

training set	
Name	Classification
<chem>FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(NCc2c3n(ccc3ccc2)C)ccc1</chem>	1
<chem>O=C([O-])[C@]1([C@H]2CC[C@@H]3C(=CC[C@@](C3)(C=C)C)[C@@]2(CCC1)C)C</chem>	0
<chem>FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2cc(OC(F)(F)F)ccc2O)CCCC)cc1</chem>	0
<chem>Clc1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(OC2cc(S(=O)(=O)C)ccc2)ccc1</chem>	0
<chem>Clc1c2ncc(C)c(c2ccc1)-c1cc(OC2cc(ccc2)C(O)(C)C)ccc1</chem>	0
<chem>Clc1c2nc(C)c(nc2ccc1)-c1ccc(cc1)-c1cc(S(=O)(=O)C)ccc1</chem>	1
<chem>FC(F)(F)c1c2ncc(C(=O)c3ccccc3)c(c2ccc1)-c1cc(OCc2ccc(cc2)[C@@H](Cc2ccc(cc2)-c2ccc</chem>	0
<chem>FC(F)(F)c1c2ncc(C(=O)c3ccccc3)c(c2ccc1)-c1cc(OCc2ccc(cc2)[C@@H](Cc2ccc(cc2)C(C)(C</chem>	0
<chem>FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2ccccc2)CC)cc1</chem>	0
<chem>Clc1c2ncc(C)c(c2ccc1)-c1cc(OC2cc(ccc2)C(=O)NC)ccc1</chem>	1
<chem>O[C@]12C[C@@H](O)CC[C@]1(C)[C@]1(O)[C@H]([C@@H]3CC[C@H]([C@H](C)[C@H]4</chem>	0
<chem>Clc1cc(ccc1N(Cc1ccccc1)CC(F)(F)F)C(O)(C(F)(F)F)C(F)(F)F</chem>	0
<chem>Clc1ccc(cc1)-c1n(nc2c1cccc2C(F)(F)F)Cc1ccc(cc1)C(F)(F)F</chem>	0
<chem>FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(ccc1)COc1c2c(ccc1)c(ccc2)CC(=O)[O-]</chem>	1
<chem>FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(ccc1)CNc1cc(C)c(cc1C)CC(=O)[O-]</chem>	1
<chem>Clc1cc2c3CC[C@H](Cc3[nH]c2cc1)[C@](S(=O)(=O)c1ccccc1OC)(C(OC)=O)C</chem>	0
<chem>S(=O)(=O)(C)c1cc(OC2cc(ccc2)-c2n3c(nc2C(C)C)C(=CC=C3)C(F)(F)F)ccc1</chem>	1
<chem>FC(F)(F)c1cc(ccc1)-c1oc(C)c(n1)CN(CC)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F</chem>	0
<chem>FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2cccn2)CC)cc1</chem>	0
<chem>Clc1ccc(OC2cc(S(=O)(=O)C(C)C)ccc2)cc1-n1c2c(nc1C)c(Cl)ccc2</chem>	1
<chem>S(=O)(=O)(C)c1cc(OC2cc(ccc2)-c2n3c(nc2Cn2ccnc2)C(=CC=C3)C(F)(F)F)ccc1</chem>	1
<chem>S(=O)(=O)(N(C)c1ccc(cc1)[C@@H](C(F)(F)F)c1n(ccc1)CCOCC)c1ccccc1</chem>	0
<chem>FC(F)(F)c1c2ncc(C(=O)c3ccccc3)c(c2ccc1)-c1cc(OCc2ccc(cc2)C(=O)[O-])ccc1</chem>	0
<chem>S(=O)(=O)(C)c1cc(OC2cc(ccc2)-c2c3c(nc2C)c(ccc3)C(F)(F)F)ccc1</chem>	0
<chem>FC(F)(F)c1c2ncc(C(=O)c3ccccc3)c(c2ccc1)-c1ccc(OCc2ccc(cc2)C(=O)[O-])cc1</chem>	0
<chem>S(=O)(=O)(C(C)C)c1cc(OC2cc(ccc2)-c2n3c(nc2C)C(=CC=C3)C(F)(F)F)ccc1</chem>	1
<chem>O[C@H]1CC[C@]2([C@@H](CC=C3C2=CC[C@@]2(C)[C@@]3(C)[C@H](O)C[C@@H]2)C</chem>	0
<chem>OC1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(OCCC=C)O)C)cc1</chem>	0
<chem>S(=O)(=O)(C)c1cc(OC2cc(-n3c4c(nc3)c(ccc4)C(F)(F)F)ccc2)ccc1</chem>	1
<chem>Clc1cc(ccc1)-c1oc(C)c(n1)CN(CC)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F</chem>	0
<chem>Clc1cc(ccc1OCCCOc1ccc2c(oc2C(F)(F)F)c1CCC)CC(=O)[O-]</chem>	0
<chem>FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(ccc1)CNc1c2c(ccc1)c(ccc2)CC(=O)[O-]</chem>	1
<chem>Clc1cccc(C(F)(F)F)c1COc1cc(ccc1)-c1c2c(nnc1Cc1ccccc1)c(Cl)ccc2</chem>	1
<chem>S(=O)(=O)(CC)c1cc(ccc1)-c1cc(ccc1)-c1c2c(nc1C)c(ccc2)C(F)(F)F</chem>	1
<chem>S(=O)(=O)(C)c1cc(OC2cc(ccc2)-c2n3c(nc2C[NH+])2CCCCC2)C(=CC=C3)C(F)(F)F)ccc1</chem>	1
<chem>Clc1c2nc(n(c2ccc1)-c1cc(OC2cc(S(=O)(=O)CC)ccc2)ccc1)C</chem>	1
<chem>Fc1c(cccc1C(F)(F)F)COc1cc(ccc1)-c1c2c(nnc1Cc1ccccc1)c(ccc2)C(F)(F)F</chem>	1
<chem>FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(CC)C[C@@H](O)c2ccccc2)cc1</chem>	0
<chem>FC(F)(F)c1c2ncc(C(=O)c3ccccc3)c(c2ccc1)-c1cc(OCc2cc(ccc2)C(=O)[O-])ccc1</chem>	0
<chem>S(=O)(=O)(C)c1cc(OC2cc(-n3c4c(nc3C)cccc4)ccc2)ccc1</chem>	1
<chem>OC1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)N[C@@H]2C[C@@H]3C[C@H]([C@H]2C)C</chem>	0
<chem>FC(F)(F)c1c2ncc(C(=O)c3ccccc3)c(c2ccc1)-c1cc(OCc2ccc(cc2)[C@@H](Cc2ccccc2)C(=O)[</chem>	0
<chem>FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2ccccc2)CC(F)(F)F)cc1</chem>	0
<chem>FC(F)(F)c1noc2c1ccc(OCCCN(C)c1ccccc1)c2CCC</chem>	0
<chem>FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2ccccc2)C)cc1</chem>	0

Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)NCC2(CCCCC2)c2ccccc2)C)cc1	0
S(=O)(=O)(C)c1cc(ccc1)-c1ccc(cc1)-c1nc2c(nc1C)c(ccc2)C(F)(F)F	1
Clc1cc(N(CCCOc2ccc3c(oc3C(F)(F)F)c2CCC)C)ccc1CC(=O)[O-]	0
Clc1c(cccc1C(F)(F)F)COc1cc(ccc1)-c1c2c(nnc1Cc1cccc1)c(ccc2)C(F)(F)F	1
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](CO)c2ccccc2)CC)cc1	0
S(=O)(=O)(C(C)C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2)c(ccc3)C(F)(F)F)ccc1	0
FC(F)(F)c1noc2c1ccc(OCCCN1nnc3cc(ccc13)CC(=O)[O-])c2CCC	0
S(=O)(=O)(C)c1cc(ccc1)-c1cc(ccc1)-c1c2c(ncc1)c(ccc2)C(F)(F)F	1
Clc1c2nc(n(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)C(C)C)ccc2)ccc1)C	1
FC(F)(F)c1noc2c1ccc(OCCCN(CC)c1ccc(cc1)CC(=O)[O-])c2CCC	0
Clc1ccccc1S(=O)(=O)[C@@](C(OC)=O)(C)[C@@H]1CCc2c([nH]c3c2cc(Cl)cc3)C1	0
FC(F)(F)c1c2ncc(C(=O)c3ccccc3)c(c2ccc1)-c1ccccc1	0
Clc1ccc(Oc2cc(S(=O)(=O)C)ccc2)cc1-n1c2c(nc1)c(ccc2)C(F)(F)F	1
Clc1c2nc(n(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)C)ccc2)ccc1)C	1
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)NCC(C)(c2ccccc2)c2ccccc2)C)cc1	0
Clc1c2nccc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)C)ccc2)ccc1	1
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2n3c(nc2C(C)C)C(=CC=C3)C#N)ccc1	1
S(=O)(=O)(C(C)C)c1cc(Oc2cc(-n3c4c(nc3C)c(ccc4)C(F)(F)F)ccc2)ccc1	1
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(OCCCC=C)=O)C)cc1	0
Clc1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)N2CCCC2)ccc1	1
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](C(=O)N2CCCC2)c2ccccc2)CC)cc1	0
S(=O)(=O)(C)c1cc(ccc1)COc1cc(ccc1)-c1n2c(nc1C(C)C)C(=CC=C2)C(F)(F)F	1
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](COCC(=O)N(C)C)c2ccccc2)CC)cc1	0
FC(F)(F)c1c2ncc(C)c(c2ccc1)-c1cc(ccc1)CNc1c2c(ccc1)c(ccc2)CC(=O)[O-]	1
Clc1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)NCCC)ccc1	1
S(=O)(=O)(C)c1cc(ccc1)-c1cc(ccc1)-c1c2c(ncc1CC)c(ccc2)C(F)(F)F	0
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2n3c(nc2C(C)(C)C)C(=CC=C3)C(F)(F)F)ccc1	1
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](C(OC)=O)c2ccccc2)CC)cc1	0
O=C(NCC1(CCCCC1)c1ccccc1)[C@@]1([C@@H]2CCc3c(cccc3)[C@]2(CCC1)C)C	0
Clc1c(cccc1C(F)(F)F)COc1cc(ccc1)-c1c2c(nnc1Cc1cccc1)c(Cl)ccc2	1
Clc1c2nnc(Cc3ccccc3)c(c2ccc1)-c1cc(OCc2c(cccc2F)C(F)(F)F)ccc1	1
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)NCCc2ccccc2)C)cc1	0
FC(F)(F)c1c2nnc(Cc3ccccc3)c(c2ccc1)-c1cc(OCc2n(c3c(c2)cccc3)C)ccc1	1
FC(F)(F)c1noc2c1ccc(OCCCN1c3c(CC1=O)cc(cc3)C(=O)[O-])c2CCC	0
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](C(=O)N(C)C)c2ccccc2)CC)cc1	0
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(Oc2ccc(OC)cc2)ccc1	0
S(=O)(=O)(C)c1cc(Oc2cc(-n3c4c(nc3C)c(ccc4)C(F)(F)F)ccc2)ccc1	1
FC(F)(F)c1c2ncc(c(c2ccc1)-c1cc(Oc2ccc(cc2)CO)ccc1)-c1ccccc1	1
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)NCC23CC4CC(C2)CC(C3)C4)C)cc1	0
FC(F)(F)c1noc2c1ccc(OCCCNc1ccc(cc1)CC(=O)[O-])c2CCC	0
S(=O)(=O)(CC)c1cc(Oc2cc(-n3c4c(nc3C)c(ccc4)C(F)(F)F)ccc2)ccc1	1
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(C(CC)(C(OC)=O)c2ccccc2)CC)cc1	0
S(=O)(=O)(N(C)c1ccc(cc1)C(O)(C(F)(F)F)c1n(ccc1)Cc1ccccc1)c1ccccc1	0
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(NCc2n(c3c(c2)cccc3)C)ccc1	1
S(=O)(=O)(CC)c1cc(Oc2cc(-n3c4c(nc3C)c(ccc4)C(F)(F)F)ccc2)cc(F)c1	1
Clc1cc2c3CC[C@H](Cc3[nH]c2cc1)[C@](S(=O)(=O)c1ccc(F)cc1)(C(OC)=O)C	0
S(=O)(=O)(NC)c1cc(ccc1)-c1ccc(cc1)-c1nc2c(nc1C)c(ccc2)C(F)(F)F	1

FC(F)(F)c1noc2c1ccc(OCCCN1c3c(nc1)cc(cc3)CC(=O)[O-])c2CCC	0
Clc1cc(CN(CCCC)c2ccc(cc2)C(O)(C(F)(F)F)C(F)(F)F)c(O)cc1	0
S(=O)(=O)(C)c1cc(Oc2cc(-n3c4c(nc3Cc3ccc(F)cc3)c(ccc4)C(F)(F)F)ccc2)ccc1	0
FC(F)(F)c1noc2c1ccc(OCCCN1c3c(CC1=O)cc(cc3)CC(=O)[O-])c2CCC	0
Clc1cc(ccc1N(Cc1ccccc1)CC)C(O)(C(F)(F)F)C(F)(F)F	0
O[C@@]12[C@H]([C@@H]3CC[C@H]([C@H](C)[C@H]4C[C@@]4([C@H](C(C)C)C)C)[C@	0
Clc1ccc(cc1COc1cc(ccc1)-c1c2c(nnc1Cc1ccccc1)c(Cl)ccc2)C(F)(F)F	1
Clc1cc(ccc1N(C(CC)(C(OC)=O)c1ccccc1)CC)C(O)(C(F)(F)F)C(F)(F)F	0
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)NC23CC4CC(C2)CC(C3)C4)C)cc1	0
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N2CCCC2(C(OC)=O)c2ccccc2)cc1	0
Clc1cc(ccc1)-c1oc(C)c(n1)CN(CC(F)(F)F)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F	0
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)N2[C@H](CCC2)c2ccccc2)C)cc1	0
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1ccccc1)(F)C(=O)N(C)C	1
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C(=O)N)c(ccc3)C(F)(F)F)ccc1	1
ClC=1c2n(C=CC=1)c(-c1cc(Oc3cc(S(=O)(=O)NC)ccc3)ccc1)c(n2)C(C)C	1
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2ccncc2)CC)cc1	0
FC(F)(F)c1noc2c1ccc(OCCCN(C)c1ccc(cc1)C(=O)[O-])c2CCC	0
Clc1cc(ccc1N(Cc1ncsc1)CC)C(O)(C(F)(F)F)C(F)(F)F	1
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)NCCC)ccc1	1
Clc1c2nnc(Cc3ccccc3)c(c2ccc1)-c1cc(NCc2c3n(ccc3ccc2)C)ccc1	1
S(=O)(=O)(N(CC(F)(F)F)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F)c1ccccc1	0
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(OCc2ccccc2)=O)C)cc1	0
Clc1cccc(C(F)(F)F)c1COc1cc(ccc1)-c1c2c(nnc1Cc1ccccc1)c(ccc2)C(F)(F)F	1
Clc1ccc(Oc2cc(S(=O)(=O)CC)ccc2)cc1-n1c2c(nc1)c(ccc2)C(F)(F)F	1
FC(F)(F)c1noc2c1ccc(OCCCN(C)c1ncc(cc1)CC(=O)[O-])c2CCC	0
FC(F)(F)c1c2ncc(C(=O)c3ccccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)CC(=O)[O-])ccc1	0
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(CCc2ccccc2)CC)cc1	0
S(=O)(=O)(C)c1cc(Oc2cc(-n3c4c(nc3C(C)C)c(ccc4)C(F)(F)F)ccc2)ccc1	1
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1cc(OC)ccc1)(F)C(OC)=O	0
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)NC(=O)C23CC4CC(C2)CC(C3)C4)C)cc1	0
Clc1cc(ccc1N([C@@H](COc1ccc(cc1)C(OC)=O)c1ccccc1)CC)C(O)(C(F)(F)F)C(F)(F)F	0
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](COCC(OC)=O)c2ccccc2)CC)cc1	0
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2ccccc2)Cc2ccccc2)cc1	0
S(=O)(=O)(C)c1cc(ccc1)-c1cc(ccc1)-c1c2c(ncc1C(C)C)c(ccc2)C(F)(F)F	0
S(=O)(=O)(CCC(O)(C)C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)ccc1	1
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)N2[C@H]3[C@H]([C@@H]4[C@H]2CCC	0
Clc1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)NCC)ccc1	1
Fc1cccc(C(F)(F)F)c1COc1cc(ccc1)-c1c2c(nnc1Cc1ccccc1)c(ccc2)C(F)(F)F	1
FC(F)(F)c1noc2c1ccc(OCCCN(C(=O)C)c1ccc(cc1)CC(=O)[O-])c2CCC	0
S(=O)(=O)(N(C)c1ccc(cc1)C(OC)(C(F)(F)F)c1n(ccc1)CCOC)c1ccccc1	0
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2ccc(O)cc2)CCCC)cc1	0
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2Cc2ccccc2)c(ccc3)C(F)(F)F)ccc1	0
S(=O)(=O)(C(C)C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C(=O)N)c(ccc3)C(F)(F)F)ccc1	1
Clc1cc(ccc1O)CN(CCCC)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F	1
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C(=O)N)c(F)ccc3)ccc1	1
Clc1cc(Oc2cc(ccc2)-c2c3c(ncc2C(=O)N)c(ccc3)C(F)(F)F)cc(S(=O)(=O)C)c1	1
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N2CCCC2(C(OC)=O)c2ccccc2)cc1	0

Clc1ccc(Oc2cc(S(=O)(=O)C(C)C)ccc2)cc1-n1c2c(nc1)c(ccc2)C(F)(F)F	1
FC(F)(F)c1noc2c1ccc(OCCCN1c3c(cc(cc3)CCC(=O)[O-])cc1)c2CCC	0
Clc1cc(cc(OC)c1O)CN(CCCC)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F	1
S1\C(=C)c2ccc(cc2)CNc2cc(ccc2)-c2c3c(ncc2C(=O)c2cccc2)c(ccc3)C(F)(F)F)\C(=O)[N-]C:	0
Clc1cc(S(=O)(=O)[C@](F)(C(OC)=O)[C@@H]2Cc3c([nH]c4c3cc(Cl)cc4)C2)ccc1	0
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1cccc1)(F)c1onc(n1)N(C)C	0
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](COC)c2cccc2)CC)cc1	0
O(C(=O)C)c1cc2c(CC[C@H]3[C@@]2(CCCC3(C(OC(=O)[C@@]2([C@@H]3CCc4c(cc(O	0
S(=O)(=O)(C)c1cc(ccc1F)-c1cc(ccc1)-c1c2c(ncc1)c(ccc2)C(F)(F)F	1
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](COCc2cccc2)c2cccc2)CC)cc1	0
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2)c(ccc3)C(F)(F)F)ccc1	1
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1cccc1)(F)c1onc(n1)C(OC)=O	0
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C(=O)NC)c(ccc3)C(F)(F)F)ccc1	1
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](C(=O)[O-])c2cccc2)CC)cc1	0
FC(F)(F)c1cc(ccc1)-c1oc(C)c(n1)CN(CC(F)(F)F)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F	0
S(=O)(=O)(CCC)c1cc(Oc2cc(-n3c4c(nc3C)c(ccc4)C(F)(F)F)ccc2)ccc1	1
S1\C(=C)c2ccc(cc2)CNc2cc(ccc2)-c2c3c(ncc2C(=O)c2cccc2)c(ccc3)C(F)(F)F)\C(=O)[N-]C:	0
Oc1cc2c(CC[C@H]3[C@@]2(CCCC3(C(=O)CC(=O)[C@@]2([C@@H]3CCc4c(cc(O)cc4)[	0
S(=O)(=O)(CC)c1cc(ccc1)-c1cc(ccc1)-c1c2c(ncc1)c(ccc2)C(F)(F)F	1
FC(F)(F)c1c2ncc(Cc3cccc3)c(c2ccc1)-c1cc(OCc2c3n(ccc3ccc2)C)ccc1	1
S(=O)(=O)(N(C)c1ccc(cc1)C(O)(C(F)(F)F)c1n(ccc1)CCOCC)c1cccc1	0
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)NC23CC4(C[C@H](C2)C[C@H](C4)C3)C(OC	0
Clc1cc(ccc1N(Cc1nc(oc1C)-c1cc(Cl)ccc1)CC)C(O)(C(F)(F)F)C(F)(F)F	0
FC(F)(F)c1noc2c1ccc(OCCCN1ncc3cc(ccc13)CC(=O)[O-])c2CCC	0
S(=O)(=O)(N(C)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F)c1cccc1	0
ClC=1c2n(C=CC=1)c(-c1cc(Oc3cc(S(=O)(=O)N(Cc4ccc(OC)cc4)C)ccc3)ccc1)c(n2)C(C)C	0
FC(F)(F)c1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(OCc2ccc(cc2)[C@@H](CC#CCC)C(=O)[O-	0
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2n3c(nc2C)C(=CC=C3)C(F)(F)F)ccc1	1
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)N2CCC(CC2)\C=C/C)c2cccc2)C)cc1	0
Clc1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)N2CCOCC2)ccc1	1
FC(F)(F)c1c2ncc(c(c2ccc1)-c1cc(NCc2ccc(cc2)CC(=O)[O-])ccc1)-c1cccc1	0
S(=O)(=O)(C)c1cc(ccc1)Cc1cc(ccc1)-c1n2c(nc1CC)C(=CC=C2)C(F)(F)F	1
S(=O)(=O)(N(C)c1ccc(cc1)[C@@H](C(F)(F)F)c1n(ccc1)CCOC)c1cccc1	0
Clc1cc(ccc1SCCCOc1ccc2c(onc2C(F)(F)F)c1CCC)CC(=O)[O-]	0
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2n3c(nc2-c2cccc2)C(=CC=C3)C(F)(F)F)ccc1	1
FC(F)(F)c1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(OCc2ccc(cc2)C(CC#CCC)(CC#CCC)C(=O)[(	0
FC(F)(F)c1noc2c1ccc(OCCCN(C)c1ncc(cn1)CC(=O)[O-])c2CCC	0
test set	
FC(F)(F)c1noc2c1ccc(OCCCN1c3c(cc(cc3)CC(=O)[O-])cc1)c2CCC	0
s1cc(nc1)CN(CC)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F	1
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)NC2C3CC4CC2CC(C3)C4)C)cc1	0
FC(F)(F)c1noc2c1ccc(OCCCN(C)c1ccc(cc1)CC(=O)[O-])c2CCC	0
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1cc(F)ccc1)(F)C(OC)=O	0
Clc1cc(ccc1N([C@@H](CO)c1cccc1)CC)C(O)(C(F)(F)F)C(F)(F)F	0
S(=O)(=O)(C)c1cc(Oc2cc(-n3c4c(nc3CC)c(ccc4)C(F)(F)F)ccc2)ccc1	1
S(=O)(=O)(CCCO)c1cc(Oc2cc(-n3c4c(nc3C)c(ccc4)C(F)(F)F)ccc2)ccc1	1
FC(F)(F)c1c2ncc(Cc3cccc3)c(c2ccc1)-c1cc(OCc2ccc(cc2)C(CC#CCC)(CC#CCC)C(=O)[(	0
FC(F)(F)c1noc2c1ccc(OCCCN(C)c1ncc(cn1)CC(=O)[O-])c2CCC	0

S(=O)(=O)(C)c1cc(Oc2cc(-n3c4c(nc3C3CC3)c(ccc4)C(F)(F)F)ccc2)ccc1	1
OC[C@]1([C@H]2CC[C@@H]3C(=CC[C@@](C3)(C=C)C)[C@@]2(CCC1)C)C	0
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(ccc1)CNc1c2c(cccc2)c(cc1)CC(=O)[O-]	1
O(C(=O)C)c1cc2c(CC[C@@H]3[C@@]2(CCCC3(C(OC(=O)[C@@]2([C@@H]3CCc4c(cc(O)C)C1c2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1ccccc1)(F)c1onc(n1)C#N	0
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)N2CCC(CC2)c2ccccc2)C)cc1	0
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1ccccc1)(F)C(=O)NC	0
Clc1c2nnc(Cc3ccccc3)c(c2ccc1)-c1cc(NCc2c(cccc2F)C(F)(F)F)ccc1	1
FC(F)(F)c1noc2c1ccc(OCCCN(C)c1ccc(cc1C)CC(=O)[O-])c2CCC	0
FC(F)(F)c1noc2c1ccc(OCCCN1c3c(cc(cc3)C(=O)[O-])cc1)c2CCC	0
Clc1c2ncc(C(=O)N)c(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)C)ccc2)ccc1	1
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)N[C@H](C)C23CC4CC(C2)CC(C3)C4)C)cc1	0
Clc1cc(ccc1N(CCc1ccccc1)CC)C(O)(C(F)(F)F)C(F)(F)F	0
Oc1cc2c(CC[C@@H]3[C@@]2(CCCC3(C(=O)NC(=O)[C@@]2([C@@H]3CCc4c(cc(O)cc4)[	0
Oc1cc2c(CC[C@@H]3[C@@]2(CCCC3(COC(=O)[C@@]2([C@@H]3CCc4c(cc(O)cc4)[C@	0
Clc1c(cccc1C(F)(F)F)CNc1cc(ccc1)-c1c2c(nnc1Cc1ccccc1)c(Cl)ccc2	1
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(ccc1)CNc1ccc(CC(=O)[O-])c(C)c1C	1
s1c(cnc1N(CCCOc1cc2c(onc2C(F)(F)F)c1CCC)C)CC(=O)[O-]	0
Oc1cc2c(CC[C@@H]3[C@@]2(CCCC3(C(OC(=O)[C@@]2([C@@H]3CCc4c(cc(O)cc4)[C@	0
S(=O)(=O)(CC)c1cc(Oc2cc(ccc2)-c2n3c(nc2C)C(=CC=C3)C(F)(F)F)ccc1	1
FC(F)(F)c1noc2c1ccc(OCCCN(C)c1cc(ccc1)CC(=O)[O-])c2CCC	0
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1ccccc1)(F)c1oc(nn1)C	1
S(=O)(=O)(N(C)c1ccc(cc1)C(O)(C(F)(F)F)c1n(ccc1)CCOC)c1ccccc1	0
S(=O)(=O)(C)c1cc(Oc2cc(-n3c4c(nc3C)c(ccc4)C(F)(F)F)ccc2)cc(F)c1	1
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C(=O)N)c(ccc3)C(F)(F)F)cc(F)c1	1
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1ccccc1)(F)c1oc(nn1)N(C)C	0
Clc1cc(ccc1N([C@@H](COc1ccc(cc1)CCC(OC)=O)c1ccccc1)CC)C(O)(C(F)(F)F)C(F)(F)F	0
Clc1cc(ccc1N(Cc1nc(oc1C)-c1cc(ccc1)C(F)(F)F)CC)C(O)(C(F)(F)F)C(F)(F)F	0
FC(F)(F)c1c2nccc(c2ccc1)-c1cc(ccc1)CNc1c2c(ccc1)c(ccc2)CC(=O)[O-]	1
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C(=O)N)c(ccc3)C)ccc1	1
FC(F)(F)c1c2ncc(C(=O)c3ccccc3)c(c2ccc1)-c1cc(OCc2ccc(cc2)[C@@H](CC#CC)C(=O)[O-])	0
FC(F)(F)c1noc2c1ccc(OCCCN(C=O)c1ccc(cc1)CC(=O)[O-])c2CCC	0
FC(F)(F)c1noc2c1ccc(OCCCN(C)c1ncc(nc1)CC(=O)[O-])c2CCC	0
S(=O)(=O)(CC)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C(=O)N)c(ccc3)C(F)(F)F)ccc1	1
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)N[C@H]2[C@@H]3CC[C@@H](C2)C3)C)cc	0
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@H](CO)c2ccccc2)CC)cc1	0
FC(F)(F)c1c2ncc(C(=O)c3ccccc3)c(c2ccc1)-c1cc(OCc2ccc(cc2)C(CC#C)(CC#C)C(=O)[O-])cc	0
Oc1cc2c(CC[C@H]3[C@](CCC[C@]23C)(C(=O)N[C@H]2[C@@H]3C[C@@H](CC2)C3(C)C	0
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2n3c(nc2CC)C(=CC=C3)C(F)(F)F)ccc1	1
O[C@@H]1CC[C@@H]2C(=CC[C@H]3[C@@]4(CC[C@H]([C@@H](CC\C=C(\C(=O)[O-])/ ClC=1c2n(C=CC=1)c(-c1cc(Oc3cc(S(=O)(=O)C)ccc3)ccc1)c(n2)C(C)C	0
FC(F)(F)c1noc2c1ccc(OCCCCc1ccc(cc1)CC(=O)[O-])c2CCC	0
Clc1c2nc(n(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)C)ccc2)ccc1)C(C)C	1
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(N(Cc2ccc(cc2)CC(=O)[O-])C)ccc1	0
FC(F)(F)c1c2nnc(Cc3ccccc3)c(c2ccc1)-c1cc(OCc2c3n(ccc3ccc2)C)ccc1	1
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1ccccc1)(F)C(OC)=O	1
O=C(CC(=O)[C@@]1([C@@H]2CCc3c(cccc3)[C@]2(CCC1)C)C)C12CC3CC(C1)CC(C2)C3	0

S(=O)(=O)(C)c1cc(ccc1)-c1cc(ccc1)-c1c2c(ncc1CCC)c(ccc2)C(F)(F)F	0
S(=O)(=O)(CCC)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C(=O)N)c(ccc3)C(F)(F)F)ccc1	1
external test set	
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2ncnc3c2cccc3C(F)(F)F)ccc1	1
S(=O)(=O)(CC)c1cc(Oc2cc(ccc2)-c2ncnc3c2cccc3C(F)(F)F)ccc1	1
S(=O)(=O)(C(C)C)c1cc(Oc2cc(ccc2)-c2ncnc3c2cccc3C(F)(F)F)ccc1	1
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2ncnc3c2cccc3C(F)(F)F)cc(F)c1	1
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2nc(nc3c2cccc3C(F)(F)F)C)ccc1	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)C)ccc2)ccc1	1
S(=O)(=O)(C)c1cc(ccc1)-c1cc(ccc1)-c1nc(nc2c1cccc2C(F)(F)F)C	1
S(=O)(=O)(C)c1cc(ccc1)-c1cc(ccc1)-c1nc(nc2c1cccc2C(F)(F)F)CC	1
S(=O)(=O)(C)c1cc(ccc1)-c1cc(ccc1)-c1nc(nc2c1cccc2C(F)(F)F)-c1cccc1	1
Clc1ccc(Oc2cc(S(=O)(=O)C)ccc2)cc1-c1ncnc2c1cccc2C(F)(F)F	1
Clc1ccc(Oc2cc(S(=O)(=O)CC)ccc2)cc1-c1ncnc2c1cccc2C(F)(F)F	1
Clc1ccc(Oc2cc(S(=O)(=O)C(C)C)ccc2)cc1-c1ncnc2c1cccc2C(F)(F)F	1
S(=O)(=O)(C)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(CC)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(C(C)C)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(C)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)cc(F)c1	1
S(=O)(=O)(C)c1cc(ccc1)COc1cc(-c2ncnc3c2cccc3C(F)(F)F)c(F)cc1	1
Clc1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)cc(S(=O)(=O)C)c1	1
Clc1ccc(Oc2cc(S(=O)(=O)C)ccc2)cc1-c1nc(nc2c1cccc2C(F)(F)F)C	1
Clc1ccc(Oc2cc(S(=O)(=O)CC)ccc2)cc1-c1nc(nc2c1cccc2C(F)(F)F)C	1
Clc1ccc(Oc2cc(S(=O)(=O)C(C)C)ccc2)cc1-c1nc(nc2c1cccc2C(F)(F)F)C	1
Clc1ccc(Oc2cc(F)cc(S(=O)(=O)C)c2)cc1-c1nc(nc2c1cccc2C(F)(F)F)C	1
Clc1ccc(Oc2cc(F)cc(S(=O)(=O)CC)c2)cc1-c1nc(nc2c1cccc2C(F)(F)F)C	1
Clc1ccc(OCc2cc(S(=O)(=O)C)ccc2)cc1-c1nc(nc2c1cccc2C(F)(F)F)C	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(F)cc(S(=O)(=O)C)c2)ccc1F	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(F)cc(S(=O)(=O)CC)c2)ccc1F	1
Clc1c2ncnc(c2ccc1)-c1cc(OCc2cc(S(=O)(=O)C)ccc2)ccc1F	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)CC)ccc2)ccc1F	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)C(C)C)ccc2)ccc1F	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)CCCO[C@H]3OCCCC3)ccc2)ccc1F	0
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)CCCO)ccc2)ccc1F	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)C)ccc2)ccc1F	1
Clc1ccc(Oc2cc(S(=O)(=O)C)ccc2)cc1-c1ncnc2c1cccc2OC	1
Clc1ccc(Oc2cc(S(=O)(=O)C)ccc2)cc1-c1ncnc2c1cccc2Cl	1
S(=O)(=O)(CCCO)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(CCCCO)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3n(nc2Cc2cccc2)C(=CC=N3)C(F)(F)F)ccc1	1
S(=O)(=O)(CC)c1cc(Oc2cc(ccc2)-c2c3n(nc2Cc2cccc2)C(=CC=N3)C(F)(F)F)ccc1	1
S(=O)(=O)(CCCO)c1cc(Oc2cc(ccc2)-c2c3n(nc2Cc2cccc2)C(=CC=N3)C(F)(F)F)ccc1	1
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2n3N=CC=C(c3nc2Cc2cccc2)C(F)(F)F)ccc1	1
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2n3N=CC=C(c3nc2CC)C(F)(F)F)ccc1	1
S(=O)(=O)(CC)c1cc(Oc2cc(ccc2)-c2n3N=CC=C(c3nc2CC)C(F)(F)F)ccc1	1
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2n3N=CC=C(c3nc2C(C)C)C(F)(F)F)ccc1	1
Clc1ccc(Oc2cc(S(=O)(=O)CCCC#N)ccc2)cc1-c1ncnc2c1cccc2C(F)(F)F	1

Clc1ccc(Oc2cc(S(=O)(=O)CCCC#N)ccc2)cc1-c1ncnc2c1cccc2Cl	1
Clc1ccc(Oc2cc(S(=O)(=O)CCCC(=O)N)ccc2)cc1-c1ncnc2c1cccc2Cl	1
Clc1ccc(Oc2cc(S(=O)(=O)CC#N)ccc2)cc1-c1ncnc2c1cccc2C(F)(F)F	1
Clc1ccc(Oc2cc(S(=O)(=O)CC(=O)N)ccc2)cc1-c1nc2c(cccc2C(F)(F)F)cn1	1
Clc1ccc(Oc2cc(S(=O)(=O)CC(=O)[O-])ccc2)cc1-c1ncnc2c1cccc2C(F)(F)F	1
Clc1ccc(Oc2cc(S(=O)(=O)NC)ccc2)cc1-c1ncnc2c1cccc2Cl	1
Clc1ccc(Oc2cc(S(=O)(=O)N)ccc2)cc1-c1ncnc2c1cccc2Cl	1
Clc1ccc(Oc2cc(S(=O)(=O)NC)ccc2)cc1-c1ncnc2c1cccc2C(F)(F)F	1
Clc1ccc(Oc2cc(S(=O)(=O)N)ccc2)cc1-c1ncnc2c1cccc2C(F)(F)F	1
S(=O)(=O)(NC)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)NC)ccc2)ccc1F	0
S(=O)(=O)(CCCC#N)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(CCCC(=O)N)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(CCCC(=O)[O-])c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(CCC[NH3+])c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(CCCCC#N)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(CCCS(=O)(=O)C)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(CCCCC(=O)N)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(CCCC[NH3+])c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
S(=O)(=O)(CCCCNS(=O)(=O)C)c1cc(Oc2cc(-c3ncnc4c3cccc4C(F)(F)F)c(F)cc2)ccc1	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)C)c(cc2)C(=O)N)ccc1F	0
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)CCC[NH3+])ccc2)ccc1F	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)CCCC#N)ccc2)ccc1F	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)CCCNS(=O)(=O)C)ccc2)ccc1F	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)CCCCNS(=O)(=O)C)ccc2)ccc1F	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)CCCCC#N)ccc2)ccc1F	1
Clc1c2ncnc(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)CCCCC(=O)N)ccc2)ccc1F	1
Clc1ccc(Oc2cc(S(=O)(=O)CCCC#N)ccc2)cc1-c1nc(nc2c1cccc2C(F)(F)F)C	1
Clc1ccc(Oc2cc(S(=O)(=O)CCCCC#N)ccc2)cc1-c1nc(nc2c1cccc2C(F)(F)F)C	1
Clc1ccc(Oc2cc(S(=O)(=O)CCCNS(=O)(=O)C)ccc2)cc1-c1nc(nc2c1cccc2C(F)(F)F)C	1
Clc1ccc(Oc2cc(S(=O)(=O)CCCCNS(=O)(=O)C)ccc2)cc1-c1nc(nc2c1cccc2C(F)(F)F)C	1

delete

Name	ratio
FC(F)(F)c1c2ncc(C(=O)c3ccccc3)c(c2ccc1)-c1cc(OCc2ccc(cc2)CC(=O)[O-])ccc1	3.400
FC(F)(F)c1c2ncc(C(=O)c3ccccc3)c(c2ccc1)-c1cc(OCc2ccc(cc2)[C@@H](CC=C)C(=O)[O-])c	3.200
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(OCc2ccc(cc2)CC(=O)[O-])ccc1	5.000
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(OCc2cc(C)c(cc2C)CC(=O)[O-])ccc1	3.667
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(ccc1)COc1cc(C)c(cc1C)CC(=O)[O-]	7.750
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(ccc1)CNc1ccc(cc1)CC(=O)[O-]	6.714
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(ccc1)CNc1c2c(ccc1)c(ccc2)C(=O)[O-]	4.486
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2ccccc2)CCCC)cc1	4.250
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2cc(ccc2)CCO)CCCC)cc1	7.667
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2ncccc2)CCCC)cc1	4.000
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2ccncc2)CCCC)cc1	3.600
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2ccccc2O)CCCC)cc1	4.500
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2cc(O)ccc2)CCCC)cc1	5.333

Fc1cccc(CN(CCCC)c2ccc(cc2)C(O)(C(F)(F)F)C(F)(F)F)c1O	5.125
Clc1cc(Cl)cc(CN(CCCC)c2ccc(cc2)C(O)(C(F)(F)F)C(F)(F)F)c1O	3.069
Clc1cc(cc(OC)c1OC)CN(CCCC)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F	6.600
Clc1cc(cc(Cl)c1O)CN(CCCC)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F	6.000
Clc1cc(cc(Cl)c1)CN(CCCC)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F	6.500
Clc1cc(cc(Cl)c1OC)CN(CCCC)c1ccc(cc1)C(O)(C(F)(F)F)C(F)(F)F	5.667
Clc1cc(S(=O)(=O)[C@@](C(OC)=O)(C)[C@@H]2CCc3c([nH]c4c3cc(Cl)cc4)C2)ccc1Cl	2.817
Clc1cc(S(=O)(=O)[C@@](C(OC)=O)(C)[C@@H]2CCc3c([nH]c4c3cc(Cl)cc4)C2)ccc1	5.467
Clc1cc(S(=O)(=O)[C@](F)(C(OC)=O)[C@@H]2CCc3c([nH]c4c3cc(Cl)cc4)C2)ccc1	3.226
Clc1cc2c3CC[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1cc(F)ccc1)(F)C(OC)=O	3.476
BrC1cc(S(=O)(=O)[C@](F)(C(OC)=O)[C@@H]2Cc3c([nH]c4c3cc(Cl)cc4)C2)ccc1	3.333
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1ncccc1)(F)C(OC)=O	3.089
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1cccc1)(F)C(OC)=O	6.450
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1cccc1)(F)c1ocnn1	4.694
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1cccc1)(F)c1oc(nn1)C1CC1	3.494
Clc1cc2c3C[C@H](Cc3[nH]c2cc1)[C@@](S(=O)(=O)c1cccc1)(F)c1onc(n1)C	7.778
FC(F)(F)c1c2ncc(Cc3cccc3)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(OC)=O)ccc1	4.358
FC(F)(F)c1c2ncc(c(c2ccc1)-c1cc(Oc2cc(ccc2)CO)ccc1)-c1cccc1	3.357
Clc1c2ncc(c(c2ccc1)-c1cc(Oc2cc(cc2)CO)ccc1)-c1cccc1	4.337
FC(F)(F)c1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(OC)=O)ccc1	>2.29885057471264
FC(F)(F)c1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(ccc2)CO)ccc1	4.857
FC(F)(F)c1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(cc2)CO)ccc1	4.226
Clc1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(OC)=O)ccc1	4.338
Clc1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(ccc2)CO)ccc1	4.917
FC(F)(F)c1c2ncc(Cc3cccc3)c(c2ccc1)-c1cc(Oc2ccc(O)cc2)ccc1	4.107
S(=O)(=O)(C)c1ccc(Oc2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)cc1	3.643
S(=O)(=O)(C)c1cccc1Oc1cc(ccc1)-c1c2c(ncc1C)c(ccc2)C(F)(F)F	>1.78571428571429
Clc1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)C)ccc2)ccc1	3.091
S(=O)(=O)(CC)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)ccc1	3.813
S(=O)(=O)(CCC)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)ccc1	8.846
S(=O)(=O)(C(C)C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)ccc1	4.389
S(=O)(=O)(CC(C)C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)ccc1	7.531
S(=O)(=O)(CCC(C)C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)ccc1	9.077
S(=O)(=O)(CCCO)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)ccc1	3.357
S(=O)(=O)(CCOC)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)ccc1	5.938
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)ccc1OC	6.829
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)cc(F)c1	3.474
Clc1cc(Oc2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)cc(S(=O)(=O)C)c1	9.333
S(=O)(=O)(CCCO)c1cc(Oc2cc(ccc2)-c2n3c(nc2C)C(=CC=C3)C(F)(F)F)ccc1	>5.31914893617021
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2n3c(nc2Cc2cccc2)C(=CC=C3)C(F)(F)F)ccc1	7.284
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2n3c(nc2C[NH+])2CCCC2)C(=CC=C3)C(F)(F)F)ccc1	>3.584229390681
S1CC[NH+](C1)Cc1nc2n(C=CC=C2C(F)(F)F)c1-c1cc(Oc2cc(S(=O)(=O)C)ccc2)ccc1	4.500
S(=O)(=O)(C(F)(F)F)c1cc(Oc2cc(ccc2)-c2n3c(nc2C(C)C)C(=CC=C3)C(F)(F)F)ccc1	>5.15463917525773
ClC=1c2n(C=CC=1)c(-c1cc(Oc3cc(S(=O)(=O)N)ccc3)ccc1)c(n2)C(C)C	>7.35294117647059
S(=O)(=O)(Cc1cc(Oc2cc(ccc2)-c2n3c(nc2C(C)C)C(=CC=C3)C(F)(F)F)ccc1)C	>5.3475935828877
S(=O)(=O)(C)c1cc(OCc2cc(ccc2)-c2n3c(nc2CC)C(=CC=C3)C(F)(F)F)ccc1	>3.42465753424658
S(=O)(=O)(C)c1cc(ccc1)-c1ccc(cc1)-c1n2c(nc1C(C)C)C(=CC=C2)C(F)(F)F	>6.02409638554217

O=C(NC(=O)[C@@]1([C@@H]2CCc3c(cccc3)[C@]2(CCC1)C)C1(CCCCC1)c1cccc1	3.500
FC(F)(F)c1noc2c1ccc(OCCCOc1ccc(cc1)CC(=O)[O-])c2CCC	7.300
Clc1cc(ccc1N(CCCOc1ccc2c(ocn2C(F)(F)F)c1CCC)C)CC(=O)[O-]	3.706
FC(F)(F)c1noc2c1ccc(OCCCN(C)c1cc(C)c(cc1)CC(=O)[O-])c2CCC	4.500
FC(F)(F)c1cc(N(CCCOc2ccc3c(ocn3C(F)(F)F)c2CCC)C)ccc1CC(=O)[O-]	3.333
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(Cc2ncccc2)CC)cc1	3.261
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](C(=O)NC)c2cccc2)CC)cc1	0.509
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](C(=O)N2CCOCC2)c2cccc2)CC)cc1	3.857
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(C(C(OC)=O)(C)c2cccc2)CC)cc1	6.250
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N(C(C(=O)N(C)C)(C)c2cccc2)CC)cc1	3.333
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](COCCO)c2cccc2)CC)cc1	0.375
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](COCC(=O)[O-])c2cccc2)CC)cc1	0.678
FC(F)(F)C(O)(C(F)(F)F)c1ccc(N([C@@H](COCC(=O)NC)c2cccc2)CC)cc1	0.581
Clc1cc(ccc1N([C@@H](COc1ccc(cc1)CC(OC)=O)c1cccc1)CC)C(O)(C(F)(F)F)C(F)(F)F	6.667
Clc1cc(ccc1N([C@@H](COc1ccc(cc1)CC(=O)[O-])c1cccc1)CC)C(O)(C(F)(F)F)C(F)(F)F	5.000
Clc1cc(ccc1N([C@@H](COc1ccc(cc1)C(=O)[O-])c1cccc1)CC)C(O)(C(F)(F)F)C(F)(F)F	5.000
Clc1cc(ccc1N([C@@H](COc1ccc(cc1)CCC(=O)[O-])c1cccc1)CC)C(O)(C(F)(F)F)C(F)(F)F	8.571
Clc1c(cccc1C(F)(F)F)C[NH+](CC(c1cccc1)c1cccc1)CCCOc1cc(ccc1)CC(=O)[O-]	8.333
FC(F)(F)c1c2ncc(Cc3cccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)CC(=O)[O-])ccc1	4.000
FC(F)(F)c1c2ncc(C)c(c2ccc1)-c1cc(NCc2ccc(cc2)CC(=O)[O-])ccc1	3.721
FC(F)(F)c1c2ncc([C@H](O)c3cccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)CC(=O)[O-])ccc1	6.809
FC(F)(F)c1c2ncc(C#N)c(c2ccc1)-c1cc(NCc2ccc(cc2)CC(=O)[O-])ccc1	4.438
O=C(c1cnc2c(cccc2C)c1-c1cc(NCc2ccc(cc2)CC(=O)[O-])ccc1)c1cccc1	3.273
O=C([O-])Cc1ccc(cc1)CNc1cc(ccc1)-c1c2c(ncc1Cc1cccc1)c(ccc2)C	4.200
Fc1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)CC(=O)[O-])ccc1	6.118
O=C(c1cnc2c(cccc2)c1-c1cc(NCc2ccc(cc2)CC(=O)[O-])ccc1)c1cccc1	4.221
Clc1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)CC(=O)[O-])ccc1	3.333
Clc1c2ncc(Cc3cccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)CC(=O)[O-])ccc1	3.571
FC(F)(F)c1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(NCc2cc(ccc2)CC(=O)[O-])ccc1	5.600
FC(F)(F)c1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(NCc2ccc(OCC(=O)[O-])cc2)ccc1	5.325
FC(F)(F)c1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)C(=O)[O-])ccc1	3.043
FC(F)(F)c1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)[C@H](C(=O)[O-])C)ccc1	5.846
FC(F)(F)c1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)C(C(=O)[O-])(C)C)ccc1	4.526
FC(F)(F)c1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)[C@@H](O)C(=O)[O-])ccc1	3.953
FC(F)(C(=O)[O-])c1ccc(cc1)CNc1cc(ccc1)-c1c2c(ncc1C(=O)c1cccc1)c(ccc2)C(F)(F)F	3.872
FC(F)(F)c1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)CC(=O)N)ccc1	7.857
FC(F)(F)c1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)CCO)ccc1	6.296
FC(F)(F)c1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(NCc2cccc2)ccc1	5.356
FC(F)(F)c1c2ncc(C(=O)c3cccc3)c(c2ccc1)-c1cc(NCc2ccc(cc2)CO)ccc1	7.070
FC(F)(F)c1c2nn(Cc3cccc3)c(c2ccc1)-c1cccc1	6.805
Fc1ccc(cc1)-c1n(nc2c1cccc2C(F)(F)F)Cc1ccc(cc1)C	7.800
Clc1cc(F)ccc1Cn1nc2c(cccc2C(F)(F)F)c1-c1ccc(F)cc1	7.458
Fc1cccc1Cn1nc2c(cccc2C(F)(F)F)c1-c1ccc(F)cc1	7.515
Clc1cccc1Cn1nc2c(cccc2C(F)(F)F)c1-c1ccc(F)cc1	9.281
Fc1ccc(cc1)-c1n(nc2c1cccc2C(F)(F)F)Cc1ccc(F)cc1	6.469
Clc1ccc(cc1)Cn1nc2c(cccc2C(F)(F)F)c1-c1ccc(F)cc1	6.914
Clc1cc(F)c(cc1)Cn1nc2c(cccc2C(F)(F)F)c1-c1ccc(Cl)cc1	6.842

Clc1cc(F)ccc1Cn1nc2c(cccc2C(F)(F)F)c1-c1ccc(Cl)cc1	8.400
Clc1ccccc1Cn1nc2c(cccc2C(F)(F)F)c1-c1ccc(Cl)cc1	9.475
Clc1ccc(cc1)-c1n(nc2c1cccc2C(F)(F)F)Cc1ccccc1F	8.000
Clc1ccc(cc1)-c1n(nc2c1cccc2C(F)(F)F)Cc1ccccc1C(F)(F)F	9.688
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)NC(C)C)ccc1	7.400
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)N(CC)CC)ccc1	4.286
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)N2CCCC2)ccc1	4.615
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)N2CCCCC2)ccc1	6.897
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)N2CCOCC2)ccc1	7.895
Clc1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)NC(C)C)ccc1	3.570
Clc1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)N(CC)CC)ccc1	9.000
Clc1c2ncc(C)c(c2ccc1)-c1cc(Oc2cc(ccc2)C(=O)N2CCCCC2)ccc1	8.333
Clc1c2nnc(Cc3ccccc3)c(c2ccc1)-c1cc(OCc2ccccc2)ccc1	3.913
Clc1ccccc1COc1cc(ccc1)-c1c2c(nnc1Cc1ccccc1)c(Cl)ccc2	6.571
Clc1c2nnc(Cc3ccccc3)c(c2ccc1)-c1cc(OCc2cc(ccc2)C(F)(F)F)ccc1	6.200
Clc1cccc(C(F)(F)F)c1COc1cc(ccc1)-c1c2c(nnc1-c1ccccc1)c(Cl)ccc2	5.108
Clc1c(cccc1C(F)(F)F)CNc1cc(ccc1)-c1c2c(nnc1-c1ccccc1)c(Cl)ccc2	9.421
Clc1c2nnc(c(c2ccc1)-c1cc(NCc2c3n(ccc3ccc2)C)ccc1)-c1ccccc1	6.200
FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(NCc2c3[nH]ccc3ccc2)ccc1	3.526
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C(=O)NCC)c(ccc3)C(F)(F)F)ccc1	9.403
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C(OCC)=O)c(ccc3)C(F)(F)F)ccc1	3.300
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C(=O)[O-])c(ccc3)C(F)(F)F)ccc1	5.933
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C#N)c(ccc3)C(F)(F)F)ccc1	6.091
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2-n2nnnc2)c(ccc3)C(F)(F)F)ccc1	5.027
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C[NH3+])c(ccc3)C(F)(F)F)ccc1	5.779
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C=[NH2+])N)c(ccc3)C(F)(F)F)ccc1	5.815
S(=O)(=O)(C)c1cc(Oc2cc(ccc2)-c2c3c(ncc2C(=O)N)cccc3)ccc1	>3.50877192982456
Clc1c2nc(n(c2ccc1)-c1cc(Oc2cc(S(=O)(=O)C(F)(F)F)ccc2)ccc1)C	9.150
S(=O)(=O)(C)c1cc(Oc2cc(-n3c4c(nc3C(F)(F)F)c(ccc4)C(F)(F)F)ccc2)ccc1	3.923
S(=O)(=O)(C)c1cc(Oc2cc(-n3c4c(nc3CC(C)C)c(ccc4)C(F)(F)F)ccc2)ccc1	4.000
S(=O)(=O)(C)c1cc(Oc2cc(-n3c4c(nc3-c3ccccc3)c(ccc4)C(F)(F)F)ccc2)ccc1	4.273
Clc1ccc(Oc2cc(S(=O)(=O)C)ccc2)cc1-n1c2c(nc1C)c(Cl)ccc2	3.784
Clc1ccc(Oc2cc(S(=O)(=O)CC)ccc2)cc1-n1c2c(nc1C)c(Cl)ccc2	3.429
Clc1ccc(Oc2cc(F)cc(S(=O)(=O)C)c2)cc1-n1c2c(nc1C)c(Cl)ccc2	9.362
Clc1ccc(Oc2cc(S(=O)(=O)C(F)(F)F)ccc2)cc1-n1c2c(nc1C)c(Cl)ccc2	5.000
S(=O)(=O)(CC)c1cc(ccc1)-c1ccc(cc1)-c1nc2c(nc1C)c(ccc2)C(F)(F)F	>7.57575757575758
S(=O)(=O)(C)c1cc(ccc1)-c1ccc(cc1)-c1nc2c(nc1CC)c(ccc2)C(F)(F)F	9.167
S(=O)(=O)(C)c1cc(ccc1)-c1ccc(cc1)-c1nc2c(nc1C)c(ccc2)C#N	>3.34448160535117
S(=O)(=O)(C)c1cc(ccc1)-c1ccc(cc1)-c1nc2c(nc1C)c(OC)ccc2	>2.53164556962025
S(=O)(=O)(C)c1cc(ccc1)-c1cc(ccc1)-c1c2c(ncc1C)c(ccc2)C(F)(F)F	5.000
S(=O)(=O)(C)c1ccc(cc1)-c1cc(ccc1)-c1c2c(ncc1C)c(ccc2)C(F)(F)F	>2.8169014084507
S(=O)(=O)(C)c1cc(ccc1)-c1cc(ccc1)-c1c2c(ncc1Cc1ccccc1)c(ccc2)C(F)(F)F	4.667
S(=O)(=O)(C)c1ccc(cc1)-c1cc(ccc1)-c1c2c(ncc1Cc1ccccc1)c(ccc2)C(F)(F)F	3.413
S(=O)(=O)(C)c1cc(ccc1C)-c1cc(ccc1)-c1c2c(ncc1C)c(ccc2)C(F)(F)F	3.750
S(=O)(=O)(C)c1cc(ccc1OC)-c1cc(ccc1)-c1c2c(ncc1C)c(ccc2)C(F)(F)F	>1.58982511923688
S(=O)(=O)(C)c1cc(ccc1F)-c1cc(ccc1)-c1c2c(ncc1C)c(ccc2)C(F)(F)F	5.882
S(=O)(=O)(C)c1cc(-c2cc(ccc2)-c2c3c(ncc2C)c(ccc3)C(F)(F)F)c(F)cc1F	3.030

<chem>S(=O)(=O)(C)c1cc(-c2cc(ccc2)-c2c3c(ncc2)c(ccc3)C(F)(F)F)c(F)cc1F</chem>	5.102
<chem>O(C(=O)[C@@]1([C@@H]2CCc3c(cc(O)cc3)[C@]2(CCC1)C)C)c1cc2c(CC[C@H]3[C@](CC</chem>	3.103
<chem>FC(F)(F)c1c2ncc(Cc3ccccc3)c(c2ccc1)-c1cc(Oc2cc(ccc2)CO)ccc1</chem>	6.410