

Ce1ee(C)ec2ee3e2(c2)[C@H]([C@@H](O)[C@H](O)[C@H](O)NCC)3ee1C
Ce1necnl CSC[C@H](C)OC(=O)lceeeel
C[C@H](C)CCCCC1n1nec2ee3(C)ee2e1=O
Cn1eene1[C@H](O)CN1nec2[nH]e(C)=O[O-]ee12
COC(=O)CC1CC(NC(=O)N2ceecOC)ee2C1
COC(=O)[C@H]1CN(C(=O)N)C[C@@H]2C[C@@H](C)=O[O-]CC2[C@H]1C
CC(=O)[C@H](NC(NC(=O)N)lceee(C)C)lceee1
C1ee3e[C@H](C#N)k2ee2e(C)N2nec2ee(F)nn2n1
C1nmmCC2CC2k1e1e[n-]e[O-]n-]e1=O
Ce1ee(C#N)ee1COlceec(C#N)=Oe(C)C1
C[C@H]1CCC[C@H]1(C)C1nec2ee(F)k2e(=O)[n-]1
C[C@H]1NC(=O)C[C@H]1e1necOC[C@H]2CCN(C)C2mo1
CCleee3(CCN(C)=O)ee2ee2N)ee1
Ce1ee(N)k(-e2n)[nH]k(Ce3en[n-]e[O-]n2)ee1
N#CC1necelC1=Ce2ee(F)k2COC1
Ce1ee(-e2neC3CC3)k(-e3ceee3)j[n-]2e1
CC[C@H](C)OC[C@H]1NCCe2e(-e3ee4ee4e3)eece21
COC(=O)[C@H](C)C1e2e3e3e3e2e(=O)[n-]1m(C)k(-O)n3C
C[C@H](O)C[N]([H+])CC[C@H](e2nm2C2ceee(C)k2)C1
CC[C@H](N)C1(O)C[NH+]C(C)=O(N)ee2e(Br)ee2C1C1
FC(F)Oee2[nH]k3e2e1)CCCC3)CCCC
e1ee2ee(-e3m)[nH]j3ee2e1
[NH3+]C[C@H]1C[C@H]1e1eeOC(=O)N2CC(C)=O)CC2ee1
COle1(O)eeee1-e1ee2e1e1[C@H]1C[C@H](O)C[NH2+]CC2
CO[C@H]1CC2nec3(C)C(NC)k(C)k2ee3e2C1
Ce1ee3e(Cn2m3C3ee3e3e3e2e)O
C1nec(NC(=O)N)C[C@H](O)C(C=O)O)2e2ee212
CCN(C(=O)OC1e3ee1C)C(=O)[C@H]1CC1(F)F
Ce1ee(Ce2m(C)H)3CCOC3)nm2ee(C)n1
N#C[C@H]1CCC[C@H]1e2ee(-e3m)[n-]j3)2nec1
CNC[C@H](NC(=O)N)lenn(-e2ee2e)k(C)C(=O)O-]
O=C1CC2ee1ee(-e3ee)1n2C1COC(CO)C1)C2
CCC1CN2ee(-e3ee)OC3)k(C)N)2)CC1
CC(=O)[C@H]1CCe2ee3e(C)k(C)k3e21
Felceee(-e2noe(C=C)ee3nec[n-]j3)ee1
CO[C@H](C)CCC(=O)Nn1e(C)ee1-e1ee2ee2e2e1
Ce1nec(C[C@H](C)C)nm2ee2CN2CC[C@H](F)C2m1
O=C1CC(Cn2m3e2CC[C@H]2[C@H](CO)[C@H]2)CC3)C1
N[C@H]1C[C@H]2[NH2+](N)C(=O)C(C)F[C@H](F)C(F)F)C[C@H]2[C@H]1O
C[C@H](NS(C)=O)k1ee2ee3e3e2[nH]1)OCC(=O)N3
COC(=O)k1ee(C)ee2ee(C(=O)N3e3nec3)j[nH]e12
COCC(=O)N1eece(-e2nm)C[C@H]3CCCN3)C2m2e1
C[C@H]1C1eenn1n1e1e(C)Oe2ee2e2m1
Ce1ee3(O)k2[nH]k3e3e1e2C1eece(F)k1-3
COleee(C[NH3+])ee2ee(CO)k3ee3e3e2e1
Ce1ee(-e2n)[n-]k(C)ee3e3e(C)k3)2e2(=O)n1C
Ce1ee(-e2ee)CCC(=O)O-]n2nec2ee(F)nm2)ee1
O=C(N)C[C@H]1CCS(=O)O)C1)Oe1ee(F)ee1O
Cn1e(C=C)ee2ee(Ne3nec)k2)knelC1
Cn1nec(C=C)ee2ee3ene3nec1)ee1CC1
N[C@H]1CCC[C@H]1n1e(C)O2(C)OCCCCC2)nm1
C[C@H]1C[C@H]1C[C@H]1n1nec1CC(=O)k2ee2e2C)n1
CC[C@H](C)C[C@H](C)C1e1e(-e2nc3ee3e2e2)m1
C[C@H](C)C1e1e(-e2ee3[nH]e)O)N)k3e2n1n)N(C)C(C)CCO
C[C@H]1C[C@H]1(C)O)CC1N)H+)C(=O)N1e1(Br)ee1C#N
Ce1ee(C)k(S=O)O-]N)C(=O)[C@H](CO)k(C)C1
CC(=O)k1ee(NC(=O)N)2ee2e(C)C)C)C1
CC(=O)[C@H]1CN(C(=O)N)k2ee2(F)ee2e2)C[C@H]1C
N#CC1ee(O)ee(Ne2e(C#N)ee2e2C#N)ee1
CCleee3(NC(=O)N)C2m2n1n)H)2e1
N1ee(F)ee1OC(=O)C1=C=C=C=C=C1
C=C1)C[C@H]2[C@H]3[C@H]4[C@H]5[C@H]6[C@H]7[C@H]8[C@H]9[C@H]10[C@H]11[C@H]12[C@H]13[C@H]14[C@H]15[C@H]16[C@H]17[C@H]18[C@H]19[C@H]20[C@H]21[C@H]22[C@H]23[C@H]24[C@H]25[C@H]26[C@H]27[C@H]28[C@H]29[C@H]30[C@H]31[C@H]32[C@H]33[C@H]34[C@H]35[C@H]36[C@H]37[C@H]38[C@H]39[C@H]40[C@H]41[C@H]42[C@H]43[C@H]44[C@H]45[C@H]46[C@H]47[C@H]48[C@H]49[C@H]50[C@H]51[C@H]52[C@H]53[C@H]54[C@H]55[C@H]56[C@H]57[C@H]58[C@H]59[C@H]60[C@H]61[C@H]62[C@H]63[C@H]64[C@H]65[C@H]66[C@H]67[C@H]68[C@H]69[C@H]70[C@H]71[C@H]72[C@H]73[C@H]74[C@H]75[C@H]76[C@H]77[C@H]78[C@H]79[C@H]80[C@H]81[C@H]82[C@H]83[C@H]84[C@H]85[C@H]86[C@H]87[C@H]88[C@H]89[C@H]90[C@H]91[C@H]92[C@H]93[C@H]94[C@H]95[C@H]96[C@H]97[C@H]98[C@H]99[C@H]100

CC[C@H](C1Nnc1-e1eeFkce1C#N)(=O)[O-]
CC(C)[C@H](C)[C@H](NC(=O)OCC(F)F)C@H(F)F)C(F)C(=O)[O-]
CC(C)[NH3+]C(=O)Nc1cc1c(C2C9N9CCCC2)nm1
CCc1[n]nc1C(=O)NC1=[NH+]N(C)C(=O)C1
CC(C)[C@H](C(=O)C1c(C)[NH2]c2c1m1m2c(C(=O)[O-])c1C1CC1
Cc1ee2ee2Cc3ccc3C#N)nc2e1F
O=C1CC[C@H](n2cc[C@H](B3CCCC[C@H]3)O)nm2)C1
Cc1ee2C(nc-n2ccc3ccc(Br)3c2=O)n1
CC(C)C(O)C(=O)N[C@H](CC1Nnc1CC2CCCC2)C1CO(C)C(=O)[O-]
CC(C)C(=O)N[C@H](C)[C@H](C1nc1c2cmm(C)2C(=O)[O-])nm1
C[C@H](H)S[C@H](C2ccc2[NH2+])C@H(H)1e1ccc1
CC(C)C(=O)N1CCN(C)C@H(O)COC[C@H](N)C2CCCC2)C1(O)C1
C=Cn1e1ccc1-e1en(C)C[C@H](H)2CCOC2)nm1
Cc1ee2ee2C(Cn3cmm3)cc2e1
CC(C)C1c1c(C)nc1[n-]e1=O)ccc(F)k1C
COC(C)CNC(=O)Oe1ccc(C(F)F)Fk1C1C(=O)OJC
C[C@H](H)C2nc2-c3ccc(Cn3)1[n-]e2(C)C1C
CC(C)C[C@H](C)N@H(=H)C1C1mm(C)C@H(H)2NC(=O)CNC2=O)c1C
CC(C)CC1e1c-2ccc2COC2COC2)nm1)O(C)N(=O)
COC[C@H](NH2+)=1c1ccc(Cnec1C(N)=O)1mm1[n-]1
CCOC(=O)[C@H](C)O)N1C(=O)Nc1ccc(O)C1
CC(C)1nc(Cn2mm2)[C@H](2)(C)C2(C)C1eo1
Cc1e1[n-]c1m1e1-e1n1[n-]c1n2cmm2)1
C[C@H](H)NC(=O)N(C)C(=O)[C@H](O)CCOC1c1ccc(C)cc1
NC(=O)1cc1(O-)=1cc1c(C)3(O)C(C)C[C@H](NH3+)C1)C3)cc2e1
Cc1ee2ee2nc-e3c(C)1cc(C)nc3=O)cc1e2
CC1(C)CC(=O)[C@H](O)c2cc(e-c3mm[n-]n3)cc2)C1
CC1(C)CNC(=O)NCCN2COC2)C1(O)N-]C1=O
Cc1ee2e2(e1)Cc1e-2[nH]e2cc(C)cc1e2
Cc1ee2NC(=O)N(C)C[C@H](2)C[C@H](O)C1N@H(=H)2(C)F)1
e1mm(C2CCCC2)C1COC1CC[NH2+]CC1
Cc1mm(CCCC2CCCC2)C1[NH2+][C@H](H)CCCC[C@H]1N
C[C@H](H)1ccc1n1nnc1-2ccc2F)nm1
e1ee2e2(c-3mm[n-]n3)1)COC2
COC(=O)N(C)C[C@H](C)1mm1C1ccc(O)c1
N#Cc1ccc1-e1nc2e2[nH]1)C(C)C[C@H](2)C(N)=O
N#Cc1ccc(F)2cc(C)N-]S[NH-](O)=O)cc1e2
COc1ccc(F)cc1-e1c1mm1[C@H](H)CCC[C@H](H)O
C[C@H](H)CCOCC1n1Ncc2e2(C)C1cc2e1=O
CC(C)C[C@H](n1e-N(C)=O)[C@H]2C(C)C[C@H](3)C3)2)mm1(C)C(C)C(C)C
O=C(O-)[C@H](C)N@H(=H)C1(O)CCc2ccc2)C(=O)N1
CCOC(=O)[C@H](H)S[C@H](C2ccc2[N]C@H(H)1e1ccc1
O=e1[n-]e-n2ccc3cc(C)ccc3e2=O)nc1F
NC(=O)[C@H](H)CCC2ccc3(Br)C1ccc3nc21
Cn1eccc1S1nmm1[C@H](H)CC2nc2n1
CCCC1(C=O)Nc2mm2)[C@H](H)C[C@H](2)CCC2(F)F)CC1
C[C@H](H)C[NH+]C(C)C1Nc1cc2e1[n-]1)C[C@H](H)CCCC[C@H](H)1C2
O=C1CCN(C2n[n-]c(C)C@H)3C4CCCCn2)C1
C[C@H](H)C(C)C(C)C[C@H](O)1e1cc1c(C)N=O)c1
Cc1ee2C(c2)h1[C@H](H)Nc1ccc3cc2e1
C[C@H](H)C(F)N@H(=H)C1(O)Nc1ccc2ccc2e1[C@H](H)CCOCC1
N[C@H](H)CCCC[C@H](C)C(=O)Nc2ccc3e2C)CCC3=O)C1
Cc1ee2C(c=C)C2ccc(C)N=O)nm1
Cc1eenc-2e2m(C)C[C@H](O)C3ccc(C)cc3)nm2)nm1
CCCCe1nc-2ccc(C)cc2)C(=O)2ccc1e2
CCNc1ee2s(C)C(=O)N3CCC[C@H](H)4[C@H](H)4)cc2e1
Cc1ncc(C=C)2ccc3nec(N)3c2)C1C1
C[C@H](N-]S(N)=O)O)c1ee2cc(C#N)C(=O)[O-]e2o1
C[C@H](O)C(=O)N(C)C1mm(C)C2C(C)C(=O)CC2)nm1
Cc1ee2Nnc1C=C1ncc2ccc2n1
Cc1eecc2cc(C3ccc(N)3)cc1e2
CC(C)Oe1ccc1O(C)N(C)C[C@H](H)CCCS1(=O)=O
C[C@H](H)CCN(C2em(C)C)H)CCCC[C@H](3)C(N)nm2)C[C@H](H)CO
CCC1=NO[C@H](C)CNC1=O)2ccc2C1
O=C(O-)[C@H](H)CC(=O)[N@H(=H)C]C[C@H](H)2C2ccc2)C(=O)N1
C[C@H](C#N)N1C1[NH+]C1(O)C2ccc2)CC1
O=C(C)1mnc-2ccc2e2)1)1)N1C(O)C1
Cc1[n-]c1NC(C)C[C@H](C)Nc1-e1cc(F)k1F
C[C@H](H)C[C@H](O)c2ccc3c2)C[C@H](H)2cc(C)nm2)NH2+]CC3)CCN1
NC(=O)OCCn1cc-2ccc3cc[nH]3c2)nm1
CC(C)[H]C[C@H](H)C1C1(=O)Nc1cc(C)C2)C2)nm1
COc1nec-2nccc3(C#N)cc(F)k3c2=O)nm1
CC1cc1(O-)]mnc1C=C1ncc2m[nH]2n1
CCNc1eence1NC(=O)[C@H](H)CC(=O)C[NH2+]1
C[C@H](H)CC(C)C(=O)2ccc(O-)]c2F)C(N)O1
Cc1ee2CC(C)C[C@H]2NCCC3(C)C)C)ccc32)1
C[C@H](H)CCN1C(=O)COe1ccc2ccc1e2
N#Cc1ccc-2nccc3ccc(C)k3c2=O)c1
CC(C)[C@H](C)C[C@H](N)C1nc1C(=O)N@H(=H)2C[C@H](H)3C(C)C)nm1
Cc1mnc(C2=C3ccc(C)C)C=C)C2)1
O=C(O-)]c1ee2[nH]c1C(=O)[N-]k3=CCNCC3)cc2e1
Cc1e1[C@H](H)O)c2ccc3cc22)nm1[nH]e1=O
Cn1mnc(C)cc1OC1(=O)Nc1cc(C)C2)cc1
CS(=O)=[O]C[C@H](C)C[C@H](H)C1ncc1eccc1NCCC2
CC1ccc-2ncc(C)C(=O)N(C)C[C@H](H)C)C)C)C)nm2)cc1
C[C@H](H)C[C@H](C)C(=O)O)N(C)C2ccc3e(=O)N(H)cc3c2)C1
Cc1ee2(O-)]n-]e1-n2nc(C)cc2-2ccc2)O-]1
CCN1CC(C)C[C@H](H)C[C@H](O)C)S1mnc-2ccc(C)nm2)1
O=C1C=C(C)C2ccc(F)2)CN1
Cc1ee2CNC(=O)N@H(=H)2CCNCC2CC3)cc1
COc1ccc-2ncc(C)C)C3cc[nH]3)nm2)1
Cc1e1(O-)]ccc1-1nnc(C)cc2ccc2e1=O
COc1e1C)C)C)cc2e3e1n2)C[C@H](H)C(C)C)O)CC3
C=C(C)C1ccc(O)C2ccc(F)2)nm1
O=e1e2cc(B)ccc2em1-e1cc(F)nm1
CC(C)C(C)C(=O)Cn1mnc(C)C[C@H](H)C[C@H](H)2CCCCO2)1
C[N-]S(=O)=[O]Cn1mnc(C)C(=O)N[C@H](C)C1ccc(C)cc1

Ce1neen1[C@@H]1CCCN(C[C@H]CO)O[C@H]2CCC[C@H]2[NH3+]C1
O=C1CN(CCN2ccc[nH]3c2)CCO1
C[C@]([O])c1ccc[n1]c1ccc(C#N)n1
C=C1cenc2nen-c3ccc(OC)c3c2
COC(=O)c1cc-c2ccc(C)cc2n1C(=O)[C@H]1COCCO1
O=C1CN1CC=CC1=O)N(C=O)Ne1ccc-c2ccc2cc1
COC1nc(CNC(=O)C2=C(C)C(=O)CC2)nol
C1c(C)ccc1N(C)=O)C1nme(CCN)[H+][C]C(C)[H]C(O)C1C
C1c[nH]C(C)[H]C(NC(=O)C)[C@H]2[C]C[C@H]2[C]C[C@H]2C1
C[C@H]1CN(C)[C@H]C(=O)[N][H+][2C][C@H]3CC[C@H]3CN3C2C1
COc1ccc1-n1ccc(CCO(=O)CC(C)C)nm1
CC[C@H]C1[C@H]C(O)C1c1ccc(C)cc1
O=C(NC[C@H]1CC[C@H]1F)C1O[C@H]1CS(=O)=O)C1[H]1O
C1cc2[nH]jcc(C3=CCNC3)c2cc1C
CC1ccc(C(O)N(-c2ccc3ccc(F)cc3)n1
CN1CCC2(C)1CC(=O)c1cc(O)cc1O[C@H]1[C]C(C)[H]O(C)1O2
C[C@H]c1nc2(c-COCC2)[nH]1c1ccc1
O=C(NC)C1en(-c2cc(Br)ccc2F)nm1)OCCF
Ne1ccc(-c2ccc2/C=C/c2ccc(F)cc2)n1
COC(=O)[C@H]C1ccc1N(C)=O)n1cc1Cn1
Ne1ccc1-c1[nH]2ccc(N)c12
C[N][H+][C]C(C)C(C)C(=O)Ne1ccc2c1NCCC2
Ce1ccc(C@H]2N[C]C@H]1)c3ccc(C)cc3S[C@H]2C)cc1
CC1cmm(C)[C@]2(O)CC3c3mcc2c1
CN1ccc(F)cc1N(C=O)[C]C1[C]C[C@H]C(O)C1[H]1C
CN1ccc(F)cc1N(C)C(C)C(O)1c2c1
CS1ccc(NC(=O)N2C(=O)N1C(=O)[C@H]F)C(C)[H]2O)C1
CCC(C)C1c1nc2C2cc(C)[nH]2)no1
C[C@H]1n1nc2(c1C1C1)C(=O)c1ccc1-2(C)F(F)F
COCC(C)C1N(C)Nme1N(C)N(=O)k2n[n]-k2C2n1
COC(=O)c1cc(F)2ccc(CO)[C@H]C(C)N(C)C1[nH]2c2c1
COC(=O)C1(NC(=O)N2CC[C@H]3CNC(=O)C[C@H]3)C2)CC1
O=c1c2ccc3c2[nH]1[C@H]1CCOCC1CN3
C1ccc(-c2cc(N)S(C)(=O)no)2n1
N(C=O)OCC1nme1[C@@H]1(O)CC(C)C@H]1C
O=c1c2(C)kccc2enn1C[C@H]1COCCO1
CO1ccc(Ne2n(C)C)ccc2c1C
COC(=O)[N][H+][C]C(H)C1c1nc(C)[C@H]2CC[C@H]C(C)C[C@H]2C)nm1
CO1cc2n(C)[H]3[C@H]C1[C]C[C@H]3C3C3)cc2c1N(C)C(O)
C/C=C/C1c1cc(NH)k2[nH]jcc2c1c1cmm1
CO1ccc2[nH]jcc(C3=CC1NH2+JCC3)k2c1
CC[C@H]C(C=O)C1c1nc(-c2ccc(C3)C3)en2)no1
C1ccc(COC)[C@H]C(O)S(C)2c2C1Cn2C1C
C[C@]([NH3+])C(S)[C@H]C(O)C[C@]([O])c1ccc1(F)F(C)F(C)O([O-])
N#Cc1ccc(F)F(C)OCC1C)nm1
C1ccc2(cc3cc(C)SC4=[NH+][C]N4)cc3)2n1
Ne1ccc1C(=O)N1C[C@H]1N(C)C2C2[C]C@H]N(C)1
c1ccc(C2=C3c3cc(c3)CC3C4)CC2c1
N(C)=O)N(C)C=C1nc(-c2ccc(N)k2)no1
CC[C@H]1CC[C@H]C1(O)N)N(H)1c1ccc1C(N)O
C1ccc(-c2ncc(C)[H]C(C)N(C)N)O)2nm1
N(C=O)c1ccc1N(C)2cc(=O)cc2C1C1
C[C@H]C(C)N(=O)nm1cc1-c1ccc(C#N)c1
N#Cc1ccc1-c1ccc2[nH]2c1O
CC[C@H]C(NC(=O)c1nnc(C)[C@H]2CC[C@H]O)CC2c1C
CO1ccc(N(C)2(C(=O)N)CC2)S(C)C(=O)O)nH]1
C[C@H]C(C)N(C=O)CC1nmm1C1ccc(C)N1
CC[C@H]1[C]C(C)[H]N2c1C[C]C2[C]2[C]C[C@H]4[C]C[C@H]C(C4)C2)C3C1
N#Cc1ccc2c2c3c(C)cc(C)k3)cc2
COC(=O)[C@H]S(C)[C@H]O(C)C(C)C[C@]([O])C(O)c1F)ccc1F
CC(C)C(O)C(=O)c1nc(C)C(C)[H]2CC[C]C[C@]2(C)C1[NH3+]nm1
CO1ccc(-n2n3c(c2-c2ccc(C)2)C(=O)CC3)cc1
CO1ccc2nm(C[C@H]C)3c3m(C)k3(=O)k2c1[O-]
C[C@H]O(C)[C@H]CO)O1ccc(C#N)k1c1ccc(C)C(C)cc1
N#Cc1ccc(-n2ccc3cc(C)ccc3c2)O)nc1
C1nme(N)1-c1nc(-c2ccc2CC)nm1
CO1ccc2c(O)n(-c3nm[n]-)j3ccc2c1
Ce1ccc2c3c(m1)2[C]C@H]1CC[C]C[C@H]31
C=C1c1ccc1N(C)C1ccc1C=C
C[C@H]C(NC(=O)C)1ncc(C)[C@H]2[C]C2C2)1
CCC1ccc(OC(=O)N)[C@H]COC2nm[nH]2)cc1
C1ccc(F)nc1-c1ccc2(O)ccc2s1
C1ccc(=O)ccc(C)[H]O)c2ccc2C(C)C)[nH]1
CN1CC2ccc3ccc(F)cc3n2[C@H]F(C)1
[NH3+][C]c1ccc(-c2[nH]3ccc3c2C2=CCNCC2)k1
CN(C)en[C@H]2COCC[C@H]2C)nm1c1ccc1
C[C@H]1[C]C@H]1(C#N)C(=O)N[C]C@H]1CCCC(C)C1
CO1ccc2n3c(c1)2[C]C@H]C(C)C)CC3
C1ncc1-c1nmm1CCOCC1CC(=O)C1
Ce1ccc2cc(C)3(O)CC[C]C@H]N(C)3[nH]12
CC(C)C)ccc(OC)[C@H]O)C(C)[H]N2c2nm[nH]2)cc1
C1ccc(N)C[C@]2(O)C1[C]C[C@H]C(C)C)C2)1
F(C)F1nccc1-c1nH]c(C2CCC2)n1
Ce1ccc2(O)M3c2c1)[C@H]C(NH3+)C(C)C(C)3
CN1c(-n2me(C)2CC[N]-)S(C)C(=O)no)2ccc21
C[C@H]C(C(=O)N)CC[C@H]2[C]C@H]O)C(C)[H]C(C)[H]2C1N(C)C
C1nmm(C)[H]C2c2ccc2c1CN1C[C]C@H]O)C(C)C@H]1C
CO1ccc2[nH]3c2c1C1C1C[C@]([C]N)CC3
CC(=O)N(C)O)N(C)O)N(C)O)C(C)C
Ce1ccc(-n2cc(C)3c(Br)ccc2c2)O)c1
C1nmm(C[C@H]C(N)C)C(C)C1O)C1)CCCCO1=O
CC[C@H]1[C]C@H]C(C)C1[H+][C]1c1ccc1CCSC1CO1
CC1c1cc(C)kccc2c3nc12C=CC1C
CN1nme1S(C)en(C)C1[C]C@H]2CCCO2)nm1
C1cc2[nH]jcc(C3=CCNC3)c2cc1F
Ne1ccc(O)1c(NC(=O)C)[C@H]2[C]3CCC[C]C@H]3)2n1
COC(C)C(C)N(C)O)N(C)[C]C1ccc1

CcO1ccc(-c2noc([C@H](CF)NC(C)=O)n2)c1
Cc1ccc2c(C)k([C@H]3CCCC3=O)n1H]2c1
CC[C@H](H)C(C)=O)N1CC[C@H](H)C2mm2CCSC(C)(C)C1
N#C[C@H](H)OC(=O)eloen1)elccc(O)1
CC(C)ccc2(cen2+2cccen2)c1
CO1ccc(C)cc1[C@H](CO)Oelccc(O)el(C)1
Cloncel1Cn1cc(CCN2CC(O)2)mm1
O=C(N=C)C=leccc1N[C@H](H)CC[C@H](O)
Clccc2[nH]3c12[C@H](H)OC1ccc(O)C3
N#C1c1(O)kenc1O[C@H](H)1CC[C@H](H)2C[C@H](H)2CC1
CC1c(C)ccc2(-c3m(C)nc3F)ccc2c1C1
CCO[C@H](H)CC(C#N)Cn1cc([C@]2(C)CCCC(C)(C)O2)mm1
CC[C@H](H)1CC[C@H](C@)1(O)1e1ccc(C#N)k(N)1
CC(=O)C1c1(C)H]2ccc3ccc3c12
C=C(C)C1c1(-c2ccc(C=O)[O-]2)2m1H1
CO1ccc(C)cc1/C=C/1c1ccc(C)2en1
Nc1mH]2ccc2c1C1=CCNCC1
C[C@H](c1m1n1)N(C)C(=O)O1ccc(Br)cc1
N#C1ccc(-n2ccc(-O)1)H]1cc12en1
CC1ccc(Cn2mnc2C=C(O)C2C)2o1
CC(C)Cn1cc(CCN2ccc(F)2)mm1
CCO1c1en1N(C)=O[C@H](H)NH2+|CC[C@H](H)C
O=C1CC=C(C)2ccc(C)2FCC1
Clccc1Nen1(-c1n1n-1c([C@H](C)OC(C)C)1
O[C@H](H)CC1CC1)1c1cc(CN2ccc2)mm1H1
CC[N@H+](C)1cc1(C)C@H]2[C@H](H)OC2(C)C)mm1|C[C@H]1CCOC1
C[C@H](H)1CCOC1)1n1ccc2ccc(Cl)2c1=O
Clccc1SCC[C@H]2CCCC2)ccc1O-1
C[C@H](H)1C=C(C)ccc(C)1=O)C(F)2c1C=C(O)1
CO(C=O)1c1([C@H](H)S[C@H](NH2+)|C@H](c3[nH]C)C(C)C(=O)OC)c3C[C@H](C)S)2c1C
CO(C=O)1CC(C)2cc3c(O)1-ccc3o2c1
CO(C=O)[C@H](H)N(C)=O)N1C[C@H](H)NH3+|CC(F)(F)C(C)(C)C
CC[C@H](H)S[C@H](H)2ccc2[NH2+]|C@H]1ccc1
CC[C@H](H)1CC=C(2ncc([C@H](C)O)3CC3)2)CC1
C=C(O)OC1mm1(C)H]2CCNCC2(C)C1COC1=C(O)
Clmm1(-c2nccc2C)1c1=O)2ccc1C1c12
N1ccc(N)1C(O)CNC(=O)O[C@H](H)1C[C@H]F
CC1=CNC(=O)N[C@H](H)C(C)C(C)C)SCCO1
C=CN1ccc(N)C[C@H](H)O)2ccc2)c1F
Clccc(-c2cc(C)ccc2O)1n1C[C@H]2CCCCO2)1
C[C@]1(N)2mnc2-2ccc2CCCF)CO(C=O)C1
Clccc(C=C)2ccc(N)C)2c12)2mH]2c1
Clccc1Se2nccc2(C)F)F)cc1
Clccc(C@H)(O)C[C@H](H)S[C@H](H)2[C@H](H)OC(C)O)C@H]2C)C(O)O)1-cc1
C[C@H](H)1CC[C@H](H)CC(=O)N(C)C(C)O)CCN(C)C)N1
O=C(NCC[C@H]1CCCO)1N)N(H+)1CC12CCN2
CO1ccc2ncc(-c3ccc4n3CCCC4)mm1(C)C(C)CC3)2c1
N1ccc(Cn2mnc3n-1)ccc3c2)cc1
CN=[S](C)C(=O)1ccc1(-c1n1C)ccc1=O
CC(C)C(O)C1[C@H](H)1c1cc([C@H]2CCCCN2)1n-1
CCN(C=O)C[C@H](H)C[C@H](H)N2ccc3ccc3C1
Clccc1cc1(C)O)N[C@H](H)C(C)F)C1
C[C@H](H)1C[C@H](H)C(C)O)O)C1
FC(F)F)1ccc2cc3c(nc2c1)CC(C)1CC1C3
N#C1ccc(N)1c1cc(N)1ncc1N
CO1ccc(-n2mnc(C)2CCCC(=O)N2CC2)ccc1
Clccc(C[C@H](C)O)C[C@H](H)C)OCC(N)O)C)N1
CCN(C=O)1ccc2ncc([C@H](C)O)CC1
c1ccc2ncc(-c3ccc4ccc4c3)cc2c1
O1ccc(C=C)2m1n-1)2cc1
N1ccc(C2c(C)mm2C)CCCC2)cc1
C=C[NH2+](c1ccc2c(C)O)NCC(N)O)cc2c1
CO(C=O)1ccc2cc([C@H](C)O)CC[C@H](H)3CCO3)1nH]2cc1F
N1ccc(-c2nccc3ccc3)cc2=O)1
F1ccc(-c2ncc(Cn3ccc3)1n)2)1
O=C(N)C(O)CO)1ccc2ccc(O)2]2m1H1
Clccc(C)cc1O)C1nmm1C
C[C@H](H)C(C)O)C[C@H](H)C1c1(-c2ccc(O)N2)1n-1
CC(C)C(C)C)C1nmm1(-c1ccc(CN)C)C1
CC(C)C(C)C@H](H)CO)NH2+|ccc(C#N)CC2)1
O=C(O)1ccc2cc(CN3C)CC3)cc12
CC[C@H](H)CO1ccc2c1(C=O)C1(CCN(C)(C)C)CC1)O2
O=C(C[C@H](H)COCCN1)NCC1ccc1
C[C@H](H)O)C(O)N1C[C@H](H)N)CC[C@H](H)C#N
CO(C[C@H](H)CO)1nmm1(-c1ccc(O)CC(C)C)1
C[C@H](H)1c2ccc(-c3ccc3C#N)2CCN1C
C=C1ccc1(-c1m1n1(C)C@H](H)C#N)S(C)C(O)=O)1
Clccc2ccc(C@H)(N)3ccc3)cc2c1
CC[C@H](H)C)CC1c1ccc2c(C)C)cc2]2m1H1
O=C(C)ccc1N1C[C@H](H)C(F)F)C1
Clccc2[nH]3c12[C@H](H)C[C@H](H)C3=O
Clccc2(-c3ccc(F)cc3)CCOC2)mm1C
C=C(O)C[C@H](H)C[C@H](H)C)CCN1C(O)N1c1cc(C)ccc1C1
Clccc(NC(O)2)ccc(C#N)2C)1C1
Clccc(O)cc(C=C)CC2)CC1
CO(C@H)(C)C(O)N1c1m1nH]2c1C[C@H](H)2CCNCC2)1
Clccc2ncc3c(cc2c1)C[C@H](H)O)C[C@H](H)C3

COC(=O)C@H(C)C1[n]j[e]-c2e(C)cc(C)[n]-j2=O)n1
COCCc1nmm-c2ccc2CO(C)C@H]2C[C@H](C)C2)c1COO
CC[C@H](C)[C@H](N)C(=O)O1cc(F)cc(C)1=C(O)OC
CC(=O)Nc1[n]-j[e]c2ccc1[O-]
CC(C)C@H](OCC(=O)[O-])j1c1cc2ccc3c2[n]H1)C(=O)OC3
CC(=O)C@H(C)COC(=O)C@H]N(C)C1cc(F)cc1
CC(=O)C@H(C)CSCc1ncc2(C)C(C)CC2n1
O=C(O)C[C@H]N]CCCN1C(=O)OCC(F)F(C)C@H](F)C(F)F
CC(C)C(C)C1nc(CN)C(O)C(F)F]nH1
C[C@H](O)C(C)C(F)F]cc(C)N)n1
C1cc(C)cc1-n2nnc(C(=O)[O-])j2C(C)C(C)O)c1
CCC[N@H+]C(=O)N(C)C@H](C)C1cccs1)C1CC(C)C(C)C1
C1cc(-c2ccc(C)C@H](C)O)cc2)C1ccn1
CC1(C)C(C)C=C2enon2)C1(C)C
[NH3+][C]c1cc1cc(NC(=O)c2ccc2)c1
[NH3+][C]c1cc1cc(-c2nm[C@H]3C[C@H]3F)n2)c1
COCC(=O)N@H+]C(C)C(C)C1nmm1[C@H]1C@H]N(C)C@H](C)C(C)O)C1
CC(C)[N@H+]C(C)C(F)C1c2ccc(OCC(=O)N)C2nH1
CC1nnc(-2nnc(C)C2)j2)N)CC
CC(C)C[C@H](NH3+)[j]c1nc1-c2cc(N)no2)no1
CC(C)O(C)C@H]1C)C(C)C@H]1c1ccccc1=O
C1cc(C)cc(NC(=O)C)H2CC(=O)N2)n1
O=C(O)C1nmm(C)C@H]2CCO2)c1-c1ccccc1
CC1nmm(-c2ccc(C)F)C2)c1CNH2+][C]CCCC1
C1cc1cc2CC2)n1C1CCCC1
C[C@H](O)C(=O)O1c1nmm1C[C@H]1C[C@H](F)C1
O(C)C@H]1CCCC[C@H](O)C@H]1NH2+][C]c1ccccc2ccn12
CC[NH2+][C]c1ccccc2cc(CN(C(=O)C)F)F)cc12
C1nc(C)cc(Nc2(O)N)nc1H2=O)n1
CC(=O)OC1c1ccccc2C)cc1C
CC(C)C@H](CO)O1cc1cc(C)C(N)j1c1ccccc1
NCC(C)C@H](O)1cc1-c2ccc3c2(C)CN3]n[n]-j1
CCCC@H](C)C[NH2+][C@H](C)C1nmm1C1CCCCO1
CCC(=O)Nc1ccccc2(=O)n-kt[C@H]3C[C@H]3F)nc12
C[C@H](C(=O)N)C1nHnHj1C(C)C@H]23CC2)C@H]23)Cn1
C1ccccc1Nc1c[nH]j2ccc12
C[C@H](NH2+)[C]C@H]1C[C@H](C)N(O)1c1ccccc1
C[C@H]1CC(C)C(C)N1C(=O)N(=O)C(C)C(C)C
COCC(=O)C1C(C)C(O)C(C)C@H]N]H3+][C(=O)[O-]C(C)C)CCOCC1
CCC(=O)1ccccc(Nc2(F)ccccc2)N)C1
NCC(=O)CN(C)CC1en(-c2cc(F)B)ccc2)C)n1
c1nmm[C@H]2CC(C)C@H]23CC1NH2+][C]c1CCN(C)C1)C1CC1
C1nc1N)ccc1-c1ccc1F
Nc1ccccc2cc(Cc3(C)C)cc3)C)cc2c1
C1=C(Nc2ccc2)Nc2ccc2)CC1
C1c(F)ccc1-c1(F)ccc1C(=O)[O-]
CCCC1nmm(Cc2ccc(C)C(C)C)2)c1C[C@H](C)O
CC(=O)1c(C)nc(O)j2c(C)N)1C
N#C(C)C@H]1CN(C2C(C)C@H]3CC(C)C@H]2)CCO1
COCC(=O)C@H](C)C(N)C(=O)N1c1ncc1C#N
CCN1CCCC1cc3cc(F)O-]ccc3o2)CC1
CON1CC2[nH]j3c(F)cc(C)C)cc2C1
C[C@H](N)C1CCCC1)1cc1ccc2cc(C)C)2s1
CC(C)C@H](O)C@H]1)C(C)C(=O)C(C)C1)1cc1cc(C)cc1)C@H](O)C(=O)OC
COCC(=O)C@H](C)C1[nH]j2c(F)cc(C(=O)[O-])jccc2c1C
CC(C)C(N)S[C@H](C)C1ccccc2c1)OCCO2)C@H](C)O
CC(C)C(N)C(=O)C@H](C)N)C@H]1CCO1)C(C)C
C1cc1cc2(O)C(C)C1CC2)cc1C#N
C1cc(C)C(=O)O(C)C@H]CN2CC(F)C2)ccc1C1
N#C(C)C@H](O)1ccccc1)1ccccc1=O)n1
O=C(O)COC1nmm1C1CC2)CCCC21
O=C(C1nHnHj(-c2ccen2)n)C@H]1C[C@H]1F
CNc1ccccc1Nc2ncc3n[n]-j2)cc3e1
CS(=O)C1ncc1ccccc2n1
CC(C)C@H](C)C(C)COC1en(Cc2ccc2)2)n1
C=C1ccccc2-CC[C@H](O)C)C2)c1C
C[C@H]1CC(C)C@H]N2C(=O)NCCN2=O)C[C@H]1C
C1nc1cc(C)C=C2c(C)mm(C)C2)C]nH1
Cn1ccc1-c1cc2c1ccc3cc3)2]nH1
C[C@H](H)OCC(C)C1nmm1C1nccccc1=O
NC1=[NH+]2ccc(C3=CC(=O)CC3)cc2C1
Nc1cc(-c2n[n]-j[C@H]3CNCCO3)n2)nc1
C1nc1cc(N)cc(-c2ncc3n2CCN3)n1
CC(C)C@H](O)C(=O)Nc1cc(C)C@H]N)CC(=O)[O-]
O1ccccc1C=C2ccc(C)mm2)cc1
CC1CCCC(N=O)NCC[NH+]C)C)CC1
Cn1cc(C)C(=O)1cc1O[C]C[NH2+][C@H]1C(C)C@H]O)C1
C[C@H](O)1ccccc(O)C(C)C)S2c(C)ccc2C)cc(O)C1
C[C@H](N)C1=[NH+]CCN1C1en(C=C)C2CC2)n1
C[C@H]1CC[N@H+]C(=O)C(=O)N(=O)C(C)C@H]1C#N
C[S@H](O)CCC(=O)N(C)C@H]1C[C@H]1ccccc(O)1)cc1
C[NH+]C(C)C=C1nHn-j[C2=CCCCC2)C1
CO[C@H](C)C(=O)Nc1nc(C)C)1)C1CC1
CC(C)C@H](O)C@H]N)Nc1cc(C)C(=O)1cc(O)1
C1nHn-j(N)1-c1nc2[n]n-2cc1
C1nmm(CN2CCC(=O)CC2)1CO(C)C@H](C)C(C)C
Cn1nc(C#N)1-c1nHnHj[C@H](H)F)CC2C2)2)n1
C[NH+]C)C1ccccc(Nc2cc(F)cc2)cc1
CO1cc(CCN)cc2cc(CCN(C)C(=O)[O-])jcc12
COCC(=O)C1nc(-c2nm[n]2)2]n-1c1C
COCC(=O)C@H](O)C(C)C@H]1(O)CC2CC(C)C@H](C)C21
CCC(C)C@H](C)C(=O)N(C)C@H](C)C1ccccc(O)1
O1ccccc1C=C2ccc3ncc2)2)n1
CC(=O)N]S(=O)C1ccccc1cc1
C=C=C1ccccc1C=C2c(N)ccc2F)cc1
C1ccccc2ncc(-c3cc(C)C(C)C)3)nc(C)2c1
C=C1ccccc1)1c1ncc(C)C)O1

Cc1nnn[C@H](O)c2ccc(C)cc2c1COC1C[NH+]C)C1
Coc1ccc2cnn[C@H]3C[NH2+]C3c(=O)c12
CCCC(=O)N[S](=O)(=O)c1ccc2nnc12
Cc1cc(-n2cc(C)C)cc2c#Nnm1
CC(C@@)(C)C(O)C@H(C)lcc(CNC(=O)CC#N)nm1
CC(C@H)C(C)N(C)C[C@H](C)Clc1n[C@H](C)COC(=O)C(C)Cm1
Cc1cc(C)C(=O)C2ccc2C#Nc1
O[C@H](C)Sc1ccc(C(F)(F)F)l1cc1
CC(=O)[C@H]1COC(=O)[C@H]1O[C]C[C@H]1CCCC[NH2+]1
CS(=O)(=O)NC1cc2ccc(F)F)2c1
CC[N@@H-](C)C(=O)NC(C)C[C@H](H)CCOC2CCC2C1
CC(=O)N[C@H]1CCN(C(=O)C2cmm(C)2)C1
CCOC(=O)[C@H](C)COc1ccc2nc[nH]2c1C
Cc1cmm(CC(=O)OC2(C)CCC(=O)C2)c1
CC(C)N1CC/C=C/c2ccc(C(=O)O)k2c1
Cc1cc(-e2ccc2F)nc(C(=O)C[C@H](C)C2CC2)m1
CC(=O)c1ccc(C)nc(O)c1c#N
CC(C)O(C)Cn1cc[C@H]2CCC(=O)C2m1
Cc1cc(O)cc(C#N)Nc1C(=O)C@H]1[C]C@H]1C
C[C@H](C)C(C)CNC(=O)N1C2CC[NH+]C1)C2
C[NH2+]C1c1(-e2ccc2nmm1)[C@H]1CCOC1=O
C=C1cc(Cc#N)nc1N[C]C@H]1O)c1cc1c
Cc1ccc(O)C(=O)N2CC[C@H](H)[NH3+]1[C]C@H]1O)C2c1
CCCC[C@H](NH2+)C1c1m[C]C@H]2CCCOC2m1
COC(=O)[C@H]1[C]C[C@H]1N(C)O[C]2[NH3+]C1)C2
Nc1Nc1Nc1OCC2(C)C2)C3)1
CC[N@@H-](C)CCF1c1n[C]C@H]2CCCNC2)1
COC(=O)C@H]1CO)nm1ncc(C[NH2-])[C@H]2CSC[C@H]2(C)C1C
O=C1CCN[C@H]2c2cc(C)CSC3)1n-1)2c1
Coc1ncc1C=C/c1ccc(C)C)1n-1)2c1
CC(C@H]1Cn1m(C)C1Cn1m(C#N)1)N(C)C
Oe1ccc(23CC(C)C2)CC3)1
Oe1ccc(F)C1[C]C(C)C(C)C(=O)N1ccc(C)C1c1C
Cc1cc(C2c1m(C)2)mm1C
CN(Ce1n-1)C=C(C)C(C)1)CC1CCC1
CC(C)c1ccc1-c1n[n]n-1
CO[C@H]1CCC[C@H]1n1ncc2ccc(C)2c1=O
COC(=O)N[C]C(C)C1n-1)C[C@H]1C(C)C(C)C1
C#Nc1Nc1Nc1N(C)C[C@H]1C2cmm[nH]2)1
C[C@H](NH3+)CCN1mcc(-c2[n-]ncc2)1
Cc1mnn(-e2ccc2CO[C@H]1C)C[NH+]1C)C1COC[C@H]1CCCCO1
C[C@H]1[C]C@H]1CN[C]C@H]1)S(=O)(=O)C(F)F)F)C1
CCO[C@H]1C(C)C(=O)N1ccc2mm2c1
Cc1ccc(C)cc2ccc(C)C3)2c1
C=C(F)1cc2ccc(B)F)2c1=O)1n-1)CCC
Coc1cc2c(C3-CNCC3)c[nH]2c1
CC[C@H](O)C(=O)Nc1ccc1cc1
O=C1CC[C@H]1O)C(=O)C2(F)CCC2)CO1
Nc1ccc(O)n-1c1C[C@H]1C1C[C]C@H]1O)C1
C[C]C@H]1c1n[C]C(C)C[C@H]1O)C2)mm[nH]1)C(C)C)O
Coc1ncc(N2C[C@H]1CCC[C]C@H]2C2)CO1
C[C@H]1CN(C)O)C@H]2[C]C@H]1C)C@H]2[C]C@H]3)CC(C)C@H]1)C)O
Cc1cc(F)nc1N(C)O)C@H]1CCCCO1
Nc1m(-c2cno2)cc1C1CCCC1
CC(=O)N1Cc2ccc(C)cc(C)3)nc2C1
CC[C@H](C)CC(=O)Nc1ccc2cc1n[nH]2cc1C
C[C@H]1CCC[C]C@H]1O)C2)C(C)C@H]1O)C@H]2O)C1
CN1ncc(COC(=O)K2(NH3+)CCOCC2)1
CC1ccc(Ce2m[n]n-1)2c1
CNc1cc(F)nc1C=C(c2cncn2)CCC1
C[C@H]1CC=C(C2c1n(C)C(C)C)O)2)CC1
CC(C)OC(=O)c1ccc(-c2ncc1-n-1)2c1
Cc1ccc2cc(Cc3c1m(C)3)2c1F
Cc1ncc(C)C(=O)N[C]C@H]2[C]C@H]1C)C2)1
COC1ccc(NC(=O)Nc2ccc(C)cc2)cc1
COC(=O)c1cc(-e2ccc(O)C2)2m1-c1nnc(C)S1
C/C(=C)C1ene(C)C1e1cccc1
Oe1ccc(C@H]2N[C]C@H]1C3ccc(O)CC3)S(C)C@H]2)C2c1
CN(c1cc2c1)CCN2)C1)CCCC[C]C@H]1O
Nc1ncc(Nc2ncc(F)2)O-1)1
CC[C@H]1(C)C[C]C@H]1C(=O)NC(=O)NH2)CC1(C)SC)CC1
CCC(C)C(C)C(N)C(=O)O)C1ccc1F
COC(=O)C1Cc2ncc(NCCC(C)C)O)1n-1)2c1
CC(C)H(N)CC(=O)c1cc1n[nH]2)O)F)1
Cc1mnn[C@H]2CC[C]C@H]1H2O)C(=O)c2ccc12
O=C(O)1ccc(S(C)C@H]1CO)C[C@H]2CCO)cc1O-1
Cc1cc(C2c1ncc(C)C@H]3CCSC3)2)C1
Cc1ccc(NC(=O)O)C@H]2CCCOC2)1
Cc1ccc(C#N)C(N)C(C)C(=O)1
CCNC(=O)c1ccc(-c2mnn2)C1[C]C@H]1C)C2)1
Coc1ncc(C=C/c2ccc3ccc2)2c1
COC(=O)C(C)C1ncc(F)[C@H]1C)C(C)C(N)1
Cc1ncc(N)cc(O)1c1n[C]C@H]1C(=O)C2CC2)C(C)C1
Cc1ccc2ncc(-c3nccc3)nc21
CNCC1nmm1C1C(C)C)CC1C
Cc1ncc(-c2ncc3[nH]2)CCC3=O)1
NCCN(CO)c1ccc2c1CC[NH2-]1[C]C@H]2)1ncc(C)1
CC(C)C@H]1C)C@H]1C(=O)O)1ncc2ccc(N)C)cc2c1=O
CC(C)C[NH2+]C(=O)NC(=O)CC(C)1CCOC1
COC(=O)NC(C)C(=O)Nc1ccc(C#N)1
CC[C@H]1(C)C(C)C@H]1)1ncc1(C)C2)2m1
Cc1ccc(-e2ccc3ncc3)2c1
N#CC1ncc(F)C@H]1O)2ccc(CO)1n2)1
C[C@H]1[C]C@H]1F)C[NH3+]1[C]C@H]1CNC(=O)N-1)C1=O
C=C(C)N1ccc(-e2cc(C)C)2c1
CC(O)C@H]1C)C@H]1C1ncc1C1ccc(C)1
C[C@H](O)C(C)C1n-1)C=C2C[NH2+]C2m1

CCCOe1ecel[C@H](CO)Oe2e(F)eecc2CCjcl
[C@H](O)(CCF)C[C@H](O)COC12CC2CC2
CC1(S=O)=O)N2CC[C@H](H)2c2nfnj2n2CC1
CC[C@H](C)C(C)C=C(O)[N@H+][C@H](O)(CF)C1
CS(=O)=O)CNC(=O)N1CCC[C@H](F)C1
elence-c2enc2-c2en[n]-j2e1
COC(=O)C[C@H](C)C1[n]m2m2(C)=C(C)C1
C(C)Cn1eeC=C2Cn1C[C@H](H)C[C@H](H)C2C2m1
NC1=C[C@H](NH2+)[C]2c2eC1m2n2COC1
CC(C)CN(C)[C@H](C)Cn1ene2nfnHj2e1
COlence[C@H]2[C@H](C)=O)OC2C2m1
[C@H](NH2+)[C@H](C)N(C)=O(O)-[C@H](C)CCCC1-O
CS(=O)=O)[N@H+][C]2CC[C@H](C)CCN=O
[C@H](e1nfnHj)N(C)C(=O)C(C)C
C[C@H]1C[C@H](n2nec2eecc1)k3e2=O)C1
[C@H](C)C1mnm1CC=C(F)NCCF
CC(C)C1e1cCCn1m1[C@H](H)CC[C@H](H)O
[C@H](H)NCC[C@H](O)C(O)N(C)C[C@H](H)C(C)C1
COC(=O)C[C@H](C)C1NCC2eecc(C=O)N(C)CCN)ec21
Cce1ec(C)C)ne[O-]c1C8N
Cce1ec(C=C)N[H]2CC2CC2(c=O)n-1
Cce1nec2eecc[C@H](H)CCN3)jn2j1
CC(=O)[C@H](CO)N1mne[C@H](H)2CC(C)C2m1
[C@H](H)C[C]C2e2n3c[nH]2)CC3C1
CC[C@H](C)[C@H](O)C1eC1mnm1CC1eeC(O)Cec1
CC[C@H](O)CNC1mnm1C1enfnHj1
Cce1nec2eecc2COC2CC2ec1N
F[C@H](H)CC[C@H](H)CN[C@H](H)2CC[C@H](H)CC[C@H](H)2C1
COC(=O)N(C)=O)NH2+][C]1CC(C)N(C)
[C@H](O)CNC12c2eecc[O-]k3e2)CC1
COlececc1Nn1e(C)ce1-c1eecc1
[C@H](e1necno1)[C@H](O)C1eece1N
Cce1nec1Nc1-c1eeC(F)N1
CCC(=O)N(C)CC(=O)N(C)=O)C(C)C(C)C
N#CC1eecc2e1)CCN2
O=C[C@H](C)CCN(C)[C@H](O)(CF)F
CC(C)Cn1ec[C@H]2CC2C(C)C1[C@H]2OCC#Nn1
COleceNj1-c2eecc2C#Nn1
C[C@H](C)C1e2eeC(O)Cce2e1C#N
CCN1eecc1Nc1eneC1e(N)N1
C=Cee1ec(C)H(O)2e2Cm2N)ec1
CC(C)C(C)=O)1e1ec(F)F)C1=O
CO[C@H](e1cCmnm1-c1eecc(C)C)C(C)C
N#CC1eece1N[C@H](H)C[C@H](H)C(C=O)NCC1
CCC[N@H+][C]C[C@H](N)C(O)C[C@H](H)C(C)C#N(C)[C@H]C
O=C(F)C1nfn-j1-c2nec[n]-j2n1
O[C@H](H)CSC1CCCC1)C1(O)CCCC1
CS[C@H](C)C(C)=C2eecc(N)C2)C1
Cce1nm-c2eecc(C)ee2e2nec21
Cce1eecc1-c1eeC(N)=O)ee1O
O=C(O)Cce1ec[nH]1[C@H](H)CC[C@H](O)C1
CCCC[C@H](C)C(C)C(O)C(O)N(C)C[C@H](O)C(C)C
NC(=O)[C@H](C)[C@H](N)2e2e[nH]2)C1
CC1eeC=C(C)C@H(H)C(C)N=O)no1
CC(C)C[C@H](H)CCCC[C@H](O)[C@H](H)C(C)N=O
CS(=O)=O)[N@H+][C]C(C)C1C1eeC[C]n-jn1
C=Ceecc[C@H](O)CC(F)F)F)C1
Cce1eeC(Oe2eefnHj)2ee1F
Cce1eeC[C@H](C)N(C)=O)N2CC2m1CCOC(=O)[NH+][C]C
COC(=O)[C@H](NH3+)[C]1nfn-j1[C@H]2CC2CC2C2m1
CO[C@H](H)1c2e[nH]3ceefnHj)ee4e23[C@H]1OC
CC(C)F)CNC(=O)N1CCCC1
CC(=O)N1eecc(S=O)=O)[N-][C@H](H)C(O)ec1
CC(C)Sce1nec[C@H]2CC2C(N)=[NH+][C]2n1
[C@H](H)N)eecc[C@H](H)F)C#N)ec1
FC(F)eeCOe2e[nH]2)ec1
COCC(=O)[N@H+][C]C1ee1nec(C)CC2C2m1
[C@H](H)C[C]C[C@H](NH3+)[C]C(O)N(C)C[C@H]2C(O)O)C1
Cce1ee-c2nec(C)C(C)C[nH]2)ec1
C=C=C1e1cCmnm1C[C@H](H)N(C)=O(O)-[C]C(C)C
Cce1en(N)Oe2e(F)ee2e2N)en1
CC(F)C(C)1e1-c2eecc(N)C2m1n-1
C(C)=C(C)C1eecc1Nc1en2eecc2n1
CC(C)C[C@H](C)C1ee2ee(O)ee2[nH]1
O=C(O)C[C@H](C)CC[NH2+][C]C@H][C@H]2C[C@H](H)C2
CC[C@H](C)C1e1nec(S=O)=O)N(C)C1C1C1
CC[N@H+][C]CC1=O)N(C)[C@H]2C[C@H](H)C(C)C1-O
C[NH2+][C]eeC(C=C)2nec(C)ec2Cm1
Cce1nfn-j1[C@H](O)C[C@H](CO)CN2CC2C2=O)N1
CNC(=O)N(C)CC1e1nfn-j1(C)C(O)N1e1cC1
[C@H](H+)[C]C[C@H](C)C(O)N(C)C[C@H]2C[C@H]3C(C)C2C1
CC(C)C[C@H](C)N1mnm1C[C]C@H(H+)[C]C(C)N=O
N#CC1=C(NC(=O)N2eecc2)OCC1
CC(C)C[C@H](C)C1mnm1[C@H](H)C(C)=O(O)-[C]1n1
Cce1en-c2nec2e2nec1N)eecc1
CCSC1(c2nec(C3=CCOC3)jn2)CC1
C=C[NH2+][C]eecc1N(C)=O)C[C@H](H)C[C@H](O)C1
Cce1nec(C=C)2eCmoeC1
CC[C@H](H)C(C)=O)N1nec(C)=O(O)-[C]ee1-c1eecc1
CC(=O)Nc1ee2[nH]1e-c3eecc1)k3e2e1
C(C)C(O)C1mnm1[C]C[C]C1-CCCCO1
C=C(C)C1e1nec[C@H](H)2C2C2C2m1n-1
[C@H](C)C(O)C2moe2)CC[C@H](H)[NH3+]
COC(=O)C1e1-c2nec(C)2[n]-je1CC
Cce1nm(C2C2)C1C1eecc1
Cce1nec1-c1eeC(N)O)1e1
CC[C@H](C)C1n1ec(C)C1-c1eecc1C1

CC1(C)C[C@H](O)CC[C@H]1(O)C(C)C@H(O)CC#N
Ce1e(C)ceecNC(=O)COC1CC1
Ce1nc2c2nc[C@@H](C)C(C)C(C)Csc2n1
CCN1CC2c2nc[C@@H](O)C3CCCC3)2)C1
CO(C)C@H(C)CCOC(=O)N(C)C@H(C)C@H(C)C(C)C@H1O
C[C@H]1CO[C@H]1CN2C[C@@H](C)C@H(C)C(=O)O]1C@H(C)C2C1
CCe1e(C2C2)ml-1c1e1e(C)C)k1
CCC(C)C@H]1[C@H]1[NH2]-j1e1nc2e(n-1)C1(=O)CC2
COe1nc(O)nc(NC2CC2)C@H]2COC[C@H]2Cn1
CC(C)C@H]1(Ne1nc2e2nc12)(C)N(=O)C1CC1
[CH2]CCN(C)C@H(C)C1e1e(O-)]n1-1)S(N)(=O)=O
CC(=O)N[C@H](N)C@H]1C[C@H]1CCCC(=O)O]1C1C)C)C
CCe1e(C)C(=O)nH]2e1e2e(F)k(C)1e12
Ce1nc1(C=C)C@H(C)C2CCN(C)C2)1
CCO(C)C@H(C)C1c1nm1[C@@H](C)C1e1c1m1
C[C@H](O)C(=O)N[C]C@H(C)S(NH-)](=O)=O(C)F(F)F
C=Ne1e(C)C(=O)N(=O)COCFnm1
C[C@H]1CCC(=O)C[C@@H]1(C)C@H(O)C(=O)2F[C]C@H]2(C)CO(C)1
O=C(Ne1e(F)k(C)1e1)l1e1m1
CC(C)C@H(O)C)CNC(=O)1e1e1
Ce1e1e(C)ce1N1C(=O)1e1e1
CC(C)CO)C1n1n-1[C@@H](C)FCC(=O)O]1-1
Ce1e1(C)N(C)C@H(C)COCFnm1C1e1s1
CNC(=O)C1n1e(C)C1CC[NH2]-]C@H]1CC[C]C@H(C)C1
Ce1e1e2nc2e(O)n2)1
Ce1e2e(C)O3nc(C)1n2]c1e1e1
C=C(N)CCCC[C@H](C)C1e1e1
CCCe1nc(C=C)2m(C)C2)C1
CCCC1CC(C)OCe2sm2C(C)C)C1
COC[C]C@H]1(NH3+)1C(=O)O]C@H]1CCCC(=O)C(C)C)C1
Ce1e2nH]e1e2C1O1e1e1
CC(C)C@H]1[NH2]+]C@H]1CCC[C]C@H]1C(=O)OC)1nc(C)N1
CO(C)C@H(C)COC(=O)C1n1m(C)C1=C(N)CCC(C)C)F
C[C@H]1(C2CC2)C[C@H]1[NH2]+]e1e1m1
CCe1nc(N)ce1-2nc2e2OC)n1
COe1e(F)2e23e(nH)2e1]1C@H]1C(C)C)C)C3
CO(C)C(=O)C@H]2[NH2]+]C[C@H]1C[C@H]3C[C@H]3)CC1
CCN(C)C1e1e1e(C)C@H]1C@H(C)N(C)C@H(C)C(=O)O]1-1
CCCe1nm(C2e2e2C)1C1(=O)OC
CCC(C)C@H]1e1nc(C)C=C)B(m-1)N1CCCC1
Ne1e1(NC(=O)N]1C(=O)C)F(F)F)nm1
O=1e2nc2e2c1m1[C@H]1C[C@H]1(O)C1
CCN1CCC(C)C@H]1e2nc(C)C@H]1(O)C(NH-)]C(C)nm2)C1
Ce1e1e1(C)1N1C(=O)C[C]C@H]1(C)C)O
Ne1e1nc(N)C@H]2CCCS(=O)C2)C1
C[NH2]+]C@H]1CCC(C)C@H]1Oe1e1e2nc2e1
Ce1nc(C)N1e2nc2(O-)]e2C1
COe1e1e1(NC(=O)O)CC(=O)N)CC1
CC(C)C@H]1CCN1C(=O)N(C)C@H]1CCOC1
CC(C)C@H]1(N)1m1m1[C@H]1C)C(C)C@H]1C)N
Ce1nc1nc1-1c1nc(C2C[NH2]+)C2)ml
CCN1C[C@H]1C(N)C@H]1+2CC(C)C@H]1(O)CCN(C)C2)C1-O
CC(C)C@H]1C)C@H]1C)N(C)C(=O)N(C)C@H]1(NH3+)1CC(=O)O]1-1
N1C1e1-2nc2e2NC(=O)C(NH3+)1c1
NCC(=O)N(C)1e1e2e(C)1e21
Ce1e1e1(C[NH2]+]2e(C)C2e2-2e2c2)nc1
CC(C)CNC(=O)C2=C(NH3+)1CC2C)COC1
CCCO(C)C@H]1C1e1e1C)nm1[C]C@H]1C@H]2COC[C]C@H]2)1
C/C=C(C)1e1e1CN2CC2)1e1C(C)C
C[C@H]1C@H]1CCNC(=O)C1(N)H+]](C)C@H]1F(S)F(=O)(=O)C)F)F
CC(C)C@H(C)N(=O)C1nc1(C)C@H]2C(C)C@H]2O)1
CC(=O)N(C)C1n1e1e2e2C)1
Ce1e1(COC2C2)nm1[C@H]1C)C)F(F)F)C@H]1F
CCC(=O)C(C)N]1e2e2e(C)C@H]1(C)O)2e1C
COC(=O)CO]C@H]1C1e1e2e2e(C)1e21
C1CC(C)C@H]2C(C)N(H)3]C(C)C@H]3)4COC4)C(C)C@H]2C1
C[C@H]1CO(C)C@H]1C(N)H+]]1e1nc(C)N(N)1
COe1e1e(C=C)2e2e2e(C)C2)C)N1
CC(C)C(C)C@H(C)C)1c1m1[C]C@H]1CCC[NH2]-]1
e1nc2nc(NCC)N(H)3]C(C)C)1
O=C1N]N=C[C@H]1[NH2]+]1c1e1e(C)1
CCn1e1e1(CN(C)N)O)C(=O)CC)N1
CCN(C)C@H(C)CCC[C]C@H]1(C)C)C1e1e1e1
COe1e1e1(C)C@H]1O(C)C)C2(N)C(=O)C2)C@H]1(C)O)1
CC(=O)C@H]1CCC(=O)O]1N1e1nc2e1C1
Ce1e1e1-2c2m2C(C)C@H]2C(C)C@H]2)C1
CCOC(C)C@H]1CC)N(C)N(C)C@H]1CCCC1-O
C=Ce1e1e1N1C@H]1C)C@H]2C(C)C@H]2)1
CN(C)CO(C)COC(=O)N1e1e2e2e2e1
CC(C)CN(C)CO1e1e2e2e2e1nH]1
COe1e1e1C@H]2C(C)F(F)F)C@H]2F)nm1C
CCe1e1e1e1C@H]1O(C)C@H]1C(C)N(H)3]C(C)N(H)3]C(C)1
CCCC(C)C@H]1C)Cn1e1e1C@H]1(NH3+)1e2e2e2)ml
Ce1e1e1C2C2)1e1N1e1(O-)]1
COe1e1(C)C(=O)C2e2e2e(C)2)k(N)1
Ce1e1e1(NC(=O)N2C(C)N(H)3)-C2C)N1
CC(F)F)C1CCN(C)C@H]2C(C)C@H]2C2C2)C1
CC(=O)C@H(C)C@H]1C)C@H]1(C)O)1e1nc(C)1N
CCC(C)C@H]1N(C)O]N(H)3]C(C)C1n1m1-1)C(=O)OC
CC(C)CNC(=O)C@H]1C)C@H]1(N)C1(O)C1
CC(C)C@H(O)CC(=O)N1CCC(C)C@H]1CO)C1-O
CCCC(=O)N1nc(C)1CO(C)C@H]1C)C@H]1(C)C)1
CC(C)Oe1e1e1C@H]1C)S(N)C(C)C)C2C2)1
CCOe1nc(C=C)2e2e(C)N)2)nc1
C[C@H]1CC(C)C)N)1e1e1e1
N(C)C@H]1C(C)C@H]1e1e1e1(O-)]e1
C[C@H]1C(C)C@H]1NCC2e1e1e1e1(Br)2(O)C(C)C)C(C)

COC(=O)C@H(O)CC(C)=O)c1ccc(OC)nc1C
Clc1ccc2c(C@H)C[C@H]C[C@H]([NH2+])4)oc2c1
O=c1c2ccc2cnn1[C@H]1CCC1
CN(C)C1ccc(C=C)c2cc(N)[nH]2=O)c1
Cc1ccc(S(=O)(=O)N)C(=O)CC(F)Fcc1
Nc1ccc(Cl)c2c3ccc2c1C
Clc1ccc2c(C@H)C3CCCC3)sc2c1C1
C[C@H]([N+](=H+))1[C@H]2[C@H]([NH2+])CC2=O)[C@H]1C(C)C1(F)F
CC=Cc1nnc1c1CN(C@H)C[C]C1C
C[C@H]([O]C[C@H]([CO]S)CC(C)=O)[O-]c1ccc(F)cc1F
CNc1ccc(Nc2ccc2C)nc1N
CCN(C)c1ccc(-c2ccc[n-]e2=O)c1
CCc1ccc(O)N(C)C2(C(=O)NC)CC2)nn1
C[C@H]([NH2+])C1mnn1COC(=O)C1CCC1
O=S(=O)([N-]C1ccc(CO)cn1)C1C1
COCC[C@H]C)N(C)C(=O)COC1=CCCC1=O
CC(C)OCC[C@H]([NH3+])e1n[n-]c(C@H)CN(C)C(C)C1
CC1(COC2=C1(O)C=O)CC2C1
CC(C@H)O(C)C1N(C)C[C@H]2COC(=O)C[C@H]2C1
Cn1ncc1SCe2cnc2C1C
COC[C@H]C)OC(=O)N(C)C(=O)c1n[nH]-1
CC[C@H]1[C@H]C)CC[N+](=H)1C(=O)c1ccc(F)cc1
CC1mnn(-c2ccc2C)C[C@H]2[C@H]([O]C)C1CSC[C@H]([O]C)O
Cc1ccc(C=C)C2C1N(C)C[C]C1n1H1=O
N#Cc1ccc1-n1c(C)CCN1
C[C@H]1CC[N+](=H+)1C2ccc(O)N)2]CCN1
CC[C@H]1S[C@H]([O]C)C(F)F)N(C)C@H]1C(F)F)F
CC(=O)C@H]C)N1mnn1C1ccc[nH]1
Cc1mnn(CCC[C@H]N(C)C(=O)N)1c1-c1ccc(CO)1
COc1ccc(OC)CCN(C=O)OCC[C@H]C)N(C)C(C)C1
O=C(C)C([H]C)COC1)N(C)C@H]O)COC1C1
COC(=O)C(C)N(C)C(=O)N(C)C[C@H]C)C@H]C)N
O[C@H]([CCCC1O)C1)C@H]1CC(F)F)C@H]1F
COC[C@H]C)C1c1ccc2en[n-]e2c1C)C)C
CC(C)CN(C)C1mnn1C=C(C)F)C1
Cn1ncc(-n2cc2n2)C[C@H]C)C)C3c1
C[C@H]1CCN(C)C2cnc2C1C=O)C1
CC1C(C)C(C)Nc2ccc(O)c[nH]2]C1
Fc1ccc(F)C1C=C=CC1
CC[C@H]C)C1c1nnc2n1H]c1F)12[C@H]C)CN
CC[C@H]N(C)C(=O)C1ccc1C1COCOC1
CC(C)C@H]C)N(C)C(=O)N(N)H+)]CC1=O)CC[C@H]C)N
C=N(C)N(H+)c1ccc2cnc2en1]C1nccc1N
C[C@H]C)N(C)C1ccc(C)C1
CC(C)C1ncc(C)N1C1ccc1
Nc1n[nH]N(C)=O)c1ncc(O)CC#N
C[C@H]([O]C)C1C1c1ccc1Fcc1
COC(=O)c1ccc(Cc2ccc(C)N)C@H]1)C)CC#N)C3C3)nm2n1
C[C@H]1(N)CCN(C(=O)N)C2ccc2F)C1
CC(C@H)C)C(=O)O)c1ccc(C)Nc1
Cc1ccc(C=C)c2cnn(CO)2)1
CC(C)C)C(=O)C1=CC(C)=O)CC1
CC[C@H]C)C1nnc1C1c1C(=O)N(C)C@H]C)CC#N)C(N)=O
CN(C)C@H]1CCC[C@H]1c1mnn(C=C)C)CCN1
CCN(C)N(H+)C)C(=O)N(C)C1C1C1C1
Cc1ccc(-c2ccc2)nc1C#N
CC(C@H)N(C)C(=O)Nc1ccc1C)C@H]C)O
CC1mnn(C@H]2CC[C@H]2)O)c1[C@H]C)OCC1COC1
CC(=O)O)c1ccc(O)cc(C)O1
C[C@H]C)N(C)C(=O)C@H]1C)C1)C1mnn[n-]1
Cc1ccc(Cl)2n1H]c1-c1ccc(C1n)3cc2c1
F(C)F)C1ncc1C1C1c1ccc1
CC[C@H]C)S(=O)(=O)N(N)H+)C)C@H]1CCNCC(=O)C1
CC(=O)n1ccc1-c1ccc1
Cc1ccc(C(=O)CC2OCC2)cc(C)O1
CCc1[n-]c1[NH2+])C2CCC2)nc1C(F)F)F
C[C@H]C)N(N)CC(C)O)c1ccc(Nc2c[n-]2)c1
C[C@H]1CC(=O)N(C)C@H]1C(=O)N(C)C@H]1C)C@H]1(NH3+)C)C)C
Cc1ccc1-c1ncc2[n-]1)CNC2
O=C1N(C)C(F)F)C(=O)N1C@H]1C)OCC1
C[C@H]1CC[C@H]C)C(=O)O)CC2(C)N(C)=O)CC2)N(C)1
CCO[C@H]C)F)F)N1mnc(C)C1C(=O)N(C)C)N(C)1
C[C@H]12CCC[C@H]1N(C)C[C@H]C)O)CC(=O)O)1)C@H]1C2
CCN(C)=O)c1ncc(C@H]2[C@H]2)S(C)C(=O)O)n1n1
N#C[C@H]1CC[N+](=H+)1C(=O)N(C)C@H]2[C]2)C[C@H]1F
C=C1ccc(F)N1C)OCC[C@H]1C
CN(C)C@H]C)N1mnn(C)C@H]C)C@H]C)O)C1
C[C@H]1C)C@H]1N(N)H+)1C@H]2[C@H]C)C)S(C)C(=O)O)O)CCO1
CCN(C(=O)N)ccc(C)cc1C)C@H]C)C)C)C)N(H3+)
CS(=O)N(C)CC(C)N(C)C1)C@H]1C)C2CCC2
CC(C@H]1)CC[NH2+])N1(C=O)c1ccc[n-]e1=O
CC[C@H]C)C)C@H]1N(H)2+]C@H]1)CCCC=C1)N(C)C(=O)O-]
CC(C)N1C)C@H]C)C@H]1N(C)C(=O)C@H]1N(C)C2CC2)C1
CCc1ncc(NC2)CO)CC2)n1-c1CC
COC(=O)c1nnc1C)C@H]2[C@H]N(C)2c1C)C)C)O
Nc1ccc(-n2ccc(C)N(C)C)N(H3+)n2c1
Cc1mnc(C2=C)C2)O1
Nc1ncc(CO)C(=O)N)C2ccc2n1
CS(=O)N(C)C1C1)CC1)CC2(N)C(O)1C2
COC1=Ce2[nH]3ccc(Cl)c(O)ccc3c2C1
C=C1c1ccc2c1O)C@H]C)C2
O=N(C)C@H]1)C)C)O1)O)C@H]1CNOC1
CCN1ncc1Nc1ccc(C)nc1N1
C[C@H]C)O)C@H]1C)O)C1N(C)C(=O)CC1C1
CNC(=O)C1ncc1-c1ccc(C)nn1C
C[C@H]1CN(C(=O)N)C2ccc(F)cc2)C1=O
Cc1ncc(N2C)C@H]3O)C@H]2[C@H]3)F)cc1F

CN[C@H](COCc1n[nH]e(=O)n1)C1C/C=C/C
O=C1CCC(CO[C@H]2CC[C@H](O)2)CC1
CCOC(=O)NC(=O)N(CCN(C)=O)C1C/C=C/C
O=C1[C@H](NH+)(CCn2nec2CCSc2nec2)C1
COlece(Ce1c1Sc1eece(CO)n1)
Ne1eece[SC](C@H)2CC[C@H](O)2)C1
CCOlece+n2eeceCCC(=O)[O]1c2k1e1OC
CNe1eece(C)e1NC(=O)c1eece1C
C=Cle2eece(C)ee2nec1CCCC
Celeece(C[C@H]2O)C1N[CH+](C)[C@H](C)[C@H]2C)ne1
Ne1nc(N2CCCC[C@H](CF)2)ee1[O-]
Celeece(C=O)N(C)[C@H](CO)SC[C@H](O)CC2CC2)S1
CCOCleence(-e2eece2OC)e1
CCOCn1e(C)[H](C)[NH3+][nec2ee(F)C(Br)ec2e1=O
CCle1e(C)ne(C)N)1C
COlece(COC[C@H](O)CS2eece2nec2)ee1OC
Celeece(C[C@H](C)[C@H](CO)CN2CCCC=O)mo1
Celeece(CO)C1n1e1eece1
O=C(CCN(C)CC1)Celeece(C)ee1
N#C[C@H](OCe1eece1N)(C)[H](O)1eece1
Celeece(C)OC(=O)[C@H]2N)C[C@H]2CO)e1
C[C@H](F)COlecece(F)C[O-]
C[C@H](N)NC(=O)N1C[C@H]2CC[C@H]2(F)C1C(=O)[O-]
CC(=O)[N@H+][C@H](N)(C)OC(F)F[C@H]1C
C[C@H](OC(=O)N)[C@H](C)C1C1)ee1eece1
CCOC(=O)N(CCN(C)=O)N1eece1
COlece1e(C)ne(C)1C#N
CNC(=O)NCC(=O)N(CCF)[C@H]1CCCC1C/C
N#CC1eece1N1C[C@H](N)C[C@H](O)C1
CCO[C@H]1CC[C@H](N)C1NC(=O)O(C)C(F)F
CCN(c1e[O-]eece1-j1=O)[C@H]1CCN1=O
CCNC(=O)N[C@H](H)C[C@H](O)C1eece1
CC(C)CC(=O)N(C)eece1N)S1
O=C(COCe1eece1)ee1eece1
CC(=O)O(C)[C@H](CO)C1eece1C1C(=O)c1N
CC1(NC(=O)N)C2eece2)CC1
CN(CCF)Celeece(-e2eece2nec2)
Celeece(N[C@H](C)C(N)=O)eece1F
CC(C)N(COCC(=O)eece1)CC1
CC(C)[C@H](NH3+)C(=O)C[C@H]1[C@H]2CC[C@H]2[C@H]2C[C@H]2
CCleeece(C[C@H](S)C)[C@H](C)C[C@H](O)C1
C=C(Br)CNC1C(C)CC1)S(C)C(=O)
CCOC(=O)N(C)O(C)C[C@H]1C=C1(C)N1C1
C[C@H]1C[C@H](C)[C@H](O)C2CO(CO)CC2C(=O)O1
Celeece1[N@H+][C@H](C)[O]C[C@H]1C[C@H](O)C1
CCCC[C@H](C)N[CH+](C)C1eece1C1
C[C@H]1CC[C@H]1C[C@H](N)C1C(C)C1
Fe1eece1C1eece1
CN(C)C[C@H](O)C=C1C=C(C)CC=C1C
Ce1[n-]e(N(C)CC(C)C)ne1-eece1
C[C@H](N)CC1S1(=O)[O]C(F)F
[NH3+]CC(C)=O)eece1eece2
CSCCN(C)C1eece2e(C)eece2[nH]1
C[C@H](N)N(e1eece1C)C(=O)[N@H+][C@H]2CC[C@H]2H1
C[C@H](O)CCCC(=O)O[C@H]1C[C@H](C)[C@H](O)C1
O=C(NCCN1C(C)C1)C[C@H]1CC[NH2+][C1
O=C1N=C2eece(O)eece21
CCOC(=O)C1(O)CC(F)F(C)C1
C[C@H](C)C=C1=CC[C@H]1[C@H](O)1O(C)C1CC1
CNe1nc(N2CC[C@H]2)N2eece1F
Celeece(C2(O)COC(C)O)C2)eece1C
N#C[C@H](O)CCN2CCN2)O)CCN(C)C1
Celeece(N)eece1(C)(O)CC2C2)C1
C[C@H]1CC[C@H](O)C[C@H](N)CC2CC2)C1
CCN(CCO)C1eece1C(C)=C(C)C)ne1
CCN(C1n2nec2[C@H](H)C)C2e1[n-]en2)C1
C[C@H](H)C1eece1(-e2eece1)C1n1
CCN(C(=O)C)[H](F)C[C@H](O)C1eece1N
COlecece([NH2+][C@H]2CO)C[C@H](O)2)eece1F
C[C@H]1C[C@H]1C[C@H](N)C(=O)N1eece1N
C[C@H]1(N)C(=O)eece2)C[C@H](O)CC1
C[C@H]1nnc(C[C@H]2CCOC2)C1C(=O)[O-]C1(CO)CC1
C=C1eece2ee(CN)C2c3[e-n-]en3)eece1
CCCN(C)C1eece1[C@H]2CCN(C)[C@H]2N)ne1
CC(C)[C@H]1[C@H](C)C#N[C@H](O)N(C)C[C@H](C)[C@H]1C
COlece2ee(CN)C(C)CC)eece21F
C=Cleeece(NC(=O)O)C(C)F)eece1OC
O=S1(=O)[N@H+](C)[C@H]2NC[C@H](O)C[C@H]3(C)[C@H]2)CC12CC2
CO(C)[C@H](O)C(C)C(=O)eece1
CCOleeece(-e2eece1)C1n2eece1
CCNe1eece(OC(=O)N)[C@H]2C[C@H]2C)eece1
O=C1C[C@H]2C[C@H]3O(C)C[C@H]3[C@H]2C1
C[C@H](NH2+)eece1C(=O)[O-]eece1)C1CC1
Ce1n[nH]e(NC)[C@H]2CCN2)ne1(C)F)F
Celeece(F)F)C2eece(CO)2)eece1
O=C(O)C[C@H]1C[C@H](CF)C1[C@H]1C[C@H]2C[C@H]2N)C[C@H]21
C=C(N1CC(C)C)C1)eece1
C=C1eece2(O)C(O)eece2(O)n1C=C=C1
N#Cleece(C2=CC(=O)CC2)eece1
Celeece(C=C)[C@H](C)C(=O)[O-]eece1O
CCCC(C)CCN(C)O)N(C)=O)C1NH2+)CC1C1
C[C@H](O)C(CO)C1)eece1nm1CC[NH3+]
C[C@H]1N[C@H](C)[C@H](F)F[C@H]2C[C@H](O)[O-]
CO[C@H](C)C#N)C1eece1F
C1NH2+)C[C@H]1nnc(COCC(=O)O)C1O)C1C/C
C[C@H](N)CCN1C1)COleeece1F
CNC(=O)[C@H](C)N1nc1CCCC(=O)O)CC#N

C[C@H](NH3+)C[C@H](C)Nc1ccc1OCC1
CCN(C)[C@H](C)CC(=O)N[C@@H](C)[C@H](C)N(C)C1
CC[C@H](C)[C@H](C)OCC[NH+]1CCCC1
CCOC(=O)Nc1ccc(F)cc1
C1ccc(CN[C@@H]2CC[C@H]2CC(=O)O)cc1
C=CS(=O)(=O)N[C@@H](C)[C@H](O)CO[C@@H](C)C(C)CC(=O)O
C(C)(C)CC(=O)N1C[C@H]2C[NH+]1CCN1C[C@H]2C1
[NH3+]C1ccc2cc[nH]c21
C[C@H](NH3+)COc1ccc(C[C@H]2CC[C@H]2O)nm1
C[C@H](F)COC(=O)OCC(F)F(C)O
C[C@H](C)[C@H](C)[C@H](CO)[C@@H](C)O[C@H](C)[C@H](C)C(C)O
CN(C)CC[NH2+][C]1S(=O)(=O)C1ccc1
COC(C)[C@H](C)[C@H](CO)ccc1CC[NH3+]
CCc1nm(C)[C@H](C)[C@H](C)[C@H](C)OCC#N
C=C1C=C(CO)[C@H](C)C(C)C[C@H]2C[NH+]1CC2
CC[C@H](N)C[C@H](C)[C@H](O)[C@H](C)N(C)F(F)F
COC1ccc(C)nm1-c1ccc(F)cc1
C[C@H](CC(=O)O)Nc1ccc2[n-]1CCCC2
CC(F)F(C)C(=O)N(C)O=C1CC1
C[C@H](NH3+)[C@H](C)C1ccc1S(NH)1(O)=O
C1ccc2cc[nH]c21
CC(C)C(=O)CC[C@H](C)N1CCC2(CC)C1
CCN(C)O=N1C1(O)ccc1C1CC1
C[C@H](N)CCN(C)C(=O)OCC(F)F(F)C1
COC(=O)N(C)C1ccc2cc[nH]c21
COC(=O)[C@H](C)C(C)C[C@H](O)Cn1ccc1
C[C@H](NS(=O)=O)[C@H](C)N(C)C(C)C
C[C@H](C)[C@H](C)[NH+]1[C@H]1OCC(C)C(C)C1
CN(C)C1ccc(C)OCC2OCC2nm1C1CC1
COC1ccc(O)[C@H]2C[C@H](NH2+)[C]2c1
C1ccc(C)C(C)O[C@@H]1C1#N
COC(C)C1ccc(S[C@H](C)C(C)O)cc1
C[C@H](O)CC(F)1cnc(C)[C@H]2C(F)Fnm1
CO[C@H]1C[C@H](C)[C@H](C)N(C)C(C)C2C2C1
C[C@H](C)N(C)N(C)C(C)O=N1C[C@H]1CCCCO1
CC(=O)C(C)C(C)C=C1ccc(C)O=C1OCC1
C=C1C=C(N)ccc1n-1
C[C@H](N)C[C@H](C)O(C)C[C@H]1C[C@H](O)C1
C[C@H](F)C[C@H](NH2+)C1ccc1C1C1(O)O
C[C@H](CO)[NH2+][C@H](C)1cnc(C)[C@H]2C(C)O)nm1
C1ccc2cc[nH]c21
CCN(C)[C@H](C)O=C1O[C@H]1(F)C(C)C1
C1ccc1C1(O)O
C[C@H](O)C(N)C(=O)CCN(C)C1[C@H](C)[C@H](C)O
C[NH2+][C@H]1CCCC[C@H](NH)1[C@H]1OCCS1(O)=O
CCCC1(C)N2CC(n3ccc3)C2CC1
CC1ccc2n-2C=O
CC(C)C(C)N[C@H]1CCCC[C@H]1C(C)C
C[C@H](O)C1ccc(O)C[C@H](CO)C(=O)O
C[C@H](C)N1m(C)C(C)O
O=C1ccc2cc[nH]c21
CS1(C)OCC2CCOCC2CC1
C[C@H]1CCN(C)[C@H]2C[C@H](C)C2S1(O)=O
CN(C)O=C(NH+)C1CC1C1(O)C[C@H](N)C(C)C
Nc1ccc(C)N1C[C@H](F)5H(O)C1
CC1ccc(O)C[C@H](C)[C@H](NH3+)CC1
CCCC(=O)N[C@H](CO)[C@H](C)O(O)C1
COC1(C)O=C(N)C=C(S)C(O)OCC1
C[C@H](F)C(C)O=C1ccc1N
C=C1C(S)1(O)C(C)N1m(C)S(=O)C1(O)nm1
CCCC(=O)Nc1ccc(O)cc1
O=C1NC[C@H](C)C=C2ccc(F)S2O1
CO[C@H](C)C(C)O=N1N[C@H](C)C[C@H](N)C1CC1
COC(=O)C1=C(C)C[NH+]1C(C)C(C)C[C@H](N)C1
O=C(O)C[C@H]1C[C@H](C)O(O)C[C@H]1C2C2C[C@H]2+1
C#CCn1ccc1=O
COC(=O)C(C)O(C)OCC(C)C
CCCC(=O)N[C@H]1CC[C@H](C)C(C)C1=O
C[C@H]1OCC(C)C[C@H]1C=C1ccc1
O1ccc(F)C(C)C[C@H](O)C(F)F
CC[NH+]1C1ccc1S(C)O=O
C[C@H](CC)N[C@H]1C1ccc1N
C[C@H](N)C(=O)O[C@H]1C[C@H]2C[NH+]1C[C@H]1F
C[C@H](C)C(O)C(=O)N1C[C@H]2[C@H](C)N(C)C[C@H]2C1
O[C@H]1CCn2nm21
C[C@H]1(F)C[C@H](C)O=N2C[C@H](O)C(N)C2C1
CC=C(C)C1ccc(C)[C@H](C)S(C)CO1
C=C1ccc(C)cc1N[C@H](C)C(C)CO1
C[C@H](NH2+)[C@H]1C1CC1
COC(=O)[C@H]1S[C@H](C)C(C)C[C@H](NH2+)[C@H]1CC(C)C
Nc1ccc(C)C1C(C)O(C)C(C)C1
C[C@H](C)N(N)C[C@H](C)C(=O)C1C1
CC(C)[C@H](O)C[C@H](C)C(=O)N(C)C(C)C(C)C
C(C)C(C)C[C@H](C)O(C)Cn1ccc1
CCN(C)C(C)[C@H](C)1m1n-1
C1ccc(NC(=O)N(C)C)C(C)C1
C1ccc1-c2ccc2[nH]c1
C[C@H](C)O(O)C[C@H](C)[C@H](NH2+)[C@H]1CCO1
CN1ccc(C)O(C)C(C)F(F)F
C[C@H](N)C(N)C[C@H](C)C(C)N(C)C(C)F(F)F
C[C@H](C)CC(C)O(NH+)1CCCC(C)CO(C)C1
C[C@H](C)C(O)C(=O)N1C[C@H](C)[C@H](O)C(C)C1CO
CO[C@H](C)C(N)C1n-1[C@H]2C(C)O)nm1
C1ccc1-c2ccc2C1
C1ccc(NH2+)[C@H]2C[C@H]2C(C)C1n1
[NH3+][C@H](C)O=C1ccc(C)C1
COCC1(O)CC2C(C)CC[NH2+]C2C1

COC1CC[NH+]C(=O)C(C)C@H(C)C(C)O)CC1
CCN(C)=C(C)=C(C)CO)CC1
CCO[C@H](C)C[N]N@H+][C]C(=O)C(C)C(O)C(C)C
CCC[C@H](O)C(=O)N[C@H](C)C@H]CCOC1
Cn1me(C)N)ml
CC[C@H](C)C(N)N@H+][C]C(=O)C(C)C(O)C(C)C
CCC(C)OCc1n[n]-jccCOcn1
NNe1een2ene2el
COe1eeFkeelO
CCO[C@H]C[C@H]C@H]e1ne(CCN[C@H](C)CCO)nnH1
CCS(=O)=O[N@H+]C[C@H](C)C@H]C(=O)OC1
CCn1nce1CCC1CCC1
[O]-j1ee2neoc2el
CC(C)CS(=O)=O[N]-j[C]C@H]COCC(=O)N1
N[C@H]1(C(=O)O)-j)CCOC1
CS(=O)=O(N)CC[C@H]C[C]NH2+][C]1CCC1
C=CS(=O)=O[N]C@H(C)C[C@H]C[C@H](O)C1
CC[C@H](C)C[C@H](O)C(CO)C1CC1C(=O)O
CCO[C@H](C)C(c1m[n]C[C@H]C[C@H](O)C)C1
CCCC(C)C(CO)C1nec1
CC[C@H](C)C[NH3+]C(=O)N[C]C@H]CCOC1
C[NH2+][C@H](C(=O)OC1(C)C(=O)CC1)C@H](C)O
O=C(O)-j1eeFkecn1
C=C1ee1Cne1N(C)CC(C)=O
CC[NH+]1CC(C(=O)O)C2e1C1enn2C)C1
NC(=O)[C@H](NH3+)CCOC(=O)NCC1ee1O
CCN(C)C@H(C)C(C)C(=O)C(C)C(C)C1C1C1
O=C1[C@H]C(C)C(C)N@H+][C]2ee2nec2C1
CC[C@H](O)C(C)Nec1nnc1[C@H]2C[C@H](O)C2e1C
O=C(N)C(F)N[C@H]1C[C@H]C@H]O
CCC(=O)Nec1C(c1e1O)
CC[C@H](O)C(C)C1nnc1(C)C(=O)OC1e1C
CCC[N@H+][C]C#N(C)C(=O)NCC(C)C(=O)O
N[N]-jC(=O)NH2+][C@H]1C-CC1
CCCC[C@H](C)C#N(C)C[C@H](O)C@H]C(C)C
CC[C@H](C)C(c1e1C(=O)OC1nnc1C[C@H](O)C)C#N
C[C@H]1CC[C@H]CCOC(=O)C[C@H](C)CO)O1
C=C1ee1N(C)C(C)CO)C1C
Oe1ee1C(C)C1
CC(C)C[C@H]1CCC1=O
C[C@H](NH2+)[C]e1sm1C(C)C(C)C#N
C[C@H](C)N)O[C@H](C)N)O
C=CCN1ee1C(c1
Cn1ee1C=C[C@H]2CCOC2e1C1C
C=CN1ee1C(c1e1S[C@H]1C(=O)O)C[C@H](C)O
C[NH+]C(C)C1ee1n1C(=O)C1
CN1ee1ee1C1)C1(C(=O)O)-j)CC1
CCS(=O)=O(N)C1CC1)C[C@H](C)C@H]1CCCNC1
Ce1ee1Nec1C=O
COC[C@H](C)C(N)C(=O)N@H+][C]C(C)C(=O)C1
CCN(C)C[C@H](C)C(=O)N1C[C@H](F)C2(C)C1
CCC(C)C(C)C(=O)C[C@H](C)N)CCF
CN1C(=O)CC(=O)N-j)C1=O
CCC[C@H](C)S[C@H](C)C(=O)C[C@H]2C[C@H]C2
#C=C1ee1C(C)O1
N#C[C@H](NH3+)C1ee1ee1
C[C@H](N)C(C)C[C@H]C[C@H]2CC[C]N@H+][C]C(C)C
CC[C]N@H+][C]C(=O)C(=O)C(C)C1(C)C(C)C
C[C@H](O)C1CC1)C[C@H](O)C(C)C@H]1CC[C@H]1CO
CCCC[C@H](C)C(=O)C[C@H]1C(C)C(C)C(=O)
CC1CCCN=C-O)CC1
COe1ee1N@H+][C]C[C@H](O)C(C)C
CC[C@H](C)C[NH2+][C]C(C)C1ee1ee1CO
C[C@H](C)C(C)C(=O)N1C1C[C]C(C)C(F)C1
C[C@H]1CC[C@H](O)C(C)C@H]1C(C)C(C)C(=O)C1
O=C1[N]-jC(=O)C(=O)N1=O
NNe1ee2e1n-jene12
e1nH1ee1Nec1NCC1C
CC(=O)N-j)C[C@H](C)C(N)O
CC(=O)C[C@H]1CC1=O
CS[C@H]1CCN1C(=O)C[C@H]1CN(C)C(C)C@H]1C
CC[C@H]1C[C@H]1NS(C)C(=O)O
CCCC[C@H](NH3+)C(C(=O)OC[C@H](O)C(C)C)=O
C[C@H]1CC[C@H](N)C(S)N(=O)O
CN(C=O)[C@H](C)C(O)C[C@H](C)C@H]C(C)OC(C)C
CC(C)C1ee1Nec1nnc1C1CC1
N#CC[C@H](O)C(C)C@H]1CC2nme21
CCN1ee1C(C)Nec1
Ce1ee1C2C2m(-e2ee1C)2m1
[O]-j1ee1nec1N(C)C[C@H](O)C(C)O1
CO[C@H]1CCCC[C@H]1NH2+][C@H]1C(C)C(N)C1
CO[C@H]1CCC[C@H]1N(C)C(=O)C1
Ce1nec1NCC[C@H](C)C)O)ee1C1
CC[C@H](C)C1ee1ee1N@H+][C]C(C)CO)CO
CC[C@H](C)C(N)C(=O)C1(=N)CC1
COe1ee1CO2C(C)NH3+][C]2en1
C[C@H]1C[C]N@H+][C]2C[C@H](C)C(C)C2(C)C(C)O1
C=C1N=C1nec1nnc1C[C@H](C)C(C)C
O=C1N=C(O)C[C@H]2C[NH2+][C]C@H]12
CC[N@H+][C]C[C@H](C)C1n[n]-jcc[C@H](C)C@H](C)O)N1
COe1ee1N=C-O)C1
CC1nec1C=C-CC1(=O)N(C)S1
CCCN(C=O)1ee1CCC
#C(C)C(C)Oe1ee1n-jn1
#CC(=O)NH+][C]C(O)C(C)C1
CC[C@H]1C(C)C@H]1Nec1C1m1
CO(C)C[C@H](NH3+)C1ee1nec1CCN2C2C2m1

C[C@H](Cn1cccn1)N(C)S(C=O)=O (ZINC00004984177+ZINC000012357651)Gen_1_Mutant_72_66457 Gen_1_Mutant_72_66457 -5
CNCC#Cc1ccc1 (ZINC000008376898 Gen_1_Mutant_72_66457 -5
CO[C@H]1CN[C@H]1O[C@H]1O[C@H]1CCO1 (ZINC000095616493+ZINC000021953350)Gen_1_Mutant_65_491575 Gen_1_Mutant_65_491575 -5
Cc1nc1ccc1c1 (ZINC000015423947 Gen_1_Mutant_65_491575 -5
C[C@H]1O[C@H]1C(=O)N1Cc1ccc1C1 (ZINC000002383503+ZINC00001646614)Gen_1_Mutant_66_575242 Gen_1_Mutant_66_575242 -5
C[C@H](C)OC(=O)N[OH+][CCO][C@H](C)C(=O)[O-] (ZINC00013309775+ZINC000002584543)Gen_1_Mutant_12_732276 Gen_1_Mutant_12_732276 -5
CC(=O)[C@H](C)C[C@H](NH2+)[C@H](C)C(C)C[C@H](C)O(C)C(C)C (ZINC000024717911+ZINC000034195376)Gen_1_Mutant_66_943863 Gen_1_Mutant_66_943863 -5
C[C@H]1C(=O)NC(=O)[C@H]1C (ZINC000017139671 Gen_1_Mutant_66_943863 -5
Fc1ccc(C)k1F (ZINC000002526754 Gen_1_Mutant_66_943863 -5
[NH3+][CCN(C)CCC1][C@H]1C[C@H]1CO (ZINC000034518783+ZINC00004481721)Gen_1_Mutant_18_352118 Gen_1_Mutant_18_352118 -5
Nc1ccc1CC[NH3+] (ZINC000002547910 Gen_1_Mutant_18_352118 -5
CSC[C@H](C)N(C=O)C[C@H](C)C(N)=O (ZINC00007260148+ZINC000038855753)Gen_1_Mutant_23_419853 Gen_1_Mutant_23_419853 -5
C[C@H]1N[C@H](C)C[C@H](C)C(N)=O)S1 (ZINC000100218455+ZINC000307105332)Gen_1_Mutant_43_508729 Gen_1_Mutant_43_508729 -5
C[C@H]1CCC=C1C#N (ZINC000043198715 Gen_1_Mutant_43_508729 -5
CCO=C=C(O)N=C=O (ZINC000034598969 Gen_1_Mutant_43_508729 -5
CCCC[C@H](C)[NH3+]OC(=O)[C@H](C)CCCC (ZINC000026895001+ZINC000100508571)Gen_1_Mutant_27_340084 Gen_1_Mutant_27_340084 -5
CCC(=O)N[C@H](CO)lees1 (ZINC000038124651+ZINC00004531639)Gen_1_Mutant_26_345930 Gen_1_Mutant_26_345930 -5
CCCCC#CC(=O)[O-] (ZINC00001701836 Gen_1_Mutant_26_345930 -5
N#CCCCc1en[n-]k1 (ZINC000072209614 Gen_1_Mutant_26_345930 -5
CCN[C@H](C)[N@H+][CCOS1(=O)=O (ZINC000095708091+ZINC000030834289)Gen_1_Mutant_72_203920 Gen_1_Mutant_72_203920 -5
CC(=O)N1Cc1ccc1N (ZINC000039120797+ZINC00001588420)Gen_1_Mutant_23_683078 Gen_1_Mutant_23_683078 -5
CC[C@H]1(C)CCCC1=O (ZINC000034593578 Gen_1_Mutant_23_683078 -5
CCOC[C@H](C)NCC1=COCC1 (ZINC000019735453+ZINC00003884197)Gen_1_Mutant_66_927405 Gen_1_Mutant_66_927405 -5
O=C(O)C[C@H]1CCCC1 (ZINC000000406088 Gen_1_Mutant_66_927405 -5
CC(C)[C@H]1N[C@H](C)C(C)S[C@H]1C (ZINC00001569114+ZINC000039257185)Gen_1_Mutant_43_429485 Gen_1_Mutant_43_429485 -5
CC(C)C(=O)OC[C@H](C)O (ZINC000032147246 Gen_1_Mutant_43_429485 -5
CC(=C)BrCOc1nsc1CO (ZINC000012416533+ZINC000038972953)Gen_1_Mutant_19_758782 Gen_1_Mutant_19_758782 -5
Oe1ccc(C)k1F (ZINC000072265980 Gen_1_Mutant_19_758782 -5
C[C@H](O)CN(CCCN)C[C@H]1C[C@H]1F (ZINC001251970219+ZINC00001668459)Gen_1_Mutant_18_949319 Gen_1_Mutant_18_949319 -5
COCCN(C)C[C@H](CO)C[C@H](C)C(C)C[C@H](C)C[NH3+] (ZINC000042459136+ZINC00001759070)Gen_1_Mutant_1_259414 Gen_1_Mutant_1_259414 -5
CCCl(C=O)O[C@H](CO)CC[NH3+][KCC1 (ZINC000064033393+ZINC000034273814)Gen_1_Mutant_14_947619 Gen_1_Mutant_14_947619 -5
CC(=O)N(CCCC(=O)[O-])C[C@H](O)C[NH+][C]C (ZINC000001529559+ZINC00001718553)Gen_1_Mutant_18_729581 Gen_1_Mutant_18_729581 -5
O=C1NC(=O)C[C@H]2C[C@H]12 (ZINC000013401200 Gen_1_Mutant_18_729581 -5
CC[C@H](C)CCN(CCCO)C(=O)CNC (ZINC000037468701+ZINC00007849902)Gen_1_Mutant_18_260311 Gen_1_Mutant_18_260311 -4.9
CC[N+](C)CCC(=O)CC1 (ZINC000038241756 Gen_1_Mutant_18_260311 -4.9
COC(=O)C[C@H]1CCCC1 (ZINC000014684366 Gen_1_Mutant_18_260311 -4.9
C[C@H]1[NH2+]C[C@H](C)C[C@H](C)C(=O)OC(C)C(C)S1 (ZINC000005598930+ZINC000138360682)Gen_1_Mutant_43_335475 Gen_1_Mutant_43_335475 -4.9
CO[C@H](C)N(C)CO(=O)Nc1ccc1 (ZINC000040448803+ZINC000082164274)Gen_1_Mutant_35_732655 Gen_1_Mutant_35_732655 -4.9
CC(C)C[C@H](C)C(O)C(=O)[O-] (ZINC000052884036 Gen_1_Mutant_35_732655 -4.9
CC[C@H](C)OC(=O)N[C@H]1C[C@H](F)C1 (ZINC000036466127+ZINC000100482985)Gen_1_Mutant_12_404914 Gen_1_Mutant_12_404914 -4.9
C[C@H](CN)CC(=O)O[C@H]1CC[C@H]1N (ZINC000005018203+ZINC000078809022)Gen_1_Mutant_14_300414 Gen_1_Mutant_14_300414 -4.9
COC(=O)C(C)C)N=C=O (ZINC000002524695 Gen_1_Mutant_14_300414 -4.9
CN1CC(N@H+)(C)C(=O)OCFC1 (ZINC000059821916+ZINC00002040572)Gen_1_Mutant_12_625324 Gen_1_Mutant_12_625324 -4.9
COe1ccc1Ncc1C (ZINC000008698124 Gen_1_Mutant_12_625324 -4.9
#CCOCe1ccc1 (ZINC000095757830 Gen_1_Mutant_12_625324 -4.9
Nc1nccc(C=O)en1 (ZINC000004992768 Gen_1_Mutant_12_625324 -4.9
CC1(C)OC[C@H](CC=O)O1 (ZINC000038220232 Gen_1_Mutant_12_625324 -4.9
CCCC(C)C)N@H+)(CCN(C)C)C(=O)CO (ZINC000011638931+ZINC00002528224)Gen_1_Mutant_18_38002 Gen_1_Mutant_18_38002 -4.9
Nc1e(O)en[n-]k1=O (ZINC000016981804 Gen_1_Mutant_18_38002 -4.9
CC[C@H](S)[C@H](C)CO(C)C(=O)OCC[C@H](C)O)CC (ZINC000053173037+ZINC000211894466)Gen_1_Mutant_2_663676 Gen_1_Mutant_2_663676 -4.9
CC[C@H]1(C)O[C@H]1C#N (ZINC000143849850 Gen_1_Mutant_2_663676 -4.9
[NH3+][C@H]1CN(C(=O)OCC(F)F)CS1 (ZINC000167077821+ZINC000004771123)Gen_1_Mutant_12_329141 Gen_1_Mutant_12_329141 -4.9
Oe1ccc(F)k1Cl (ZINC000021304466 Gen_1_Mutant_12_329141 -4.9
N#e1ccc(C)k1F (ZINC001161693769 Gen_1_Mutant_12_329141 -4.9
CC(=O)OCClenn(C)N+)(C)Ck1 (ZINC000307415697+ZINC000031667387)Gen_1_Mutant_18_505807 Gen_1_Mutant_18_505807 -4.9
CC[C@H](C)C(=O)C(C)C(C)C(=O) (ZINC000001586735+ZINC00001648961)Gen_1_Mutant_80_55735 Gen_1_Mutant_80_55735 -4.9
C[C@H](CN1CCCC1)[NH2+][C1(C)CCC1 (ZINC000001646652+ZINC000014628922)Gen_1_Mutant_66_163040 Gen_1_Mutant_66_163040 -4.9
CC(C)C)N@H+)(CCC(=O)C1 (ZINC000037239796 Gen_1_Mutant_66_163040 -4.9
CC[C@H](C)CC)N@H+)(C)S(=O)(=O)CCO (ZINC000005998106+ZINC000037870669)Gen_1_Mutant_84_624556 Gen_1_Mutant_84_624556 -4.9
CC[N@H+](CCC(=O)C)C[C@H](C)C1 (ZINC000001235041 Gen_1_Mutant_84_624556 -4.9
CC[C@H](N)N[C@H](C)OC(C)=O)C1CC1 (ZINC000021398479+ZINC000014507405)Gen_1_Mutant_24_378281 Gen_1_Mutant_24_378281 -4.9
CNC(=O)C[C@H]1S[C@H](C)[NH2+][C@H]1C (ZINC000002038075+ZINC000167138543)Gen_1_Mutant_43_87277 Gen_1_Mutant_43_87277 -4.9
C=Cc1ccc(C)sc1OC (ZINC001240831652 Gen_1_Mutant_43_87277 -4.9
CC1(C)C=C(C(=O)[O-])C1 (ZINC000039117897 Gen_1_Mutant_43_87277 -4.9
CC1(C)OCC[C@H]1C#N (ZINC000075521441 Gen_1_Mutant_43_87277 -4.9
CO(C)C(C)C[C@H](C)C(O)CC#N (ZINC000001679564+ZINC00008681669)Gen_1_Mutant_81_564492 Gen_1_Mutant_81_564492 -4.9
Nc1ccc(F)cc1O (ZINC000021981857 Gen_1_Mutant_81_564492 -4.9
Cc1ccc(OCC2(C)CSC2)nn1 (ZINC000017058591+ZINC00003474345)Gen_1_Mutant_19_444248 Gen_1_Mutant_19_444248 -4.9
COCCS(=O)(=O)N(C)C=C(C)B)CCC#N (ZINC000116492750+ZINC000054157678)Gen_1_Mutant_72_8723 Gen_1_Mutant_72_8723 -4.9
CCOC(=O)[C@H](C)C[C@H](C)O (ZINC000014489011 Gen_1_Mutant_72_8723 -4.9
CCOC(=O)e1cccn1 (ZINC00002527148 Gen_1_Mutant_72_8723 -4.9
Nc1ccc(N)k1(O) (ZINC000032150081 Gen_1_Mutant_72_8723 -4.9
CCCC[C@H](CO)N[C@H]1C[C@H](C)CO(C)C1 (ZINC000005819872+ZINC000104675177)Gen_1_Mutant_66_586308 Gen_1_Mutant_66_586308 -4.9
C=C(C)BrCO(C=O)[C@H](C)CCC (ZINC00002569601+ZINC000100508546)Gen_1_Mutant_27_887483 Gen_1_Mutant_27_887483 -4.9
C=Cc1ccc(OC)en1 (ZINC001240826425 Gen_1_Mutant_27_887483 -4.9
CCOC(=O)C(=O)CC (ZINC000004528565 Gen_1_Mutant_27_887483 -4.9
C[C]H)CCS(=O)(=O)N(C)C[C@H](C)CCO (ZINC000003638707+ZINC000019092121)Gen_1_Mutant_84_73431 Gen_1_Mutant_84_73431 -4.8
COC(=O)C[C@H]1S[C@H](C)N[C@H]1C (ZINC000010154894+ZINC00002568011)Gen_1_Mutant_43_313862 Gen_1_Mutant_43_313862 -4.8
CS(=O)N[O-][C-][C@H]1OCCS1 (ZINC000022066026+ZINC000034310298)Gen_1_Mutant_84_398473 Gen_1_Mutant_84_398473 -4.8
Nc1ccc(S)nn1 (ZINC000033650059 Gen_1_Mutant_84_398473 -4.8
[C]N@H+)(CCCO)C1ccc1C1 (ZINC000014982472+ZINC000026476037)Gen_1_Mutant_66_134338 Gen_1_Mutant_66_134338 -4.8
Nc1ccc1N (ZINC00000395550 Gen_1_Mutant_66_134338 -4.8
CCNc1ccc(C)cc1C (ZINC000002384024+ZINC000016052656)Gen_1_Mutant_90_987564 Gen_1_Mutant_90_987564 -4.8
C[C@H]1(O)CCCC1=O (ZINC000045070441 Gen_1_Mutant_90_987564 -4.8
Nc1mm1CC1 (ZINC000017315314 Gen_1_Mutant_90_987564 -4.8
COC(=O)C[C@H]1S[C@H](C)N[C@H]1C (ZINC000059515438+ZINC00003861333)Gen_1_Mutant_43_154539 Gen_1_Mutant_43_154539 -4.8
Cc1ccc(S)nn1 (ZINC000036378430 Gen_1_Mutant_43_154539 -4.8
[NH3+][C]c1cc(O)C[C@H]2CC(F)F)cs1 (ZINC000062709807+ZINC000114498850)Gen_1_Mutant_19_786577 Gen_1_Mutant_19_786577 -4.8
Cc1ccc(SCCN(C)C)en1 (ZINC000001481997+ZINC000098175513)Gen_1_Mutant_20_805440 Gen_1_Mutant_20_805440 -4.8
CCCCS(=O)(=O)N[C@H](C)C(C)C(=O)O (ZINC000001697391+ZINC000035186321)Gen_1_Mutant_84_366353 Gen_1_Mutant_84_366353 -4.8
Cn1ccc(C=O)k1F) (ZINC00021873292 Gen_1_Mutant_84_366353 -4.8
CC(=O)NCCe1ccc(C)sc1 (ZINC000011848936+ZINC000097956655)Gen_1_Mutant_26_883223 Gen_1_Mutant_26_883223 -4.8
Cc1ccc(N=C)k1 (ZINC000004200662 Gen_1_Mutant_26_883223 -4.8
C[C@H](NH3+)C1(OC(C)C)CO1 (ZINC000001586729+ZINC000584883999)Gen_1_Mutant_19_493792 Gen_1_Mutant_19_493792 -4.8
C[C@H]1N[C@H](C)C[C@H](C)C(=O)N(C)CS1 (ZINC000035797159+ZINC000004521425)Gen_1_Mutant_43_969674 Gen_1_Mutant_43_969674 -4.8
COC(=O)C[C@H]1(F)CCO1 (ZINC000260974250 Gen_1_Mutant_43_969674 -4.8
C#CCNC(=O)C(=O)CC (ZINC001143969208 Gen_1_Mutant_43_969674 -4.8

C[C@@H](F)COC(=O)N1CCCC1	(ZINC001083809801+ZINC000000895216)Gen_1_Mutant_12_441747	Gen_1_Mutant_12_441747	-4.8
CCCC(=O)O[C@H](C)[C@H](C)CC	(ZINC000001598473+ZINC000004556489)Gen_1_Mutant_24_452730	Gen_1_Mutant_24_452730	-4.8
Ce1cc(C[O]H)(C)Nc(C)O1	ZINC000021949875	ZINC000021949875	-4.8
Ne1ncc(C)cc1F	ZINC000016158481	ZINC000016158481	-4.8
CNCC1CN(C=O)C(C)C(C)C1	(ZINC000095719246+ZINC000034264458)Gen_1_Mutant_23_579986	Gen_1_Mutant_23_579986	-4.8
C#C[C@H](OCCO)C(C)C	ZINC001217928890	ZINC001217928890	-4.8
[NH3+][C@@H](C)C(=O)N	ZINC000004738115	ZINC000004738115	-4.8
Ce1ncc(C)nc1N	ZINC000001764830	ZINC000001764830	-4.8
C#CC[NH-][C@@H](C)C	ZINC000307623344	ZINC000307623344	-4.8
CC(C)SCCN1CC[C@H](F)[C@H](O)C1	(ZINC000071255378+ZINC000037684833)Gen_1_Mutant_18_67854	Gen_1_Mutant_18_67854	-4.8
NO[C@H](C)(C=O)[O-]C1CC1	ZINC000219043456	ZINC000219043456	-4.8
O[C@H]1CCC2[C@H]2+1C2C1	ZINC000238724177	ZINC000238724177	-4.8
C[C@H](C)[C@H](C)(=O)O[C@H](C)[NH3+])COC(C)C(C)C	(ZINC000020513483+ZINC000252188314)Gen_1_Mutant_27_595779	Gen_1_Mutant_27_595779	-4.8
COc1ccccc1NN	ZINC000036222744	ZINC000036222744	-4.8
C[C@H](NH3+)CS(=O)(=O)[O-]	ZINC000002585523	ZINC000002585523	-4.7
CCCC(=O)CC(C)=O	ZINC000004552334	ZINC000004552334	-4.7
C#CCC[C@H](O)[C@H]1CO1	ZINC000043199155	ZINC000043199155	-4.7
CCCCC(=O)NCCO	ZINC000011638467	ZINC000011638467	-4.7
Ne1nem1CC(=O)[O-]	ZINC000070824964	ZINC000070824964	-4.7
Ce1nccc1CC1	ZINC000059664634	ZINC000059664634	-4.7
C[C@H](O)[C@H]1CCC[NH2+]	ZINC000034278486	ZINC000034278486	-4.7
C#CC(=O)Ne1nem1C	ZINC001143901162	ZINC001143901162	-4.7
Cn1ccc(=O)cc1C1	ZINC0000238548942	ZINC0000238548942	-4.7
C=C-CC[N-]S(C)=O	ZINC0000867469600	ZINC0000867469600	-4.7
CCCC(=O)N1CC[C@H](NH+)(CC)CC1	(ZINC000022913485+ZINC000228916001)Gen_1_Mutant_26_947459	Gen_1_Mutant_26_947459	-4.7
C[C@H](C)[C@H]1C[NH2+][C@@H]1C	ZINC000012650056	ZINC000012650056	-4.7
C#CC(=O)NC=C=C	ZINC001161884470	ZINC001161884470	-4.7
C=CCNS(=O)(=O)C=C	ZINC000114612074	ZINC000114612074	-4.7
CC[C@H](C)[C@H]1C=C=C	ZINC000062821996	ZINC000062821996	-4.7
COc1n[nH]cc1C=O	ZINC000020357655	ZINC000020357655	-4.7
CO[C@@](C)(C)[C@H]1(F)S[C@H](C)OCCO	(ZINC000163732423+ZINC000098175161)Gen_1_Mutant_20_519390	Gen_1_Mutant_20_519390	-4.7
CC[C@H](C)C(=O)Nc1ccc(C)cc1	(ZINC000102173083+ZINC000086049781)Gen_1_Mutant_26_417492	Gen_1_Mutant_26_417492	-4.7
CCC(=O)N[C@H](C)NCC	ZINC000040351499	ZINC000040351499	-4.7
[NH3+][C@H]1CSC[C@H](C)(=O)[O-]	ZINC000090569315	ZINC000090569315	-4.7
CNe1ccccc1N	ZINC000038549194	ZINC000038549194	-4.7
C[N@@H+][C@@H]1CCN[C@H](C=O)[O-]C1	ZINC000023094286	ZINC000023094286	-4.7
CNC(=O)CCCC(C)=O	ZINC000104153756	ZINC000104153756	-4.7
CC[C@H](C)(NH3+)C(=O)[O-]	ZINC000001602525	ZINC000001602525	-4.7
CCCCC[C@H](C)N	ZINC000019167664	ZINC000019167664	-4.7
CCCCC[C@H](O)CC	ZINC000002390331	ZINC000002390331	-4.7
COC(=O)C#CCCCO	ZINC000002583943	ZINC000002583943	-4.7
C[C@H](N)Ccc1n[nH]c1	ZINC000026663631	ZINC000026663631	-4.6
COc1ccc(C)nc1	ZINC000000730496	ZINC000000730496	-4.6
CC(C)N1C[C@H](C)[C@H](NH3+)C1	ZINC000074941863	ZINC000074941863	-4.6
Ce1ncc(C)C(=O)O1	ZINC000039074003	ZINC000039074003	-4.6
CC(=O)[C@H]1COCCO1	ZINC000075772369	ZINC000075772369	-4.6
C[NH2+][C-](C)[N+](=O)[O-]N	ZINC000001385212	ZINC000001385212	-4.6
[NH3+][C@H]1CCNC(=O)CC1	ZINC000083267407	ZINC000083267407	-4.6
Oc1ccc(C)cc1	ZINC000095670834	ZINC000095670834	-4.6
CC[C@H](C)C(=O)N-JN	ZINC000022161351	ZINC000022161351	-4.6
CCNe1nccc1N	ZINC000001592097	ZINC000001592097	-4.6
Ce1ncc(C=O)cc1C	ZINC000082411510	ZINC000082411510	-4.6
CC[C@H](C)OCC(N)=O	ZINC000043639468	ZINC000043639468	-4.6
CC[C@H](C)CNC(N)=[NH2+])OC	ZINC000307463101	ZINC000307463101	-4.6
CC[C@H](C)CC[C@H](C)[NH3+]	ZINC000044463400	ZINC000044463400	-4.6
O=C(C)C1ccc1	ZINC000085344405	ZINC000085344405	-4.6
C#C[C@H]1[C@H](C)C(=O)OC	ZINC000039244972	ZINC000039244972	-4.6
O=c1[n-]ccc1C1	ZINC000003209701	ZINC000003209701	-4.6
CC(C)CO[NH2+][C@@H](O)C	ZINC000035603965	ZINC000035603965	-4.5
CC(C)C[C@H](O)C(C)C	ZINC000003070122	ZINC000003070122	-4.5
Ce1ccc(C)nc1	ZINC000002559906	ZINC000002559906	-4.5
COC(=O)[C@H](C)OC1CC1	ZINC000261091725	ZINC000261091725	-4.5
[NH3+][C@H](C)C(C)C(=O)[O-]	ZINC000002035148	ZINC000002035148	-4.5
O=C(C)N1CC(O)C1	ZINC000170279545	ZINC000170279545	-4.5
[NH3+][C@H](C)C)N1CCCC1	ZINC000072233206	ZINC000072233206	-4.5
CCCN(C)C(=O)N[C@H](C)COC	(ZINC000062821998+ZINC000016489877)Gen_1_Mutant_31_5186	Gen_1_Mutant_31_5186	-4.5
C[C@H](C)[NH-]1CCCC(N)CC1)N(C)C	(ZINC000002018080+ZINC000082046523)Gen_1_Mutant_18_394778	Gen_1_Mutant_18_394778	-4.5
Ne1ccc(C)nc1	ZINC000001595944	ZINC000001595944	-4.5
C1CO[C@H](C)[C@H]2CO2)C1	ZINC000115688385	ZINC000115688385	-4.5
COC(C=O)CC(C)C	ZINC000039398104	ZINC000039398104	-4.5
CC(=O)CNC[C@H](O)CO	ZINC001252069970	ZINC001252069970	-4.5
C#CC(=O)N[C@H](C)CC	ZINC000233832562	ZINC000233832562	-4.5
NCCOCCCC1CC1	ZINC000096528545	ZINC000096528545	-4.5
CCCC[C@H](C)COC[C@H](CC[NH3+])COC	(ZINC000002015540+ZINC000068985048)Gen_1_Mutant_19_58730	Gen_1_Mutant_19_58730	-4.5
Ne1ccc(F)cc1S	ZINC000001559798	ZINC000001559798	-4.5
C#CC[C@H](C)OCC#CC	ZINC001224357966	ZINC001224357966	-4.5
O=C1C(O)CC1CC1	ZINC000034767819	ZINC000034767819	-4.4
Ne1ncc(N)nc(C)nc1	ZINC000000896288	ZINC000000896288	-4.4
CNC[C@H](O)CC(=O)[O-]	ZINC000084426046	ZINC000084426046	-4.4
C1c1ncc(C)nc1	ZINC000012650759	ZINC000012650759	-4.4
F[C@H](C)NCC12CC2	ZINC000107260796	ZINC000107260796	-4.4
CCCCC[C@H](O)CC	ZINC000002011663	ZINC000002011663	-4.4
C=C[C@@](C)(C)C[C@@](F)C1	ZINC000137128619	ZINC000137128619	-4.4
CCOC(O)C(C)C=O	ZINC000001684358	ZINC000001684358	-4.4
C=C-C[C@H](C)C	ZINC000071782872	ZINC000071782872	-4.4
CC(=O)C=C(C)O	ZINC000100009099	ZINC000100009099	-4.4
Ce1ncc(C[NH3+])sc1C	ZINC000011631691	ZINC000011631691	-4.4
CCCN(C)N(C)C(=O)=O	(ZINC0000033914540+ZINC000019365688)Gen_1_Mutant_84_695758	Gen_1_Mutant_84_695758	-4.4
CCCN(C)C(=O)C(=O)OC	ZINC000042304561	ZINC000042304561	-4.4
CC[C@H](C)CNC(O)C(=O)OC1CC1	(ZINC000034327620+ZINC000034115108)Gen_1_Mutant_19_248753	Gen_1_Mutant_19_248753	-4.4
CC(C)C[C@H](O)[C@H](C)N	ZINC000001759070	ZINC000001759070	-4.3
CN(C)C(N)C(=O)C1	ZINC000060247276	ZINC000060247276	-4.3
O=C-N[C@H](CS)C(=O)[O-]	ZINC000149266798	ZINC000149266798	-4.3
CC(C)C(N)CC1	ZINC000001613311	ZINC000001613311	-4.3
C/C=C/C1[N+](=O)[O-]	ZINC000001733879	ZINC000001733879	-4.3
C#CC#CC(C)C(C)C	ZINC000066377785	ZINC000066377785	-4.3
CC#CC(=O)N/C=C/CC	ZINC001179756274	ZINC001179756274	-4.3

CC[C@](C)(N)C(=O)CC1	ZINC000038220264	ZINC000038220264	-4.3
C=C[C@H](O)CCCC	ZINC000001562157	ZINC000001562157	-4.3
C=CCOC[C@H](CC)C(=O)[O-]	ZINC000037912056	ZINC000037912056	-4.3
C[C@H](Cl)S(=O)(=O)[O-]	ZINC000032139705	ZINC000032139705	-4.3
C[C@](O)(C)[NH3+]C(=O)[O-]	ZINC000078724735	ZINC000078724735	-4.3
CC(C)C(=O)N=C=S	ZINC000022143666	ZINC000022143666	-4.2
N/N=C/S=C=C(=O)[O-]	ZINC000604970841	ZINC000604970841	-4.2
CC(C)C[C@H]1CO1	ZINC000032182999	ZINC000032182999	-4.2
O=Ce1sc1C=O	ZINC000000334484	ZINC000000334484	-4.2
C[C@H](O)C([NH+]=C)(N)N(C)C	ZINC000306675889	ZINC000306675889	-4.2
[NH3+]C@]1(C)CCO)CCOC1	ZINC000083617766	ZINC000083617766	-4.2
CC[C@H](OC)C(=O)[O-]	ZINC000019091090	ZINC000019091090	-4.2
CCC(=O)N=C=S	ZINC000022149244	ZINC000022149244	-4.2
ClCN(C[C@H]2CO2)CCO1	ZINC000019735112	ZINC000019735112	-4.2
O=Ce1scc1Cl	ZINC000002383503	ZINC000002383503	-4.2
C=C(Cl)CNCC1CC1	ZINC000037680870	ZINC000037680870	-4.1
CC(C)NH2+ CC(C)C=O	ZINC000001675674	ZINC000001675674	-4.1
CO[C@H](CN)C(=O)[O-]	ZINC000078684455	ZINC000078684455	-4.1
CCCCCCCC1	ZINC000001686928	ZINC000001686928	-4.1
C[N+](C)CCO)CCOCC1	ZINC000000369913	ZINC000000369913	-4.1
NCCNC(=O)CCO	ZINC000116039474	ZINC000116039474	-4.1
N[N-]C(=O)CCO	ZINC000001702056	ZINC000001702056	-4.1
C#CCOC[C@H](C)OC	ZINC000034588647	ZINC000034588647	-4.1
CSCCCN=[N+]=[N-]	ZINC000005662644	ZINC000005662644	-4.1
C=C([NH2+])CC(=O)OC	ZINC000019736929	ZINC000019736929	-4.1
CCO[C@H](Cl)CC#N	ZINC001204945189	ZINC001204945189	-4.1
CC[C@H](C)[C@H](C)O	ZINC000001598473	ZINC000001598473	-4.1
COCCOCCN=[N+]=[N-]	ZINC000034115250	ZINC000034115250	-4
ClCe1sml1	ZINC000034284512	ZINC000034284512	-4
O=C1OCC[C@H]1Cl	ZINC000005134260	ZINC000005134260	-4
C[C@H](O)C(O)[O-]=S	ZINC000001692438	ZINC000001692438	-4
CCOC(=O)N=C=S	ZINC000001606013	ZINC000001606013	-4
C[C@H](N)CCCC1	ZINC000083591286	ZINC000083591286	-4
C[C@H](C)S)OCCC#N	ZINC001205620658	ZINC001205620658	-4
[N-]=[N+]=NCCCO	ZINC000038887055	ZINC000038887055	-3.9
CCN(C)[C@H](C)C#N	ZINC000044427502	ZINC000044427502	-3.9
CC(C)CO)CC1	ZINC000001765864	ZINC000001765864	-3.9
CC(=O)N=C=S	ZINC000002386803	ZINC000002386803	-3.9
CNC(=[NH2+])[C@H](Cl)Cl	ZINC000006485436	ZINC000006485436	-3.8
CCC[C@H](Cl)CC	ZINC000002013440	ZINC000002013440	-3.8
C=CCCCN=C=S	ZINC000002556867	ZINC000002556867	-3.8
O=COC[C@H]1CO1	ZINC000039251923	ZINC000039251923	-3.7
CN(C)CCC=O	ZINC000067175989	ZINC000067175989	-3.7
N[C@H]1[NH2+][N+](=S)S1	ZINC000008627995	ZINC000008627995	-3.7
C(C#N)=C.Br	ZINC000016138636	ZINC000016138636	-3.7
C=COC(=O)Cl	ZINC000002242591	ZINC000002242591	-3.6
COC[C@H](O)CS	ZINC000034257041	ZINC000034257041	-3.6
Cl[C@H](Cl)[C@H]1CO1	ZINC000001598462	ZINC000001598462	-3.6
C#CCCC1	ZINC000002242625	ZINC000002242625	-3.5
SC[C@H]1CCCCO1	ZINC000005282940	ZINC000005282940	-3.5
ClCC[C@H]1CO1	ZINC000039241060	ZINC000039241060	-3.4
ClS@]([O)CCC1	ZINC000001640818	ZINC000001640818	-3.4
OC[C@H](Cl)CF	ZINC000068590945	ZINC000068590945	-3.4
C=C(Br)CO	ZINC000002043455	ZINC000002043455	-3.2
COCCOCCS	ZINC000016194405	ZINC000016194405	-3.1
CN(C)CCCS	ZINC000033605002	ZINC000033605002	-3