SMILES	Class
CCCCC=O	1
CC[n+]1ccn(C)c1	0
CCCCCCOC(=O)c1ccccc1C(=O)c1ccc(N(CC)CC)cc1O	0
CCCO[Si](OCCC)(OCCC)OCCC	0
O=C(O)COc1cccc(Cl)c1Cl	0
CC(C)c1cccc(C(C)CC=O)c1	0
CCCCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCCCC)OC(=O)CCCCCCCCCCCCCCCC	0
CC(CC(=O)OOC(C)(C)C)CC(C)(C)C	0
CC(C)(C)C(=O)O	1
C=C(C)C(=O)OCCCCCCCCCCCCCCCCCCCCCC	0
CN(C)Cc1ccccc1Cl	0
CC(C)(C)c1ccc(O)cc1	1
O=C(O)c1cc(F)c(Br)cc1Cl	1
O=C(O)c1ccc2c(c1)C(=O)OC2=O	0
C1=CCCCCCC1	0
CCCCCOC(=O)Cc1ccccc1	0
CCCC1CO1	0
CC(C)c1cc(C(C)C)cc(C(C)C)c1	0
CCCCCCCCCCCCN1CCCC1=O	1
CCCCN	1
Nc1ccc(Cl)cc1C(=O)c1ccccc1Cl	0
C[Si](C)C	0
CCOc1nc(NC)nc(NC(=O)NS(=O)(=O)c2ccccc2C(=O)OC)n1	0
CC(C)C(=O)OCC(C)(C)C(O)C(C)C	1
C1=CC(c2ccc(C3CC=CCC3)cc2)CCC1	0
O=[N+]([O-])c1ccc(CCc2ccc([N+](=O)[O-])cc2)cc1	0
CCOC(=O)CC#N	0
CC(=O)OCc1ccccc1	0
CCCC(C)C1OCC(C)(CCC)CO1	1
CN(C)c1ccc(C(O)(c2ccc(N(C)C)cc2)c2ccc(Nc3ccccc3)c3ccccc23)cc1	0
C1=CCCC=CCC1	0
O=C=Nc1ccc(OP(=S)(Oc2ccc(N=C=O)cc2)Oc2ccc(N=C=O)cc2)cc1	0
Brc1c(Br)c(Br)c(CCc2c(Br)c(Br)c(Br)c(Br)c2Br)c(Br)c1Br	0
CCCCCCCN	1
C[C](C)C	1
NNC(=O)NN	0
O=c1occo1	1
CC1C2CC(CC2C2CCCC(O)C2)C1(C)C	0
CCCCCCCC=O	1
COc1cc(NC(=O)/C(=N\Nc2cc(OC)c(S(=O)(=O)Nc3ccccc3)cc2OC)C(C)=O)c(OC)cc1Cl	0
CCCOCC(C)OCC(C)O	0
CCc1cccc(C)c1N	0
CC(O)c1ccccc1	0
CC(=O)CC(=O)Nc1ccccc1	0

CC1COC(=O)O1	0
COC=C(C(=O)OC)c1ccccc1COc1cccc(C(F)(F)F)n1	0
CC(C#N)N(CC#N)CC#N	0
COCCCn1c(=O)c2ccc3c(=O)n4c5ccc(C)cc5nc4c4ccc(c1=O)c2c34	0
OCc1ccccc1	0
C1CN(CCOCCN2CCOCC2)CCO1	1
CCCc1nc(C)c2c(=O)nc(-c3cc(S(=O)(=O)O)ccc3OCC)[nH]n12	0
CCCCCOCCOCCOCCCCC	0
O=c1[nH]c2ccc([N+](=O)[O-])cc2[nH]1	0
COc1ccc(C(=O)c2ccccc2)c(O)c1	0
O=C1Cc2ccccc2O1	1
O=P1(Cl)OCCCN1CCCl	1
CSSC	1
Cc1cc(C)c(O)c(C)c1	0
CC(C)CCCCCN(CCCCCC(C)C)CCCCCC(C)C	1
CCCCC(CC)COP(=O)(OCC(CC)CCCC)OCC(CC)CCCC	1
O=C(OCCOCCOC(=O)c1ccccc1)c1ccccc1	0
CCCCCCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCCCCCC	0
C[N+](C)(C)C	1
CCOc1ccc(NC(=O)/C(=N/Nc2ccc(-c3ccc(N/N=C(\C(C)=O)C(=O)Nc4ccc(OCC)cc4)c(Cl)c3)cc2Cl)C(C)	0
NCCOCCO	1
CN(C)CCOCCN(C)C	1
N#CNC(=N)NCCCCCCNC(=N)NC#N	0
O=C(CCl)N(c1ccccc1)c1c(Cl)cccc1Cl	0
O=C(Nc1ccccc1Sc1ccccc1)Oc1ccccc1	1
C=C(O)C=O	0
COCCOCCOCCOCCOC	0
COc1ccccc1NC(=O)c1cc2ccccc2c(N=Nc2cc(Cl)ccc2Cl)c1O	0
O=S(=O)(O)c1cc(Nc2nc(Nc3ccccc3)nc(N(CCO)CCO)n2)ccc1C=Cc1ccc(Nc2nc(Nc3ccccc3)nc(N(CCO	0
C=Cn1ccnc1	0
CCCCCCOP(=O)(O)O	1
O=C(OCc1ccccc1)c1ccccc1	0
CC(C)(C)CC(C)(C)c1ccc(Nc2ccc(C(C)(C)CC(C)(C)C)cc2)cc1	0
CNC(=O)c1cc(Oc2ccc(NC(=O)Nc3ccc(Cl)c(C(F)(F)F)c3)cc2)ccn1	0
NNC(=O)C(N)CO	0
Cc1ccc(-c2ccccc2C#N)cc1	0
O=CC1CCC2C3CCC(C3)C12	0
C1CCCCC2=C(CCCC1)CCCO2	1
CN(C)Cc1ccccc1	1
Cc1ccc(Cl)cc1C	0
CCCCCCCCC=CCCCCCCCCNCCCNCCCNCCCN	1
CCO[Si](CCCSSCCC[Si](OCC)(OCC)OCC)(OCC)OCC	0
CCCCCCCCCCCC	1
CC(=O)/C(=N\Nc1cc(C(=O)O)ccc1Cl)C(=O)Nc1cc(Cl)c(NC(=O)/C(=N/Nc2cc(C(=O)O)ccc2Cl)C(C)=O)	0
COC(OC)C(C)(C)CC=C(C)C	1

CCOC(=O)C1CCC(C(=O)OCC)CC1	0
CCCCCCCCCCCCCCCCCOC(=O)c1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1	0
C=CC(=O)OCCN=C=O	1
C[Sn](C)(Cl)Cl	1
CC(C)(C)OC(=O)NC(Cc1ccccc1)C(O)CN(Cc1ccc(-c2ccccn2)cc1)NC(=O)OC(C)(C)C	0
CCCN(C)C	1
C[Si](Cn1cnnc1)(c1ccc(F)cc1)c1ccc(F)cc1	0
CCOC(=O)CCl	1
CCCC(=O)OCC	0
CCOC(=O)C=Cc1ccc([N+](=O)[O-])cc1	0
CC(C)CCCCCCCCCCCCCC(=O)OCC(O)COCC(O)COC(=O)CCCCCCCCCCCCCC(C)C	0
C=C(C)C(=O)OCCN1CCNC1=O	0
CC(C)(C)c1ccc(C#N)cc1	0
O=C(Cl)C(Cl)Cl	1
O=c1[nH]c2ccccc2[nH]1	0
CC(C)C(=O)c1ccccc1	0
C=CCOCC1(OC2OC(CO)C(O)C(O)C2O)OC(CO)C(O)C1O	0
CN(C)CCCN	1
C=C(C)C(=O)OC(C)(C)C	1
CC(O)c1c(Cl)ccc(F)c1Cl	0
CCN(CC)c1ccc(N=Nc2c(C#N)cc([N+](=O)[O-])cc2C#N)c(C)c1	0
Nc1c(I)c(C(=O)Cl)c(I)c(C(=O)Cl)c1I	0
C=CC=CCCC=CCC	1
CC(OC(C)(C)COC(=O)C1CC1)C1CCCC(C)(C)C1	0
NC(=O)c1ccc(Cl)c(N)c1	0
CC(C)(C)OC(=O)CBr	1
O=C(Cc1ccccc1)OCCc1ccccc1	0
Nc1ccccc1C(F)(F)F	1
COc1ccc(C)cc1NC(C)=O	0
Oc1cc(Cl)ccc1Oc1ccc(Cl)cc1	0
CCCCN(CCO)CCO	0
O=c1c2ccc3c4c(ccc(c24)c2nc4ccccc4n12)c(=O)n1c2ccccc2nc31	0
CC(C)(C)CCCCC(=O)OOC(C)(C)C	1
O=[N+]([O-])c1ccc(Cl)c(Cl)c1	0
Cn1c(=O)cc2c3c(c(Br)ccc31)C(=O)c1ccccc1-2	0
CCSC	1
Cc1cc(Cl)ccc1OC(C)C(=O)O	0
Cc1ccc(N)cc1Cl	1
CN1CCCC1=O	0
C=C(C)C(=O)OCCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
O=C(Nc1ccc(Cc2ccc(NC(=O)NC3CCCCC3)cc2)cc1)NC1CCCCC1	0
CC(C)CCCCCCCCCCCCCC(=O)OCC(C)(C)COC(=O)CCCCCCCCCCCCCC(C)C	0
CC1=CCC(C(C)(C)O)CC1	0
CCCCC(CC)C(=O)OOC(C)(C)CCC(C)(C)OOC(=O)C(CC)CCCC	0
C1CCC2CCCCC2C1	1

O=C1C(Cl)=C(Cl)C(=O)C(Cl)=C1Cl	0
CCCCC(CC)COB(OCC(CC)CCCC)OCC(CC)CCCC	1
CCCCCCCCCCCCCC(=O)OCC(O)CO	0
CCCCCCCCC(=O)OOC(=O)CCCCCCCC	0
C=CC(C)(C#CC1(O)C(C)=C2OC(C)OC2CC1(C)C)OC(C)OCC	0
CC1=C2CC(C=O)C(C1)C(C(C)C)C2	0
CC(C)(c1ccc(OP(=O)(Oc2ccccc2)Oc2ccccc2)cc1)c1ccc(OP(=O)(Oc2ccccc2)Oc2ccccc2)cc1	0
CC(C)(C)c1ccc(OP2OCC3(CO2)COP(Oc2ccc(C(C)(C)C)cc2C(C)(C)C)OC3)c(C(C)(C)C)c1	0
CCOC(=O)C1(C(=O)OCC)COC(C(C)C)OC1	0
CN(C=O)c1ccccc1	0
CCCCCCCC[Sn](CCCCCCCC)(SCC(=O)OCC(CC)CCCC)SCC(=O)OCC(CC)CCCC	1
CCO[Si](C)(CCCCl)OCC	1
C=CS(=O)(=O)CS(=O)(=O)C=C	0
N#Cc1c(F)cccc1F	0
CC(C)(CO)CO	0
Cc1ccc2[nH]c3cc4c(=O)c5cc(C)ccc5[nH]c4cc3c(=O)c2c1	0
CCCCNC(=O)CCC(NC(=O)C(CC)CCCC)C(=O)NCCCC	0
CN(C)CCO	1
CC(C)(OOC(C)(C)c1ccccc1)c1ccccc1	0
CCO[Si](CCC1CCC2OC2C1)(OCC)OCC	0
NCCNCCO	1
C=CC(=C)CCC=C(C)CCC=C(C)C	1
Cc1cc(C2C(=O)Oc3c2cc(C(C)(C)C)cc3C(C)(C)C)cc(C)c1OP1Oc2cc(C(C)(C)C)cc(C(C)(C)C)c2C(C)c2c(c...	0
CC1COc2ccccc2N1C(=O)C(Cl)Cl	0
Cc1ccc(O)c(N=Nc2ccccc2[N+](=O)[O-])c1	0
CCCCCCC(O)CCCCCCCCCCCO	0
Nc1cc(Cl)ccc1Oc1ccc(Cl)cc1Cl	0
C[Si](C)(C)O[Si](O[Si](C)(C)C)(O[Si](C)(C)C)c1ccccc1	0
Nc1ccc2cc(S(=O)(=O)O)ccc2c1	0
CCCCC(CC)COC(=O)C(C)O	1
CO[Si](CCCCCC[Si](OC)(OC)OC)(OC)OC	0
CC(CCl)OP(=O)(OC(C)CCl)OC(C)CCl	0
Cc1cn[nH]c1	1
Clc1nc(Cl)nc(Cl)n1	1
C=C(C)C(=O)NC(C)C	0
CO[Si](OC)(OC)OC	1
CCCCCC=CCCC=O	1
CON=C(C(C)=O)C1(C)OCC(C)(C)CO1	0
CCCCC(CC)COC(=O)OCC(CC)CCCC	1
COC(=O)C1CC2(C(C)C)C=CC1(C)CC2	0
O=C(O)c1ccccc1C(=O)O	0
O=C1CCCCCO1	0
CCCCCCCC(=O)O	1
O=C(CCCl)OCCCCCl	1
Cc1cc(C)c(Nc2ccc(Nc3c(C)cc(C)cc3C)c3c2C(=O)c2ccccc2C3=O)c(C)c1	0

C=CCOCC(O)COCCCC	1
C=[N+](O)CCCCCCCCCC	0
C=CC(=O)OCC	1
C=C(C)CC(C)(C)C	1
COc1cc(NS(=O)(=O)c2ccccc2)c2c(c1N)C(=O)c1ccccc1C2=O	0
C=CCOC(=O)C(C)(C)OC(=O)c1cc(N=C=O)ccc1Cl	0
CC(C)(C)C1CCC2(CC1)OCC(CCl)O2	1
Cc1cc(C(F)(C(F)(F)F)C(F)(F)F)ccc1NC(=O)c1ccccc1C(=O)NC(C)(C)CS(C)=O	0
CCC(=O)OCCc1ccccc1	0
CS(=O)(=O)c1ccc(C(O)=C2C(=O)CCCC2=O)c(Cl)c1COCC1CCCO1	0
C=C(Br)C(F)(F)F	0
COc1ccccc1NC(=O)/C(=N/Nc1ccc(-c2ccc(N/N=C(\C(C)=O)C(=O)Nc3ccc(C)cc3C)c(Cl)c2)cc1Cl)C(C)	0
CC1(C)CC(N=C=O)CC(C)(CN=C=O)C1	1
COC(=O)c1ccc(C(=O)O)cc1[N+](=O)[O-]	0
Nc1cccc(O)c1	0
COc1ccccc1N	0
CC(=O)/C(=N\Nc1ccc(-c2ccc(N/N=C(\C(C)=O)C(=O)Nc3ccccc3C)c(Cl)c2)cc1Cl)C(=O)Nc1ccccc1C	0
COc1c(C)c2c(c(O)c1CC=C(C)CCC(=O)O)C(=O)OC2	0
CO[Si](C)(CCCCl)OC	0
CCC1(CO)COC1	0
c1ccc(C2CCCCC2)cc1	1
CC[Si](OC(C)=O)(OC(C)=O)OC(C)=O	1
COC(=O)COc1nc(F)c(Cl)c(N)c1Cl	0
CCCCC(CC)COC(=O)c1ccccc1C(=O)OCC(CC)CCCC	0
CC=CC(=O)O	0
COc1ccccc1C	0
O=C1CCC(=O)N1	0
CN(C)Cc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1	0
CC(C)(CN)C(N)=O	0
COCc1ccc(-c2ccc(COC)cc2)cc1	0
CC(C)(C1CCCO1)C1CCCO1	1
CCC(CO)(CO)COCC(CC)(CO)CO	0
CC(O)COC(=O)OC1CC(C)CCC1C(C)C	0
Cc1ccc(-n2[nH]c(C)cc2=O)cc1	0
CC(C)CCCCCOP(=S)(S)OCCCCCC(C)C	1
CCC(C)Cl	0
CCOC(=O)c1[nH]n(-c2ccccc2)c(=O)c1N=Nc1ccc(-c2ccc(/N=N/c3c(C(=O)OCC)[nH]n(-c4ccccc4)c3=(	0
CCOC(=O)C(Cl)C(=O)OCC	0
CCCCCC(=O)OC	1
COC(=O)c1ccc(C(=O)OC)cc1	0
C#CCOS(=O)OC1CCCCC1Oc1ccc(C(C)(C)C)cc1	1
ClCc1ccccc1Cl	1
CC1CC=CCCCCCCCC(=O)C1	0
CCCCCCC(=O)Cl	1
CCCC=O	0

c1ccc2n[nH]nc2c1	0
Cc1ccc(Cl)cc1N=Nc1c(O)c(C(=O)Nc2cc(C)c(NC(=O)c3cc4ccccc4c(N=Nc4cc(Cl)ccc4C)c3O)cc2C)cc2	0
CO[Si](CC(C)C)(OC)OC	1
NNc1ccc(S(N)(=O)=O)cc1	0
C=CC(=O)OCC(CC)(COCC(CC)(COC(=O)C=C)COC(=O)C=C)COC(=O)C=C	0
CC(CC=O)CCCC(C)(C)O	0
CCC(C)(C)c1ccc(O)c(C(C)(C)CC)c1	1
CC(=Cc1ccc(C)cc1)CCC=O	1
COc1nc(Cl)nc(OC)n1	1
N=C(c1ccccc1)c1ccccc1	1
COc1ccccc1NC(=O)/C(=N\Nc1ccc(Cl)cc1[N+](=O)[O-])C(C)=O	0
O=C(O)c1cc(Nc2ccccc2)c(C(=O)O)cc1Nc1ccccc1	0
NC(=O)c1ccc(NC(=O)c2ccc([N+](=O)[O-])cc2)cc1	0
CC(Cl)(Cl)CC(Cl)(Cl)Cl	1
NCc1ccc(CN)cc1	1
CC(C)c1c(C(=O)Nc2ccccc2)c(-c2ccccc2)c(-c2ccc(F)cc2)n1CCC1CC(CC(=O)OC(C)(C)C)OC(C)(C)O1	0
C[Si](C)(F)CCCC#N	1
CCN(CCOc1ccc(C2CCCCC2)cc1)c1ccc(C=C(C#N)C#N)c(C)c1	0
CCCCCCCCCCCCS	1
CC(NCCCCCCNC(C)C(C)(C)C)C(C)(C)C	1
CC(C)(O)C(=O)c1ccc(Cc2ccc(C(=O)C(C)(C)O)cc2)cc1	0
NC(=O)c1cccnc1	0
Nc1nc(=O)c2c(CCc3ccc(C(=O)O)cc3)c[nH]c2[nH]1	0
CC(c1ccccc1)c1ccc(O)cc1O	1
CC(C)(C)c1ccc(O)c(C(C)(C)C)c1	1
CC(C)C(=O)OOC(=O)C(C)C	1
CC(C)C(C)(C)C(C)(C)C(C)(C)S	1
Nc1ccc(Cl)cc1Cl	0
C=C1CC(=O)CC(C)(C)C1=O	0
C#CC(C)(O)CCC(C)=C(C)C	0
O=C=Nc1ccc(Cl)cc1	1
O=C(O)c1ccc2c3c(ccc(C(=O)O)c13)C(=O)OC2=O	0
OCCCNCCO	0
CSCCC(O)C#N	0
O=C(F)c1cc(Cl)c(F)c(Cl)c1F	1
COc1cc(S(=O)(=O)Nc2ccccc2)c(OC)cc1N	0
CN1CCN(C)C1=O	0
O=P(Cl)(Cl)Oc1ccccc1	1
CCCCCC(=O)OCC(CC)(COC(=O)CCCCC)COC(=O)CCCCC	0
O=C(O)c1ccc(O)cc1O	0
Cc1ccc([N+](=O)[O-])cc1Cl	0
COc1ccc(OC)c([N+](=O)[O-])c1	0
CCCC1CCC(C2CCC(=O)CC2)CC1	0
C=CC(Cl)CCl	0
CCCCCCCCP(=O)(O)O	1

O=C(CCS)OCC(COC(=O)CCS)(COC(=O)CCS)COC(=O)CCS	0
CC(=O)N(CCN(C(C)=O)C(C)=O)C(C)=O	0
CC(C)(C#N)CC1=CCC2CC1C2(C)C	0
CCOC(=O)C=O	1
CO[Si](CCCNCCN)(OC)OC	0
CCO[Si](CCCC1CC(=O)OC1=O)(OCC)OCC	1
N#Cc1nn(-c2c(Cl)cc(C(F)(F)F)cc2Cl)c(N)c1SSc1c(C#N)nn(-c2c(Cl)cc(C(F)(F)F)cc2Cl)c1N	0
CC1(C)CC(NC(=O)c2cccc(C(=O)NC3CC(C)(C)NC(C)(C)C3)c2)CC(C)(C)N1	0
CCCCC(CC)C(=O)OC	1
CCc1ccc2c(c1)C(=O)c1ccccc1C2=O	0
CC(O)C(N)C(=O)O	0
Clc1ccccc1C(Cl)(Cl)Cl	1
Oc1ccccc1-c1ccccc1	1
CCCCOC(=O)c1ccccc1N=Nc1c(O)c(C(=O)Nc2ccc3[nH]c(=O)[nH]c3c2)cc2ccccc12	0
CS(=O)(=O)c1ccc(C(=O)O)c([N+](=O)[O-])c1	0
CC12CCC3C(CCC4C(C)(C)CCCC43C)(CO1)O2	0
Clc1ccccc1	1
CCCCCC(C=O)=Cc1ccccc1	1
C=CC(=O)OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
CO[Si](CCCN)(OC)OC	1
CCCCCCCCCC=O	1
COc1cc(N=Nc2c(Br)cc([N+](=O)[O-])cc2[N+](=O)[O-])c(NC(C)=O)cc1N(CCOC(C)=O)CCOC(C)=O	0
OCCOCCN(CCOCCO)CCN(CCOCCO)CCOCCO	0
CCC=C(C)C(O)CCCC	0
O=C(O)COc1ccc(Cl)c2cccnc12	0
CC(=O)C=C(C)O	0
CCO[Si](CC(C)CC(C)(C)C)(OCC)OCC	0
CC(C)(C)NC(=O)C1CC2CCCCC2CN1	0
CCCCOC(=O)CCCCC(=O)OCCCC	1
COCC(C)N	1
BrCCCCCBr	0
CCCCCCCCCCC#N	1
COc1ccc(C=C(C#N)C(=O)O)cc1OC	0
Cc1ccc(S(=O)(=O)O)cc1N	0
COC(=O)c1ccc(NC(=O)c2cc(Cl)ccc2Cl)cc1N	0
CC=COC	0
CCO[Si](C)(OCC)OCC	0
O=C(O)c1ccccc1SSc1ccccc1C(=O)O	1
CC(=O)Nc1ccc(F)cc1-c1ccc(Cl)c(Cl)c1	0
C=CC(=O)O	1
O=C1CC(=O)NC(=O)N1	0
CCCCCCCCSCc1cc(C)c(O)c(CSCCCCCCCC)c1	0
CCCCCCCCC(O)CO	1
O=C(O)C(O)c1ccccc1Cl	0
Clc1ccc(C(Cl)(Cl)Cl)c(Cl)c1	1

CC(CCl)OP(=O)(OCC(CCl)(CCl)COP(=O)(OC(C)CCl)OC(C)CCl)OC(C)CCl	0
CCOC(=O)C(C)(C)c1ccccc1	0
CC(CC(=O)OCCN1C(C)(C)CC(OC(=O)CC(C)CC(C)(C)C)CC1(C)C)CC(C)(C)C	1
CCc1ccccc1CC	1
CC(C)CC(C)O	1
CC(C)c1cc(Cc2cc(C(C)C)c(N)c(C(C)C)c2)cc(C(C)C)c1N	0
CCCCCCCCO	0
CCC(C)(C)OOC(C)(C)CC	1
Cc1nc2n(c(=O)c1CCN1CCC(C(=NO)c3ccc(F)cc3F)CC1)CCCC2	0
CCCCCCCC(=O)SCCC[Si](OCC)(OCC)OCC	0
COc1cc(NC(=O)c2cc3ccccc3cc2O)c(OC)cc1Cl	0
C1CCCCCCCCCC1	1
CC(C)COP(=O)(OCC(C)C)OCC(C)C	0
Cc1cnn(C)c1	0
Nc1c(Oc2ccccc2)c(Oc2ccccc2)c(N)c2c1C(=O)c1ccccc1C2=O	0
CC(=O)CC(=O)Nc1ccc2[nH]c(=O)[nH]c2c1	0
CC(C)CC(C)OP(=S)(S)OC(C)C	1
C=CNC=O	0
CNC(=S)NN	0
CCN(CC)CCCl	1
CC1(C)CC(O)CC(C)(C)N1CCO	0
CCCCOCCCC	0
Clc1cccc(C(Cl)(Cl)Cl)n1	0
CC(C)(C)OOC(C)(C)c1ccccc1	0
CCCCCCCCP(=O)(CCCCCCCC)CCCCCCCC	1
CC(CN=Cc1ccccc1O)N=Cc1ccccc1O	0
CCCCC(CC)COC(=O)C(C)Oc1ccc(Cl)cc1C	0
NCCCC(O)(P(=O)(O)O)P(=O)(O)O	1
CCCCCCCCC(=O)O	1
CC(=O)/C(=N\Nc1cc(C(=O)Nc2cc(Cl)ccc2C)ccc1Cl)C(=O)Nc1cc(C)c(NC(=O)/C(=N/Nc2cc(C(=O)Nc3c	0
CC1(C)NCCS1	1
COC(=O)CC(O)CC(O)C=Cc1c(-c2ccc(F)cc2)nc(N(C)S(C)(=O)=O)nc1C(C)C	0
O=[N+]([O-])c1ccc(O)c(CCl)c1	0
C=CC1CC=CCC1	1
CC(C)CC(C)c1ccccc1N	0
O=C(O)c1ccc([N+](=O)[O-])cc1	0
O=C(CS)OCC(O)CO	0
CCCCCC(C)=O	1
Clc1ccccc1C(Cl)Cl	1
Cc1ccc(N(C)C)cc1	0
COc1cc(N=Nc2c(Cl)cc([N+](=O)[O-])cc2[N+](=O)[O-])c(NC(C)=O)cc1N(CCOC(C)=O)CCOC(C)=O	0
CC1(C)C(=O)N(CO)C(=O)N1CO	0
CC(C)CCCCCCCOCCC#N	0
FC(F)(F)c1cccc(Cl)c1	1
C=CCc1cc(C(C)(C)c2ccc(O)c(CC=C)c2)ccc1O	1

C1COCCN1	1
C1=Cc2ccccc2Nc2ccccc21	0
Nc1cccc(Cl)c1	0
Cc1cc2[nH]c(=O)[nH]c2cc1N	0
Cc1ccc2oc(C=Cc3nc4cc(C)ccc4o3)nc2c1	0
CN(C)C(=O)C(CCN1CCC(O)(c2ccc(Cl)cc2)CC1)(c1ccccc1)c1ccccc1	0
CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCCCCC	0
C=CCBr	1
O=C(OCC1CO1)c1ccc(C(=O)OCC2CO2)c(C(=O)OCC2CO2)c1	0
Cc1ccc(S(C)(=O)=O)cc1[N+](=O)[O-]	0
CC(=O)C1(Cl)CC1	0
Cc1ccccc1Cc1ccccc1	1
CCOC(=O)C=CC(=O)OCC	0
CC(C)c1cc(C(C)C)c([N+](=O)[O-])c(C(C)C)c1[N+](=O)[O-]	0
CC(O)CC(C)(C)O	0
O=C(O)c1cc(C(=O)O)cc([N+](=O)[O-])c1	0
O=S(=O)(c1ccc(O)cc1)c1ccc(O)cc1	0
CCCSc1nc(Cl)c([N+](=O)[O-])c(Cl)n1	1
CCCCC(CC)CO[N+](=O)[O-]	0
C1=CC2C3CCC(C3)C2C1	1
CCCCC(CC)COC(=O)CC#N	0
CCO[Si](OCC)OCC	1
CO[Si](CC(C)CC(C)(C)C)(OC)OC	0
C=C(C)C(=O)OCC(C)C	0
CO[Si](OC)(C1CCCC1)C1CCCC1	1
CCOC(=O)CP(=O)(OCC)OCC	0
CCC(C)OP(=S)(S)OCCCCCC(C)C	1
CC(CC(C)(C)C#N)c1ccccc1	0
COC(=O)c1ccc(C(=O)OC)c(N)c1	0
C=CC(=O)OC	1
CCC(CC)C1CC(C)(O)CCO1	0
CCCCC(CC)COC(=O)CC(CC(=O)OCC(CC)CCCC)(OC(C)=O)C(=O)OCC(CC)CCCC	0
O=[N+]([O-])c1ccccc1-c1ccc(Cl)cc1	0
CCCCCCC(CCCC)C(=O)O	0
CCCCC(CC)COCOCC(CC)CCCC	0
COC(=O)COc1cccc(Cl)c1Cl	0
Nc1ccc(Nc2ccccc2)cc1	0
CCCCCCCCCCCCN	1
CC(O)CCC1CCCCC1	1
CCC(C)CCCC(C)CCCC(C)C	0
C=C(C)C(=O)O[Si](C(C)C)(C(C)C)C(C)C	0
CCCCCCCCCCCCCC(C)C	0
COc1nc(OC)nc(C(=O)c2cccc(F)c2N(C)S(=O)(=O)C(F)F)n1	0
C=CC(=O)OCCOCC(CC)(COCCOC(=O)C=C)COCCOC(=O)C=C	0
OCC1CN2CCN1CC2	0

CCC(CC)CC1(C(=O)O)CCCCC1	0
Nc1ccc(Cl)c(Cl)c1	0
O=C(CCl)c1ccc(O)c(Cl)c1	1
Cc1ccccc1Cl	0
O=C(O)CCC(=O)O	0
O=C1CCCN1	0
C=Cc1cc(Br)ccc1Br	1
COc1cc([N+](=O)[O-])ccc1N/N=C(/C(C)=O)C(=O)Nc1ccccc1OC	0
CCCCC(CC)CO	1
CC(C)(C)c1cc(-c2cc(C(C)(C)C)cc(C(C)(C)C)c2O)c(O)c(C(C)(C)C)c1	0
C=CC(=O)NCOCCCC	0
CC(=O)/C(=N\Nc1ccc(-c2ccc(N/N=C(\C(C)=O)C(=O)Nc3ccc(C)cc3C)c(Cl)c2)cc1Cl)C(=O)Nc1ccc(C)c	0
CCc1cc(C)cc(CC)c1N	0
CCCCCCCCCCC(CCCCCCCC)COC(=O)CCCCCCCCCCCCCCC(C)C	0
CCC(=O)OCc1ccccc1	0
CC(c1ccccc1)c1ccc(Nc2ccc(C(C)c3ccccc3)cc2)cc1	0
COB1OB(OC)OB(OC)O1	1
CCOCC	0
C=CP(=O)(OC)OC	0
CC(C)(C)c1cc(Cn2c(=O)n(Cc3cc(C(C)(C)C)c(O)c(C(C)(C)C)c3)c(=O)n(Cc3cc(C(C)(C)C)c(O)c(C(C)(C)C)C	0
COCOC	0
O=CC1=C(Cl)C(C=O)CCC1	1
Cc1ccc(C(N)=O)cc1N	0
O=C(O)CCSCCC(=O)O	0
C=c1cc(C)cc(C)/c1=C(\O)P(=O)(/C(O)=c1\c(C)cc(C)cc1=C)c1ccccc1	0
c1cc(OCC2CO2)cc(N(CC2CO2)CC2CO2)c1	0
C=C(Cl)CN=C=S	1
CCCCBr	1
CCCCCCCCCCCCCCCC[Si](OC)(OC)OC	0
CCCCCCCCC=CCCCCCCCCCCCC(=O)NCCCN(C)C	1
CCCCCCCCCCCCCCCCCC(=O)OC(CO)COC(=O)CCCCCCCCCCCCCCC	0
CCCCC(CC)COC(=O)c1c(Br)c(Br)c(Br)c(Br)c1C(=O)OCC(CC)CCCC	0
CCCCCC=CCCC(CCCCCCCC(=O)O)C(CCCCCCCC)CCCCCCCC(=O)O	0
COC1CCCC1	1
CCC(CC)CC1(C)CCCCC1	1
CCCCOCC(C)OCC(C)O	0
CCCCCCCCCCCCO	0
COC(=O)c1ccc(C(=O)Nc2cc(Cl)ccc2Cl)cc1[N+](=O)[O-]	0
CC(=O)/C(=N\Nc1ccc(C)cc1[N+](=O)[O-])C(=O)Nc1ccccc1	0
CC1CN(c2ccccc2)NC1=O	0
CCCCCC(=O)CC	1
C=C(C)C(=O)Oc1ccccc1	0
CC(C)c1cccc2c(C(C)C)cccc12	0
N#CCCN(CCC#N)c1ccc(N=Nc2ccc([N+](=O)[O-])cc2Cl)cc1	0
CCCCC(C#N)c1ccccc1	0

CCC(C)(C)OOC1(OOC(C)(C)CC)CCCCC1	1
CCCCC(CC)COC(=O)OOC(=O)OCC(CC)CCCC	1
Brc1ccccc1	1
Cc1ccc(Nc2cc(C(=O)O)c(Nc3ccc(C)cc3)cc2C(=O)O)cc1	0
Clc1ccc(C(Cl)Cl)cc1	1
COc1ccc(C(=O)c2ccccc2O)c(O)c1	0
CCCCCCCCC=CCCCCCCCC(=O)N(CCCC)CCCC	1
CCN(CC)c1ccc2c(c1)Oc1cc(N(CC)CC)ccc1C21OC(=O)c2ccccc21	0
COc1ccc(CC2CC2)cc1	1
OCCCOCC(OCCCO)C(OCCCO)C(OCCCO)C(COCCCO)OCCCO	0
CC1(C)CC(=O)CC(C)(C)N1[O]	0
ClCc1ccc(Cl)cc1Cl	0
Nc1ccc(N2CCOCC2=O)cc1	0
ClC=CCCl	1
NCC(O)CO	1
C=C[Si](OCC)(OCC)OCC	0
CN(C)S(=O)(=O)c1cc(Cl)c(N)cc1Cl	0
COC1CC(OC2C(C)OC(OC3C(C)=CCC4CC(CC5(C=CC(C)C(C6CCCCC6)O5)O4)OC(=O)C4C=C(C)C(O)C	0
CC1CO1	0
Nc1ccc(Cl)cc1C(F)(F)F	1
O=Cc1cccc2c1OC(F)(F)O2	0
COC(=O)c1cc(N/N=C(\C(C)=O)C(=O)Nc2ccc3[nH]c(=O)[nH]c3c2)cc(C(=O)OC)c1	0
CC(C=CC1=C(C)CCCC1(C)C)=CC=CC(C)=CCO	1
CN(C)CCCNCCCN	1
CCO[Si](CC(C)C)(OCC)OCC	1
CN1COCNC1=N[N+](=O)[O-]	0
O=CC1CCOC1	0
O=C1CCCCCCCCCCCCCO1	1
C=CC(=O)NC(C)(C)CC(C)=O	0
CCCCCCCCCCCCCCCC=CCC(CC(=O)O)C(=O)O	0
COc1c(Cl)ccc(B(O)O)c1F	0
O=C(O)c1cc2ccccc2cc1O	0
CCCCCCCCCCC(=O)O	0
CCC1CC2CC1CC2OC	1
N#Cc1ccccc1Cl	0
COc1cc(NC(=O)CC(C)=O)c(OC)cc1Cl	0
CCOCCOCCOC(=O)C1CCC(C(=O)OCCOCCOCC)CC1	0
CC(C)CC1CCC(CCC=O)CC1	0
CC(C)CC(C)OP(=S)(S)OC(C)CC(C)C	1
NC(=O)OC(CCl)CCl	0
CCN	1
CC(=O)C=CC1=C(C)CCCC1(C)C	0
CCOC(=O)/C(C)=C/N	1
CON=C(C(=O)OC)c1ccccc1COc1ccccc1C	0
COc1ccc(NC(=O)CC(C)=O)cc1	0

CC(=O)OC(C)(C)C	0
COC(=O)CCCC(=O)OC	0
C=CCOC(=O)C=CC(=O)OCC=C	0
COc1ccc(OC)c(NC(C)=O)c1	0
CCCCCCCCCCCCCCCCCC[Si](OC)(OC)OC	0
CCCCCCC(=O)OCC(COC(=O)CCCCCC)OC(=O)CCCCCC	1
C=C(C)C(=O)OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0
COc1nccc(C(F)(F)F)c1S(=O)(=O)Cl	1
CC1CCC(C(C)C)C(C(=O)NCCc2ccccn2)C1	0
CO[Si](C)(CC(C)CNCCN)OC	0
COC(CN)OC	1
CC1(C)CC(O)CC(C)(C)N1	1
CCCCCCCC(=O)Cl	1
CCOC(=O)C1=NOC(c2ccccc2)(c2ccccc2)C1	0
C=CCOC(=O)C(C)(C)O	0
CC(C)C(=O)OCC(C)(C)C(OC(=O)C(C)C)C(C)C	0
CCCCCCOC(CO)CO	0
c1ccc(CN2CCC(Nc3ccccc3)CC2)cc1	0
CC(C)c1cc(C(C)C)c(N=C=O)c(C(C)C)c1N=C=O	0
O=Cc1ccccn1	1
O=C1CCCCCCCCCC1	0
O=C(Nc1ccc2[nH]c(=O)[nH]c2c1)c1cc2ccccc2cc1O	0
CCCCc1nc(Cl)c(C=O)[nH]1	0
CCN(CC)c1ccccc1	1
CCCCCCCCC=CCCCCCCCC(=O)N(CCO)CCO	1
CNS(=O)(=O)c1cc(OC)c(N=Nc2c(O)c(C(=O)Nc3ccc4[nH]c(=O)[nH]c4c3)cc3ccccc23)cc1C	0
C=C(C)C(=O)OCCCCCCCCCCCC	0
CCCCCCCCCCCCCCCCCC[Si](C)(OC)OC	0
O=C1CNC(=O)N1	0
C=C(C)C(=O)OCCOCC	1
CCCCOC(=O)NC(=S)SCCCC	0
O=c1cc(O)[nH]cn1	0
CCCCCCC(C=O)=Cc1ccccc1	1
CCC(=O)OCC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C	1
O=[N+]([O-])c1cc(S(=O)(=O)Nc2ccccc2)ccc1Nc1ccccc1	0
CN1CN(C)CN(C)C1	1
C=COC(C)=O	0
C=COC(=O)c1ccccc1	1
CCO[Si](CCCCl)(OCC)OCC	0
COc1ccc(C(=O)Nc2ccccc2)cc1N=Nc1c(O)c(C(=O)Nc2ccc3[nH]c(=O)[nH]c3c2)cc2ccccc12	0
CC(=O)OCC1OC(c2ccc(C)c(Cc3ccc(-c4ccc(F)cc4)s3)c2)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O	0
CCCCOCC(C)O	1
O=NCc1ccccn1	0
CC(C)COP(=S)(S)OCC(C)C	1
C1CO1	0

COC(=O)C(C)(C)C#N	0
CCO[Si](CCl)(OCC)OCC	0
O=C(Nc1cc(Cl)c(NC(=O)c2cc3ccccc3c(N=Nc3cc(Cl)ccc3Cl)c2O)cc1Cl)c1cc2ccccc2c(N=Nc2cc(Cl)cc	0
CC(=O)C=CC=C(C)CCC=C(C)C	1
C=CC(=O)OCCC[Si](OC)(OC)OC	1
CC(=O)C=C(C)C	0
Cc1oncc1C(=O)O	0
CC(=O)N1CC(O)CC1C(=O)O	0
C=C(C)C(=O)OCCOC(=O)CC(C)=O	0
CCC=CCCCCCCCCCCCCCCOCC	1
CSc1ccc(C(=O)C(C)(C)N2CCOCC2)cc1	0
COC(=O)c1ccccc1O	0
O=S(=O)(O)c1ccc2nc(-c3ccccc3)[nH]c2c1	0
COc1ccccc1NC(=O)CC(C)=O	0
O=S(=O)(O)c1cccc2cc(Nc3ccccc3)cc(Nc3ccccc3)c12	0
NNC(=O)CCCCC(=O)NN	0
C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	0
CNC(N)=O	0
CCCCCCCCCCCCCCCC(CO)CCCCCCCCCCCCC	0
CCOc1ccccc1C(=N)NO	0
CCCCCCCCCCCCCN(CCCN)CCCN	1
COc1cc(C(F)(F)F)ccn1	0
CCC=CCCOC(=O)OC	0
O=C(Cl)c1ccc(Cl)cc1	1
COC(=O)CCc1cc(-n2nc3ccccc3n2)c(O)c(C(C)(C)C)c1	0
CC(CO)COC1CC2CCC1(C)C2(C)C	1
CCCCC(CC)COC(=O)c1ccccc1	0
CC(C)C=NCC1CCCC(CN=CC(C)C)C1	1
CC1=CCC(C(C)C)CC1	0
CCCCN(CCCC)c1ccc2c(c1)Oc1cc(C)c(Nc3ccccc3)cc1C21OC(=O)c2ccccc21	0
CCC(C)C(C)C(C)CCc1ccc(O)cc1	1
CCCCC(CC)COC(=O)CS	0
CCOC(=O)c1ccc(O)cc1	0
CCCCCC(C)OC(=O)COc1ccc(Cl)c2cccnc12	0
C=CC(=O)OCC(CCC)CCCCC	1
CS(C)=O	0
CO[SiH](CC1CCCCC1)OC	1
CCOC(=O)Cl	1
Cc1ccc([N+](=O)[O-])cc1	0
Nc1ccccc1N	0
O=C=Nc1cccc2c(N=C=O)cccc12	1
NCC1C2CCC(C2)C1CN	1
N=C(N=C(N)Nc1ccc(Cl)cc1)NCCCCCCNC(=N)N=C(N)Nc1ccc(Cl)cc1	0
Nc1cc(Cl)nc(C(=O)O)c1Cl	0
O=c1nc(-c2ccccc2)[nH]c(-c2ccccc2)n1	0

O=S(=O)(Cl)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	1
CC(C)=CC1CC(C)CCO1	1
CCCC1CC(C)(OC(C)=O)CCO1	0
CCC(C)(C)OOC1(OC)CCCCC1	1
CCC=CCC=CCC=CCCCCCCC(=O)O	0
COC(OC)OC	0
CO[Si](CC(C)C)(OC)C(C)C	1
CO[Si](CCCCl)(OC)OC	1
CC(C)(C)OOC(=O)C(C)(C)C	1
CCC(=O)N(c1ccccc1)C1CCNCC1	0
CCCCCC1C(=O)CCC1CC(=O)OC	0
Cn1c(N)cc(=O)n(C)c1=O	0
O=C=Nc1ccccc1Cl	1
CCCCC(CC)(CO)CO	0
O=c1c2ccc3c(=O)n4c5ccccc5nc4c4ccc(c2c34)c2nc3ccccc3n12	0
CCOC(=O)CC(NC1CCC(CC2CCC(NC(CC(=O)OCC)C(=O)OCC)C(C)C2)CC1C)C(=O)OCC	0
CCOc1ccccc1O	0
CCCCCCCCCC(C)=O	1
CC(O)COc1ccccc1	0
ClC(Cl)=C(Cl)Cl	1
CCCC[Sn](Cl)(Cl)Cl	1
CCCC(C)C(CCC)C(C)Cc1ccc(OP(=S)(S)Oc2ccc(CC(C)C(CCC)C(C)CCC)cc2)cc1	0
CCC(O)COC1CCCCC1C(C)(C)C	0
CC(C)COC(=O)C(C)O	0
O=C1CCC=CCCCCCCCCC1	0
CCCCCCC(O)CC=CCCCCCCCC(=O)OC	1
CCOc1cc(C=O)ccc1O	0
CC=CC(=O)OC(CC)C(C)C	0
NCC1CCCC(CN)C1	1
CC(C)(C)CC(C)(C)c1ccc(O)cc1	0
CCCCC(=O)O	1
CC(C)c1ccc2c(c1)OCC(=O)CO2	1
CN(C)c1ccccc1	0
CC(C)CC1CC(C)(O)CCO1	0
CCC(Cc1ccccc1)(C(=O)c1ccc(N2CCOCC2)cc1)N(C)C	0
Cc1cc(=O)n(-c2cccc(S(=O)(=O)O)c2)[nH]1	0
OC[P+](CO)(CO)CO	0
CCCCOCCOP(=O)(OCCOCCCC)OCCOCCCC	1
CC(C)CCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCCCC(C)C	0
CCOC(=O)CC(C)CC(C)(C)C	0
CCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCC)OC(=O)CCCCCCCCCCCC	0
COC(=O)CCC(=O)OC	0
CC(=O)CC(=O)OC(C)(C)C	0
c1ccc(COc2ccc3ccccc3c2)cc1	0
C=CCCC(=O)C1=CCCC(C)(C)C1	0

FC(F)(F)COc1cccnc1Cl	0
CCC(CO)(CO)C(=O)O	0
CCCCCCCCCCCC(=O)OCCOCC(OCCO)C1OCC(OCCO)C1OCCO	0
CCCCOC(=O)NC1CCC(CC2CCC(NC(=O)OCCCC)CC2)CC1	0
CC(CC(C)(C)C)C[Si](Cl)(Cl)Cl	1
COC(=O)c1nc(Cl)cc(NC(C)=O)c1Cl	0
O=C(OCC1CCC2OC2C1)C1CCC2OC2C1	0
O=C(Nc1ccnc(=O)[nH]1)c1ccccc1	0
O=CC(=O)O	0
C=CC(=O)OCCOc1ccccc1-c1ccccc1	0
CC(=O)/C(=N\Nc1ccccc1OCCOc1ccccc1N/N=C(\C(C)=O)C(=O)Nc1ccc2[nH]c(=O)[nH]c2c1)C(=O)N(	0
O=C=NS(=O)(=O)c1ccccc1C(F)(F)F	0
CCCCCCCCN=c1ccn(CCCCCCCCCCn2ccc(=NCCCCCCCC)cc2)cc1	1
C=C(CC(C)(C)c1ccccc1)c1ccccc1	1
Cc1cn(C2CC(O)C(CO)O2)c(=O)[nH]c1=O	0
CC(C)COC(=O)C1CCCCC1C(=O)OCC(C)C	1
O=S(=O)(O)CCCN1CCOCC1	0
CC1=NN(c2ccccc2)C(=O)/C1=N/Nc1ccc(-c2ccc(N/N=C3/C(=O)N(c4ccccc4)N=C3C)c(Cl)c2)cc1Cl	0
CCCCCCCC[Si](OCC)(OCC)OCC	1
CC(CC(C)(C)C)CC(C)(C)C	1
CCCCCCCCCCCCN(C)C	1
CC(C)(O)C(=O)c1ccc(OCCO)cc1	0
NCC(=O)O	0
CC(=O)CCCC(C)CCCC(C)CCCC(C)C	1
CC(Br)C(=O)c1ccc(OCc2ccccc2)cc1	0
Cc1cc(=O)n(-c2ccccc2)[nH]1	0
O=C(Cn1cnc([N+](=O)[O-])n1)Nc1cc(C(F)(F)F)ccc1Cl	1
CCC(O)OC(O)CC	0
C=C1C2CCC3C2C(C)(C)CCCC13C	1
O=C1CCCC=CCCCCCCCCC1	0
OCCO	0
CCOC(=O)CC(C(C)=O)C(=O)OCC	0
CCC(C)(OOC(C)(C)C)OOC(C)(C)C	1
COC(=O)CC(C(C)=O)C(=O)OC	0
O=C(O)c1cc(I)ccc1Cl	0
CCCCCCCCCCCC	1
CCCCN1CCCC1=O	0
CC(C)(C)C1CCC(O)CC1	0
CC1CCC(C(C)C)C(O)C1	0
COc1cc(NC(=O)/C(=N/Nc2ccc(-c3ccc(N/N=C(\C(C)=O)C(=O)Nc4cc(OC)c(Cl)cc4OC)c(Cl)c3)cc2Cl)C(	0
CC(C)(c1ccccc1)C(C)(C)c1ccccc1	0
CCCc1nc(C)c2c(=O)nc(-c3ccccc3OCC)[nH]n12	0
CC(O)CC(C)(C)c1ccccc1	1
COC(=O)C(C)O	1
COC(C)CCO	0

CC[AlH3](CC)CC	0
C=CC(=O)O[Si](C(C)C)(C(C)C)C(C)C	1
CCCCCC1(C)CCC(C)(C)C1=O	0
Cc1ccccc1Nc1ccc(Nc2ccccc2C)c2c1C(=O)c1ccccc1C2=O	0
CC(=O)O[Si](C)(OC(C)=O)OC(C)=O	1
CCn1c2ccccc2c2ccccc21	0
CC1C2CC(CC2C2CCC(O)CC2)C1(C)C	0
C=CC(N)=O	0
CO[Si](C)(C)CCCNCCN	1
CCNc1nc(NC(C)C)nc(SC)n1	0
CCCCN(C)C	1
CCCCCCCCCC(=O)N(C)C	1
On1ccccc1=S	0
CC(C)(C)CCCCC1(C(=O)OC(C)(C)CC(C)(C)C)OO1	1
CN(C)C(=O)Nc1ccc(Cl)c(Cl)c1	0
Cc1ccc(N)c(C)c1	0
Clc1cccc(Cl)c1Nc1ccccc1	1
CCCCCCCCCCCCCC[N+](C)(C)CCO	1
O=c1n(CC2CO2)c(=O)n(CC2CO2)c(=O)n1CC1CO1	0
OCC1CCCO1	0
CO[Si](OC)(c1ccccc1)c1ccccc1	1
COC(C)=O	0
CC(O)CNCC(C)O	0
CCCCOCCOC(=O)c1ccccc1	0
CCS(=O)c1c(C#N)nn(-c2c(Cl)cc(C(F)(F)F)cc2Cl)c1N	0
CCOC(=O)OC1CCCCC1C(C)(C)C	0
CC(C)(c1ccc(OCC2CO2)cc1)c1ccc(OCC2CO2)cc1	0
CCOC(=O)C1=NN(c2ccc(Cl)cc2Cl)C(C)(C(=O)OCC)C1	0
O=C(O)C1CCNCC1	0
CC(C)CCCCCCCCCO	1
COc1ccc(O)cc1	1
O=C1OCCO1	0
CCCC(O)CO	0
CCNC(=S)NCC	0
Fc1c(Cl)ncnc1Oc1ccccc1Cl	0
CC(=O)OC1CC2CC1C1CC=CC21	0
CCCCNCCO	1
CCO[Si](OCC)(OCC)N(CC)CC	1
CNc1ccc(C(O)(c2ccc(N(C)C)cc2)c2ccc(N(C)C)cc2)cc1	0
C=CCOc1nc(OCC=C)nc(OCC=C)n1	0
CC1=CCC(C=CC(C)(C)C(C)O)C1(C)C	1
O=C(NC(C(=O)O)C1CCCCC1)OCc1ccccc1	0
CCCCCCCCCCC1CO1	1
O=C1CCCCCN1C(=O)c1cccc(C(=O)N2CCCCCC2=O)c1	0
CC(CO)CC(C)c1ccccc1	0

CC(C)(C)O	0
CC(CC(=O)O)CC(C)(C)C(=O)O	0
C=CC(=O)OCCCCCCOC(=O)C=C	1
c1ccc2c(c1)CCc1ccccc1N2	0
C=CCCCCCCCCC=O	1
O=C1NCCN1CCO	0
O=C1C2CC=CCC2C(=O)N1SC(Cl)(Cl)Cl	0
ClCC(Cl)CCl	1
NC(=O)CCNCCO	0
O=S(=O)(OS(=O)(=O)C(F)(F)F)C(F)(F)F	1
CCCc1nc(C)c2c(=O)nc(-c3cc(S(=O)(=O)N4CCN(CC)CC4)ccc3OCC)[nH]n12	0
O=C(O)c1ccc(O)cc1	0
OCCN(CCO)CCO	0
CNS(=O)(=O)c1cc(OC)c(N)cc1C	0
CO[Si](CCCS[Si](C)(C)C(C)(C)C)(OC)OC	0
O=C(O)C=CC(=O)O	0
Nc1ccc(Cl)cc1O	0
O=Cc1ccco1	1
C=C(C)C(=O)OCCN=C=O	1
CC[Si](CC)CC	0
CON=C(C(=O)OC)c1ccccc1CCl	0
CCCCCC(CCC)COC(=O)c1ccccc1C(=O)OCC(CCC)CCCCC	0
Cc1cc(Cc2cc(C)c(O)c(C)c2)cc(C)c1O	0
COC(=O)C=C(C)C	0
Nc1c(Cl)cc(C(F)(F)F)cc1Cl	1
CC(C)CCCCCOC(=O)CS	1
CCCCCCCCCCCCCCCCCCNC(=O)CCc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1	0
Fc1ccccc1	0
C=C(C)C(=O)OCCOc1ccccc1	0
Cc1ccc(Nc2ccc(O)c3c2C(=O)c2ccccc2C3=O)cc1	0
CCCCCCCCCCCCCCCCCCN(O)CCCCCCCCCCCCCCCCCCC	0
CN(C)CCCCCN(C)C	1
CCCCc1ccc(-c2ccc(-c3ccc(CC)cc3)c(F)c2F)cc1	0
CCCCCCCc1ccc(O)cc1	1
CN(C)C(=S)SSC(=S)N(C)C	0
CC(C)OC(=O)CCC(=O)OC(C)C	0
NS(=O)(=O)c1ccc(NC(=S)Nc2ccc(F)cc2)cc1	0
CCOC(C)(C)C	0
Cc1cc(C)c(S(=O)(=O)NC2CCCCC2)c(C)c1Nc1ccc(Nc2c(C)cc(C)c(S(=O)(=O)NC3CCCCC3)c2C)c2c1C(	0
COC(CCl)OC	0
CO[Si](C)(OC)OC	0
CCOCC(C)OC(C)=O	0
CCCCCCCCCCCCCCCCOC(=O)Oc1c(Cl)cc(C(=O)OCC)cc1Cl	0
C(=Cc1ccc(-c2nc3ccccc3o2)cc1)c1ccc(-c2nc3ccccc3o2)cc1	0
CCOP(OCC)c1ccccc1	1

Cc1ccc(S(=O)(=O)CNC=O)cc1	0
O=C(O)c1ccccc1	0
C=CC(C)(O)C=CC1=C(C)CCCC1(C)C	0
CC(C)c1ccc(N)cc1	1
CCCCCCCCCCCCCCO	0
O=C(OCCc1ccccc1)c1ccccc1	0
CCOC(=O)C=C(NC)C(F)(F)F	0
COC(=O)C(C)Nc1c(C)cccc1C	0
Nc1c(Oc2ccccc2)cc(O)c2c1C(=O)c1ccccc1C2=O	0
CCCCC(CC)C(=O)OCCOCCOCCOC(=O)C(CC)CCCC	0
C=C1CCOC(C=C(C)C)C1	1
CCOc1ccc2ccccc2c1	0
CCCCCCCCCCCCCCCCC(=O)O	0
Nc1ccc([N+](=O)[O-])c(N)c1	0
COc1ccccc1OC	0
CCCCCC1=C(OC(C)=O)CCC1CC(=O)OC	0
NC(=O)c1c(F)cccc1F	0
O=C=Nc1ccc(Cl)c(C(F)(F)F)c1	1
CCOC(=O)C1(OC(=O)Cc2ccc(Cl)cc2Cl)CCCCC1	0
CCCCCCCCCCCCC	1
C=CC(=O)OCC1CCCO1	1
CCCCCCCCC=CCCCCCCCC(=O)OCC(OC(=O)CCCCCCCC=CCCCCCCCC)C1OCC(O)C1OC(=O)CCCCCCC	0
CC(C)COP(=S)(OCC(C)C)SCC(C)C(=O)O	0
Cc1ccc(-n2[nH]c(C)c(/N=N/c3ccc(-c4ccc(/N=N/c5c(C)[nH]n(-c6ccc(C)cc6)c5=O)c(Cl)c4)cc3Cl)c2=	0
C=COCCOCCOCCOC=C	0
C=C(C)COCCC=CCC	1
CC(=O)CC(=O)Nc1ccc(NC(=O)CC(C)=O)cc1	0
COc1ccc(CC(C#N)C(=O)O)cc1OC	0
CCCCCCCCCCCC[N+](C)(C)CC(O)CS(=O)(=O)O	0
O=C1C=CC(=O)c2ccccc21	1
CCCCOCCO	0
C=CCOC(=O)C(C)(C)OC(=O)c1cc(N)ccc1Cl	0
C1CCSC1	1
CO[Si](CCCNc1ccccc1)(OC)OC	0
Cc1cccc(C)c1N	1
CCCCCCCCCCCCC(=O)OC(C)C	0
CCCCCCCCCCCCCCCCCCN	1
C=[N+](O)CCCCCCCCCCCCCCC	1
C=CC(=O)OCCCOCC(C)(C)COCCCOC(=O)C=C	0
Nc1cccc(Cl)c1Cl	1
CCCCCCCCCCN(C)C	1
CCCCCCCCCCCCCCN(C)C	1
COc1ccc([N+](=O)[O-])cc1N/N=C(/C(C)=O)C(=O)Nc1ccccc1OC	0
Cc1ncoc1C#N	0
C(CCOCC1CO1)COCC1CO1	0

CCCCCOC(=O)C=CC(=O)OCCCC	1
CC1=CCCC(C)(C)C1C(C)CCC=O	1
CC(C)COC(=O)C(C)Cl	1
NS(=O)(=O)c1ccccc1C(F)(F)F	0
CCC(C)C(N)C(=O)O	0
Nc1ccccc1Cl	0
CCCc1ccc(-c2ccc(-c3ccc(CC)cc3)c(F)c2F)cc1	0
CC(C)C=O	0
COC(=O)CC#N	0
CCC=CCC(C)OC(=O)c1ccccc1O	0
C=CCCCCCCCCC(=O)NCCCN(C)C	1
Nc1ccc2[nH]c(=O)[nH]c2c1	0
O=Cc1ccncc1	1
N#Cc1ccc(-c2ccccc2)cc1	0
CC(C=O)(CO)CO	0
COc1cc(-c2cc(OC)cc(C(C)(C)C)c2O)c(O)c(C(C)(C)C)c1	0
O=C(Cl)c1ccc(Cl)cc1Cl	1
C=C(C)C(=O)O	0
CC(C)CCCCCCCCCCOCCCN	1
O=C(O)CCCCCCCC(=O)O	0
c1ccc2c(c1)CCCC2	1
C=CC(=O)OCC(CC)(COC(=O)C=C)COC(=O)C=C	1
CC(C)CC1(C)OCC(CO)O1	0
CC(C)(C)c1cccc(C(C)(C)C)c1O	1
CC(C)(C)NCc1ccccc1	1
O=c1[nH]c2ccccc2c(=O)n1CCO	0
CCCCCCOC(=O)c1ccccc1O	1
CC(=O)S	1
NCCc1ccc(O)cc1	0
COCCCN	1
O=S(=O)(O)c1ccc(O)cc1	0
CCC(C)c1cccc(C(C)CC)c1O	1
CO[Si](CCCN=C=O)(OC)OC	1
CCCCC(CC)COC(=O)C(C#N)=C(c1ccccc1)c1ccccc1	0
NC(=O)c1ccc(NC(=O)c2ccc(N)cc2)cc1	0
C=C(C)C(=O)Nc1ccc(S(=O)(=O)Nc2nc(C)cc(C)n2)cc1	0
O=C1OCCC1O	0
C=CCCCCCCCC(=O)OCC	0
CCOCCCOC(O)CC	1
Oc1cc(Cl)cc(Br)c1	1
COc1cc([N+](=O)[O-])ccc1N	0
CC(=O)CC(=O)OC(C)C	0
CC(C)CC(=O)O	1
Nc1ccc(-c2ccc(N)c(Cl)c2)cc1Cl	0
CCC(C)(C)OC	0

O=c1[nH]c2ccccc2c(=O)n1CCCl	0
O=[N+]([O-])c1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1S(=O)(=O)c1ccccc1	0
CC(CO)CCCC1CCCCC1	1
Fc1cccc(C(F)(F)F)n1	0
CCN(C(C)C)C(C)C	1
O=C(O)c1[nH]n(-c2ccc(S(=O)(=O)O)cc2)c(=O)c1/N=N/c1ccc(S(=O)(=O)CCOS(=O)(=O)O)cc1	0
CC(C)N	1
CC(C)OC(=O)C(C)OC(=O)C(C)(C)C	0
CC(=O)OCCC(C)CCC=C(C)C	1
Cc1ccccc1NC(=O)c1cc2ccccc2c(N=Nc2cc(Cl)c(Cl)cc2Cl)c1O	0
CCC(C)(O)CCC=C(C)C	1
O=C1NC(=O)C(=c2[nH]c(=C3C(=O)NC(=O)NC3=O)c3ccccc23)C(=O)N1	0
CC1(C)CC(=O)CC(C)(C)N1	1
COc1ccc(C(=O)Nc2ccc(C(N)=O)cc2)cc1[N+](=O)[O-]	0
Nc1cc(C(=O)O)cc(C(=O)O)c1	0
CC1=CCC(C)CC2CCCC2=O)CC1	0
C=CCn1c(=O)n(CC=C)c(=O)n(CC=C)c1=O	0
CCCCOCCO[Si](OCCOCCCC)(OCCOCCCC)OCCOCCCC	1
NC(CO)(CO)CO	0
COc1ccc(C(=O)Nc2ccccc2)cc1N	0
COc1cc(Br)c2c3c1OC1CC(=O)C=CC31CCNC2	0
CCSCC	1
CC12CCCC=C1C(=O)OC2=O	1
CCCCC(CC)CN	1
CCOC(=O)N1CCC(=O)CC1	0
COc1ccc2ccccc2c1	0
OC1(c2ccc(Cl)cc2)CCNCC1	1
CC(=O)Nc1ccc(NC(=O)c2cc3ccccc3cc2O)cc1	0
CCCCCCCC1=NCCN1CCO	1
COc1cc(C=O)ccc1O	0
COc1ccc(OC)c(N)c1	0
O=P(O)(O)CN(CCN(CP(=O)(O)O)CP(=O)(O)O)CP(=O)(O)O	0
CCCCCCCCCCCCCCCN(C)C	1
Cc1nc(N)nc(N)n1	0
CCCCC(CC)COC(=O)c1ccc([N+](=O)[O-])cc1	0
O=Cc1c(O)ccc2ccccc12	0
CCCCC(CC)C(=O)O	1
CCCCC	1
O[Si](O)(c1ccccc1)c1ccccc1	0
COc1cc([N+](=O)[O-])c(OC)cc1Cl	0
O=S(=O)(NS(=O)(=O)c1ccccc1)c1ccccc1	0
OCC(O)COC1CCCCC1	0
CCCCCCCCCCCCCCCC[Si](OCC)(OCC)OCC	0
OC(Cc1ccccc1Cl)(CN1NCNC1=S)C1(Cl)CC1	0
CCOC(=O)CCN(C(=O)c1ccc(NC)c(N)c1)c1ccccn1	0

CC(C)C(=O)OOC(C)(C)C	0
CC(C)(C)c1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1	0
CCC(C)NC1CCC(CC2CCC(NC(C)CC)CC2)CC1	1
Cn1c(=O)c2ccc3c4ccc5c(=O)n(C)c(=O)c6ccc(c7ccc(c1=O)c2c37)c4c56	0
COC(=O)CSP(=S)(OC)OC	0
CC(C)CC(=O)CC(C)C	0
CCC(Cc1ccc(C)cc1)(C(=O)c1ccc(N2CCOCC2)cc1)N(C)C	0
COC(=O)CCl	1
C=C(C)C(=O)OCCOCCOCCCC	0
NC(=O)c1ccc(N)cc1	0
CC(=O)CCC1=C(C)CCCC1(C)C	0
CCCCOCOCCCC	0
Clc1cccc(Cl)c1C(Cl)Cl	0
CCCCCCCCCC(=O)Oc1ccc(C(=O)O)cc1	0
COCCOCOCCOC	0
CC(C)=CCCC(C)(O)C1CC=C(C)CC1	0
COC1(OC)CCC2=C(CCC3C2CCC2(C)C(=O)CCC32)C1	0
OCC(F)(F)F	0
COc1cc([N+](=O)[O-])ccc1N/N=C(/C(C)=O)C(=O)Nc1cc(Cl)ccc1OC	0
O=C1COC(=O)CO1	1
COC(=N)N	0
C=CC(=O)OC(C)COCC(C)OC(=O)C=C	1
NC1CCc2c(c3ccccc3n2CCC(=O)O)C1	0
CCC1(CO)COC(C)(C)OC1	0
CCCCCCCCCCCCCCC(=O)OCCCCCCCCCCCCCCC(C)C	0
N#CCCN(CCOC(=O)c1ccccc1)c1ccc(N=Nc2ccc([N+](=O)[O-])cc2)cc1	0
OB(O)c1ccc2cc(O)ccc2c1	0
CCCCl	0
NC1CCCCC1N	1
C=[N+](O)CCCCCCCCCCCCC	1
CC(CCO)CCO	0
O=CCCCC=O	1
CCOC(=O)C1C(C)CCCC1(C)C	1
CC(C)NC(C)C	1
CCCCCCCCC=CCCCCCCCCCCC(N)=O	0
C[Si](Cl)(Cl)CCCCl	1
CC(=O)Nc1ccc(NC(=O)c2cc3ccccc3c(N=Nc3cc(C(N)=O)ccc3Cl)c2O)cc1	0
O=Cc1ccc(F)cc1	0
CCCCCCOCCO	1
CCCCCCCCN(C)C	1
CC(O)CN(CC(C)O)C(=O)CCCCC(=O)N(CC(C)O)CC(C)O	0
CCC(C)Oc1c(OC)cc(C=O)cc1OC	0
CCCCCCCC[Sn](SCC(=O)OCC(CC)CCCC)(SCC(=O)OCC(CC)CCCC)SCC(=O)OCC(CC)CCCC	1
CC(C)(C)N(Sc1nc2ccccc2s1)Sc1nc2ccccc2s1	0
C=CCOC(=O)C1C(C)CCCC1(C)C	1

CCCCCCCCC=CCCCCCCCCNC(=O)CCCCCCCCCCCCCCC	0
CCCC(=O)OCc1ccccc1	0
CCOCOC1CCCCCCCCCC1	1
NC(=O)CCl	0
O=C(CCl)c1ccc(Cl)cc1Cl	1
O=[N+]([O-])c1cc(Cl)c(OC(F)(F)C(F)C(F)(F)F)cc1Cl	0
O=C1CCC2COC1O2	0
OCc1cncs1	0
C=CCOC(=O)C(C)(C)OC(=O)c1cc([N+](=O)[O-])ccc1Cl	0
CC(CC=O)CC(C)(C)C	1
O=C1OCCN1CCCO	0
Cc1ccc(Cl)c(Cl)c1	0
CCCCNC(=O)OCC#Cl	0
COP(=S)(Cl)OC	1
Clc1ccc(CNC2CCCC2)cc1	0
c1ccc(-c2ccc(-c3ccccc3)cc2)cc1	0
CCCCCCCCCCCCCCCCCOC(=O)C(CC)CCCC	1
Nc1nc(=O)[nH]cc1F	0
ClC=C(Cl)Cl	1
CCCCCCCCCCCCCCCC(=O)OC(C)C	0
CC(C)(C)N	1
C[Si](C)(O[Si](C)(c1ccccc1)c1ccccc1)O[Si](C)(c1ccccc1)c1ccccc1	0
COc1ccccc1N/N=C(\C(C)=O)C(=O)Nc1ccc2[nH]c(=O)[nH]c2c1	0
COc1ccc(C(=O)Nc2ccccc2)cc1[N+](=O)[O-]	0
Cc1cccc(C)c1OP(=O)(Oc1cccc(OP(=O)(Oc2c(C)cccc2C)Oc2c(C)cccc2C)c1)Oc1c(C)cccc1C	0
CC1OCC(c2ccccc2)O1	0
COCCCOc1cc(CC(CC([N-][N+]#N)C2CC(C(C)C)C(=O)O2)C(C)C)ccc1OC	0
COc1cc(S(=O)(=O)O)c(C)cc1NC(=O)CC(C)=O	0
CC(=O)C1CC=C(C)C1(C)C	1
O=C(Nc1cccc([N+](=O)[O-])c1)c1cc2ccccc2cc1O	0
CC(C)OC(C)C	1
CC(NC(=O)Cl)C1CCCCC1	0
Cn1c(=O)c2[nH]cnc2n(C)c1=O	0
CC(C)CCC(C)Nc1ccc(NC(C)CCC(C)C)cc1	0
CC(CCl)CBr	0
Cc1c(N)cccc1Cl	1
CCOC(=O)CN(CC(=O)OCC)C(=O)Oc1c(C)c(C(=O)OC2C(C(C)(C)C)CC(C)CC2C(C)(C)C)c2nc(-c3ccc(C(C	0
CCOC(=O)C(C)OC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]	0
C=CC(=O)OCCCOCC(COCCCOC(=O)C=C)OCCCOC(=O)C=C	0
CCCCOC(=O)c1ccccc1C(=O)OCCCC	0
CCCC(C)=NO	0
CC(C)(C)C1=CC(=Cc2ccccc2)C=C(C(C)(C)C)C1=O	0
CCC(C)CCCOC(=O)CCc1cc(-n2nc3ccccc3n2)c(O)c(C(C)(C)C)c1	0
CO[Si](C)(C)OC	0
CCCCCCCCCCCCCc1ccc(OP(=S)(S)Oc2ccc(CCCCCCCCCCCCC)cc2)cc1	0

CC(=O)/C(=N\Nc1ccc(-c2ccc(N/N=C(\C(C)=O)C(=O)Nc3ccc(C)cc3)c(Cl)c2)cc1Cl)C(=O)Nc1ccc(C)cc1	0
COc1ccc(NC(=O)/C(=N/Nc2ccc(-c3ccc(N/N=C(\C(C)=O)C(=O)Nc4ccc(OC)cc4)c(Cl)c3)cc2Cl)C(C)=O)	0
CCO	0
CCCCOC(=O)c1ccc(C(=O)OCCCC)cc1	0
O=c1c2ccccc2[nH]c2cc3c(=O)c4ccccc4[nH]c3cc12	0
COc1ccc(OC)cc1	0
CCOC(CCl)OCC	0
CCCC(CC)COC(=O)CCc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1	0
CCc1ccc(C2OC3COC(c4ccc(CC)cc4)OC3C(C(O)CO)O2)cc1	0
CC(C)Cl	0
CC(C)=CCCC(C)=CCOC(=O)Cc1ccccc1	0
O=c1c2cc(Cl)ccc2[nH]c2cc3c(=O)c4cc(Cl)ccc4[nH]c3cc12	0
N#CN	0
CC1(C)CCCC2(C)C1CCC1(C)OCCC12	0
CCCCCCCCCCCCCC	1
CCCCCCCCCC	1
CCCCCCCCCCCCCCCC(=O)OCC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C	1
CCCCCCCCN1CCCC1=O	1
O=S(=O)(O)CCN(CCO)CCO	0
COc1ccccc1NC(=O)/C(=N/Nc1ccc(-c2ccc(N/N=C(\C(C)=O)C(=O)Nc3ccccc3OC)c(Cl)c2)cc1Cl)C(C)=	0
CC(=O)/C(=N\Nc1cc(Cl)c(-c2cc(Cl)c(N/N=C(\C(C)=O)C(=O)Nc3ccc(C)cc3C)cc2Cl)cc1Cl)C(=O)Nc1cc	0
CC(C)C1=CC2=CCC3C(C)(C(=O)OCC(CO)(CO)CO)CCCC3(C)C2CC1	0
CC(=O)/C(=N\Nc1ccc(-c2ccc(N/N=C(\C(C)=O)C(=O)Nc3ccccc3)c(Cl)c2)cc1Cl)C(=O)Nc1ccccc1	0