCCCl)OCCCl	0
COC(=O)CCCCC(=O)OC	0
COCCl	0
NC=O	0
OC(=O)\C=C/C(O)=O	0
OC(=O)C(O)=O	0
OC(CC(O)=O)C(O)=O	0
OC[C@@H](O)[C@@H](O)[C@H](O)C=O	0

```
ClC1=CC=C2OC3=C(C=CC=C3)N=C(N3CCNCC3)C2=C1                                          0
CC(C)[C@H](SC(C)=O)C(=O)N[C@H]1CC2=C(C=CC=C2)[C@H]2CCC[C@H](N2C1=O)C(O)=O           0
Cl.CN(C)C(=O)NC1(CCN(CC[C@]2(CN(CCO2)C(=O)C2=CC=CC=C2)C2=CC(F)=C(F)C=C2)CC1)C1=CC   0
CC(C)C1=CC=C(C=C1)C#N                                                               0
ClC1=CC=C(C=C1)C#N                                                                  0
O=C1CCCN1C1CCCCC1                                                                   0
CC(C)(C1=CC(Cl)=C(O)C(Cl)=C1)C1=CC(Cl)=C(O)C(Cl)=C1                                 0
C[C@H](CCC(=O)NCC(O)=O)[C@H]1CC[C@H]2[C@@H]3[C@H](O)C[C@@H]4C[C@H](O)CC[C@]         0
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