Supporting Information

Discovery of Neuroprotective Compounds through Machine Learning Approaches

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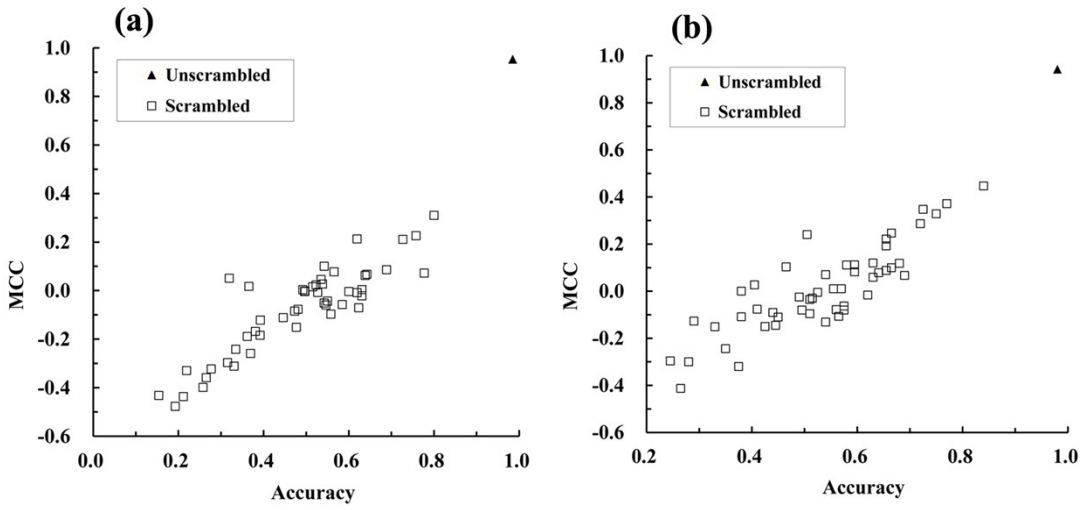
(a)
Unscrambled
Scrambled
MCC
Accuracy
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
0.0
0.2
0.4
0.6
0.8
1.0
(b)
Unscrambled
Scrambled
MCC
Accuracy
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
0.2
0.4
0.6
0.8
1.0

Figure S1.

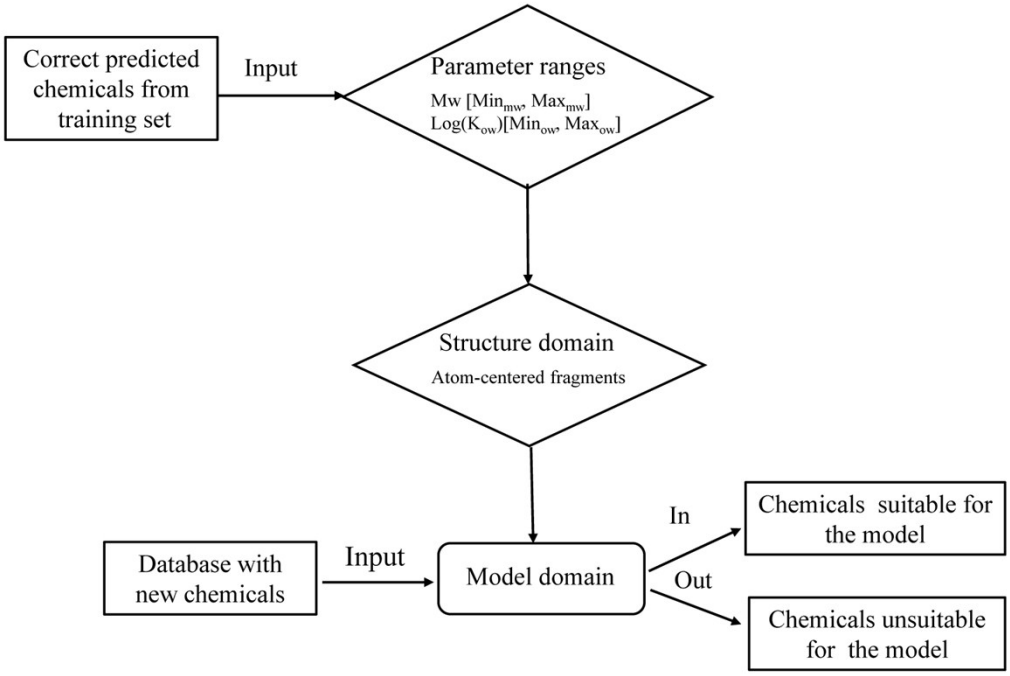
Correct predicted chemicals from training set
Input
Parameter ranges
Mw [Min$_{mw}$, Max$_{mw}$]
Log(K$_{ow}$)[Min$_{ow}$, Max$_{ow}$]
Structure domain
Atom-centered fragments
Database with new chemicals
Input
Model domain
In
Out
Chemicals suitable for the model
Chemicals unsuitable for the model

Figure S2.

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Table S1. Structures of the 1000 Compounds (in SMILE format) from the Training set together with their activities (1 or 0) for glutamate-induced models.

Name	Structure	Activity
CHEMBL2152538	Oc1cc2C[NH+]3C(N(c2cc1)C)c1c(CC3)cccc1	1
CHEMBL48310	OC1=CC(=CC=CC1=O)C(C)C	1
CHEMBL134342	S1SCC[C@H]1CCCCC(=O)[O-]	1
CHEMBL2425182	S(=O)(=O)(n1c2cc(ccc2c2c1cccc2)C(F)(F)F)c1ccc(cc1)C	1
CHEMBL565873	O(\N=C\1/CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@H](C(=O)C)[C@]4(CC3)C)CCC2=C/1)C)C(=O)[C@@H]([NH3+])C(C)C	1
CHEMBL430183	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@H]1O[C@@H]1OC=C[C@]2(O)[C@H]1[C@@](O)(C[C@H]2O)C	1
CHEMBL2334453	Clc1cc(ccc1Cl)CNC1=CC(=O)c2c(cccc2)C1=O	1
CHEMBL28862	P(=O)([O-])([O-])CCCC([NH3+])C(=O)[O-]	1
CHEMBL2425187	n1(c2c(c3c1cccc3)cccc2)-c1ccc(cc1)C(C)(C)C	1
CHEMBL397863	s1c(nnc1Nc1ccc(F)cc1)-c1ccc(O)cc1O	1
CHEMBL1641661	Oc1cc(cc(O)c1)\C=C\C=C\c1ccc(O)cc1	1
CHEMBL456235	o1c(ccc1CCCCCC)-c1cc(OC)c(O)cc1	1
CHEMBL9790	O=C1N=C2C=C(C#N)C([N+](=O)[O-])=CC2=NC1=O	1
CHEMBL543926	S1C=2CCCCC=2N(CC(=O)CC)C1=N	1
CHEMBL2387147	FC(F)(F)C(=O)N(\N=C\c1cc(OC)ccc1)c1ccc(cc1C)CO	1
CHEMBL607033	S1SCCC1CCCCc1onc(n1)Cc1c2c(OC(CC2)(C)C)c(C)c(C)c1O	1
CHEMBL1951836	O1c2c(cc(C)c(c2)C)C(=O)C(O)=C1c1ccc(N(C)C)cc1	1
CHEMBL344151	[NH2+]1[C@@H]2Cc3c(cccc3)[C@]1(c1c2cccc1)C	1
CHEMBL34792	S1SCCC1CC(=O)Nc1ccc(NC(=[NH2+])c2sccc2)cc1	1
CHEMBL1802358	O1c2cc(ccc2OC1)\C=C\1/N=C(NC/1=O)Nc1ccccc1	1
CHEMBL1096005	OC1=CC(=CC=C(C[NH+]2CCN(CC2)C(OCC)=O)C1=O)C(C)C	1
CHEMBL481060	O1c2c(cccc2)C(=O)C=C1CCc1ccccc1	1
CHEMBL551213	Oc1cc(ccc1O)\C=C\c1ccc(cc1)COC(=O)CNC(=O)c1ccccc1	1
CHEMBL2391370	O=C(NC1CCCC1)C([NH+]1CCC[NH2+]CC1)C	1
CHEMBL259223	O=C1c2c(cccc2)C(=O)C(C)=C1C\C=C(\CC\C=C(\CC\C=C(\CC\C=C(\C)/C)/C)/C)/C	1
CHEMBL257170	O1[C@H]([C@]2(C(=C(CCC2)C)C1=O)C)c1ccoc1	1
CHEMBL243623	Fc1cc(ccc1OC)C(=O)\C=C\c1cc(OC)c(O)cc1	1
CHEMBL1951856	O(CC)c1cc(nc2c1cccc2)-c1cc(O)c(O)cc1	1
CHEMBL2334454	O=C1c2c(cccc2)C(=O)C=C1C(=O)[O-]	1
CHEMBL496686	O(C(=O)C(NC(=O)[C@]1(C2CC=C3[C@H](CCC(=C3)C(C)C)[C@]2(CCC	1

	1)C)C)CO)CC	
CHEMBL1926761	S1(=O)(=O)N(CCCC[NH2+]CC2Oc3c(CC2)cccc3)C(=O)c2c1cccc2	1
CHEMBL479698	O1c2c(C[C@H](OC(=O)[C@]3(O[C@H]3C)C)C1(C)C)cc1C=CC(Oc1c2)=O	1
CHEMBL391366	S1SCCC1CCCCc1nnnn1CCc1cc(O)c(O)cc1	1
CHEMBL465508	O(C)c1cc(CO)c(N2CN(c3c(cc(OC)cc3)C2=O)C=O)cc1	1
CHEMBL2151787	Clc1cc2[nH+]c3c(CCCC3)c(NCCNC(=O)\C=C\c3cc(O)c(O)cc3)c2cc1	1
CHEMBL1215856	OC1(CC[NH+](CC1)C[C@H]1C[C@]1(C(OC)=O)c1ccc(cc1)C)c1ccccc1	1
CHEMBL499750	O(C)c1cc(ccc1O)C(O[C@H]1[C@H]2[C@](CC[C@@H]3[C@@]2(CC[C@H](O)C3(C)C)C)(C)[C@]2([C@@H]([C@@H]3[C@@](C[C@@H]2O)(CC[C@H]3C(C)=C)C)C1)C)=O	1
CHEMBL1087801	FC(F)(F)c1cc(ccc1)C[NH+](Cc1c2c(nccc2)c(O)cc1)Cc1c2c(nccc2)c(O)cc1	1
CHEMBL1641662	Oc1ccc(cc1C(C)(C)C)\C=C\c1ccc(O)cc1	1
CHEMBL444109	O1[C@@]2([C@@]34Oc5c(C(=O)C3=C[C@H](CC4C1(C)C)C2=O)c(O)c1c(O[C@@](C=C1)(CC\C=C(\C)/C)C)c5C\C=C(\C)/C)C\C=C(/C(=O)N)\C	1
CHEMBL1813353	O1c2c(CCC1(C)C)c(-c1noc(c1)-c1ccc([N+](=O)[O-])cc1)c(O)c(C)c2C	1
CHEMBL2334458	O=C1c2c(cccc2)C(=O)C=C1NC1CCCC1	1
CHEMBL430187	O1c2cc(ccc2OC1)C(=O)\C=C\c1cc(OC)c(O)cc1	1
CHEMBL202194	O1c2c(CCC1(C(=O)N1CCN(CC1)C(=O)\C=C\c1cc(OC)c(OC)cc1)C)c(C)c(O)c(C)c2C	1
CHEMBL50	O1c2c(C(=O)C(O)=C1c1cc(O)c(O)cc1)c(O)cc(O)c2	1
CHEMBL498754	P(=O)([O-])([O-])C(NC(=O)CCCCCCCCCCCCCCCCC)CO	1
CHEMBL496878	O1C(C(O)COC(=O)CCCCCNC(=O)CCCCCCCCCCCCCCCCC)C([O-])=C(O)C1=O	1
CHEMBL55934	O=C1C=CC(=O)c2c1cccc2	1
CHEMBL162460	O=C1c2c(cccc2)C(=O)C=C1N(C)C	1
CHEMBL1951841	O1c2c(ccc3c2cccc3)C(=O)C(O)=C1c1cc(O)c(N2CCCC2)cc1	1
CHEMBL2391375	O=C(N1CC[NH+](CC1)CC(=O)NCCC(C)(C)C)C1CCCCC1	1
CHEMBL56	Oc1c2CC([NH+](CCC)CCC)CCc2ccc1	1
CHEMBL2069517	O1CC[NH+](CC1)CCO\N=C(/C)\[C@H]1CC[C@H]2[C@H]3[C@H](CC[C@]12C)[C@@]1(C(=CC(=O)CC1)CC3)C	1
CHEMBL2425186	O(C)c1ccc(-n2c3c(c4c2cccc4)cccc3)cc1	1
CHEMBL402437	O1[C@H]([C@]2([C@@]3(O[C@@H]3C1=O)[C@]1([C@@H]([C@]34[C@@H](C(=O)[C@@H]1O)C(O[C@H]3CC(OC4)=O)(C)C)CC2)C)C)c1cocc1	1
CHEMBL1165316	O1c2c(CCC1(C)c1oc(nn1)Cc1cc(OC)c(OC)cc1)c(C)c(O)c(C)c2C	1
CHEMBL505393	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1Oc1c(OC)cc(	1

	cc1OC)[C@H]1OC[C@H]2[C@@H]1CO[C@@H]2c1cc(OC)c(O[C@H]2O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]2O)c(OC)c1	
CHEMBL1641654	Oc1c(cc(cc1C(CC)CC)\C=C\c1cc(O)cc(O)c1)C(CC)CC	1
CHEMBL60542	Oc1cc2c(C[C@@H]3[NH+](CC[C@@]2(C)[C@@H]3C)C\C=C(\C)/C)cc1	1
CHEMBL561200	Oc1cc(ccc1O)\C=C\c1ccc(cc1)C(=O)N1CCC(CC1)Cc1ccccc1	1
CHEMBL2069514	O=C(C)[C@H]1CC[C@H]2[C@H]3[C@H](CC[C@]12C)[C@@]1(C(=C/C(=N/O)/CC1)CC3)C	1
CHEMBL103	O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@H](C(=O)C)[C@]4(CC3)C)CCC2=C1)C	1
CHEMBL201538	O1c2c(CCC1(C)C)c(CCc1cc(O)c(O)cc1)c(O)c(C)c2C	1
CHEMBL1164503	O1c2c(CCC1(C)C)c(Cn1nnnc1CCc1cc(O)c(O)cc1)c(O)c(C)c2C	1
CHEMBL1926733	O1c2c(CCC1C[NH2+]CCCCN1C(=O)C3N(CCC3)C1=O)cccc2	1
CHEMBL1096006	OC1=CC(=CC=C(C[NH+]2CCN(CC2)c2ccc([N+](=O)[O-])cc2)C1=O)C(C)C	1
CHEMBL2152551	O(C(=O)NCCCCCCC)c1cc2C[NH+]3C(N(c2cc1)C)CCC3	1
CHEMBL556153	Oc1cc(ccc1O)\C=C\c1ccc(cc1)\C=C\C=O	1
CHEMBL305187	Oc1ccc(cc1)C(O)C([NH+]1CCC(CC1)Cc1ccccc1)C	1
CHEMBL201543	O1c2c(CCC1(CNC(=O)\C=C\c1cc(O)c(O)cc1)C)c(C)c(O)c(C)c2C	1
CHEMBL1813358	Fc1ccc(cc1)-c1noc(c1)-c1c2c(OC(CC2)(C)C)c(C)c(C)c1O	1
CHEMBL2425170	FC(F)(F)c1ccc(-n2c3c(c4c2cccc4)cccc3)cc1	1
CHEMBL2391363	O=C(N1CC[NH+](CC1)CCC(=O)NC1CCCCC1)C1CC1	1
CHEMBL572318	O=C1c2c(cccc2)C(=O)C(N)=C1C	1
CHEMBL236288	S1SCCC1CCCCc1oc(nn1)CCc1cc(O)c(O)cc1	1
CHEMBL605527	S1SCCC1CCCCC(=O)NCC1(Oc2c(CC1)c(C)c(O)c(C)c2C)C	1
CHEMBL2069526	O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@H](/C(=N/OC(=O)c5cccnc5)/C)[C@]4(CC3)C)CCC2=C1)C	1
CHEMBL2204447	O1c2c(C(=O)[C@H](O)[C@H]1c1cc3O[C@H]([C@@H](Oc3cc1)COC(=O)CCC(=O)NCCCCCCNc1c3CCCCc3[nH+]c3c1cccc3)c1cc(OC)c(O)cc1)c(O)cc(O)c2	1
CHEMBL1951865	O(C1CCCC1)c1cc(nc2c1cccc2)-c1cc(O)c(O)cc1	1
CHEMBL2334451	O=C1c2c(cccc2)C(=O)C=C1NCc1ccc(cc1)C(OC)=O	1
CHEMBL2334466	O=C1c2c(cccc2)C(=O)C=C1NCc1ncccc1	1
CHEMBL1951848	O(Cc1ccccc1)c1cc(ccc1OC)\C=C\C(=O)c1cc(C)c(cc1O)C	1
CHEMBL403868	O1[C@H]([C@]2(C([C@H](O)C1=O)=C(C)[C@@H](O)CC2)C)c1ccoc1	1
CHEMBL479684	O1c2c(C(=O)C=C1CCc1ccccc1O)c(O)ccc2	1
CHEMBL2334457	O=C1c2c(cccc2)C(=O)C=C1NCCC	1
CHEMBL561002	Oc1cc(ccc1O)\C=C\c1ccc(cc1)C(=O)NCC=C	1

CHEMBL499411	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1OC=C([C@@H]2[C@H]1C(=C[C@H]2OC(=O)\C=C/c1ccc(O)cc1)CO)C(OC)=O	1
CHEMBL1090054	O1CC[NH+](CC1)CC1=CC=C(C=C(O)C1=O)C(C)C	1
CHEMBL354201	O=C1c2c(cccc2)C(=O)C(C)=C1C	1
CHEMBL228675	O1c2c(C(=O)C=C1\C=C\c1ccccc1)c(O)ccc2	1
CHEMBL603959	S1SCCC1CCCCCn1nnc(c1)C1(Oc2c(CC1)c(C)c(O)c(C)c2C)C	1
CHEMBL466728	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1OCCCc1cc(O)c(O[C@H]([C@H](O)c2cc(OC)c(O)cc2)CO)cc1	1
CHEMBL256319	O1[C@H]([C@]2([C@@]3(O[C@@H]3C1=O)C(=CCC2)C)C)c1ccoc1	1
CHEMBL1087935	s1cccc1C[NH+](Cc1c2c(nccc2)c(O)cc1)Cc1c2c(nccc2)c(O)cc1	1
CHEMBL479697	O1c2c(C[C@H](OC(=O)\C=C(\CO)/C)C1(C)C)cc1C=CC(Oc1c2)=O	1
CHEMBL2387146	FC(F)(F)C(=O)N(\N=C\c1cc(O)c(O)cc1)c1ccc(cc1C)C	1
CHEMBL2391358	O=C(NC1CCCCC1)C([NH+]1CC[NH+](CC1)C1CCCC1)CC	1
CHEMBL2069520	O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@H](/C(=N/OC(=O)[C@H]5[NH2+]CCC5)/C)[C@]4(CC3)C)CCC2=C1)C	1
CHEMBL497730	OC1(\C=C\C(=C\C(=O)NC(C(OCC)=O)CO)\C)C(CC(=O)C=C1C)(C)C	1
CHEMBL555017	O1[C@@]2([C@@]34Oc5c(C(=O)C3=C[C@H](C[C@H]4C1(C)C)C2=O)c(O)c1c(O[C@@](C=C1)(CC\C=C(\C)/C)C)c5C\C=C(\C)/C)C\C=C(/C(=O)[O-])\C	1
CHEMBL1096354	O1c2c(CCC1(C(=O)NCC[NH+]1CC[NH+](CC1)CC1=CC=C(C=C(O)C1=O)C(C)C)C)c(C)c(O)c(C)c2C	1
CHEMBL429261	S1SCCC1CCCCCc1n[nH]c(c1)-c1cc(O)c(O)cc1	1
CHEMBL1164844	O1c2c(CCC1(C)C)c(Cc1nc(on1)-c1cc(O)c(O)cc1)c(O)c(C)c2C	1
CHEMBL551681	o1cccc1CNC(=O)c1ccc(cc1)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2425171	n1(c2c(c3c1cccc3)cccc2)-c1ccc(N(C)C)cc1	1
CHEMBL556068	S1C=2CCCCC=2N(Cc2ccccc2)C1=N	1
CHEMBL2391356	O=C(NC(C)C)C[NH+]1CC[NH2+]CC1	1
CHEMBL2391361	O=C(NC(CC)CC)C[NH+]1CCC[NH+](CC1)C	1
CHEMBL1165155	O1c2c(CCC1(C)C)c(-c1noc(c1)-c1cc(O)c(O)cc1)c(O)c(C)c2C	1
CHEMBL2425165	n1(c2cc(ccc2c2c1cccc2)-c1ccccc1)-c1ccc(cc1)C	1
CHEMBL2334459	O=C1c2c(cccc2)C(=O)C=C1NCC1CCCCC1	1
CHEMBL1641664	O(C)c1c(cc(cc1C(C)(C)C)\C=C\c1cc(O)cc(O)c1)C(C)(C)C	1
CHEMBL481657	O1c2c(C[C@H](O)C1(C)C)cc1C=CC(Oc1c2)=O	1
CHEMBL452919	O1c2c(C(=O)C(O[C@@H]3O[C@H](CO)[C@H](O)[C@H](O)[C@H]3O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)=C1c1cc(O)c(O)cc1)c(O)cc(O)c2	1

CHEMBL428020	S1SCCC1CCCCc1onc(n1)-c1cc(O)c(O)cc1	1
CHEMBL305195	Oc1ccc(cc1)[C@H](O)[C@H](C[NH+]1CCC(CC1)Cc1ccccc1)C	1
CHEMBL2387144	FC(F)(F)C(=O)N(\N=C\c1cc(OC)ccc1)c1ccc(cc1C)C	1
CHEMBL2391359	O=C(N(C)C1CCCC1)C[NH+]1CC([NH+](CC1)CC)C	1
CHEMBL2391374	O=C(NC(C)C)C([NH+]1CC[NH+](CC1)C1CCCCC1)(C)C	1
CHEMBL1951857	O(C(C)C)c1cc(nc2c1cccc2)-c1cc(O)c(O)cc1	1
CHEMBL2334462	O=C1c2c(cccc2)C(=O)C=C1N(Cc1ccccc1)C	1
CHEMBL594077	S1SCCC1CCCCc1oc(nn1)C1(Oc2c(CC1)c(C)c(O)c(C)c2C)C	1
CHEMBL1096355	OC1=CC(=CC=C(C[NH+]2CC[NH+](CC2)CC2=CC(=CC=C(O)C2=O)C(C)C)C1=O)C(C)C	1
CHEMBL2391381	O=C(N1CCC[NH+](CC1)CCC(=O)NC1CCCCCC1)C	1
CHEMBL1951843	Oc1cc(C)c(cc1C(=O)\C=C\c1cc(O)c(O)cc1)C	1
CHEMBL42905	O=C1C=C([O-])c2c(cccc2)C1=O	1
CHEMBL402945	O1[C@H]([C@]2(C([C@H](C)[C@@H](O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)CC2)=C(O)C1=O)C)c1ccoc1	1
CHEMBL138529	O1c2c(CCC1(C(=O)NCCc1cc(OC)c(OC)cc1)C)c(C)c(O)c(C)c2C	1
CHEMBL2391350	O=C(NC1CCCCC1)CC[NH+]1[C@H]2C[C@H]([NH2+]C2)C1	1
CHEMBL1164222	O1c2c(CCC1(C)c1onc(n1)-c1cc(OC)c(OC)cc1)c(C)c(O)c(C)c2C	1
CHEMBL2334460	O=C1c2c(cccc2)C(=O)C=C1NCC#C	1
CHEMBL478316	Oc1c2ncccc2c(cc1)C[NH+](Cc1c2c(nccc2)c(O)cc1)Cc1ccc(cc1)C	1
CHEMBL1983100	O=C(NC1CCCCC1)C[NH+]1CC[NH2+]CC1	1
CHEMBL2334452	FC(F)(F)c1cc(ccc1)CNC1=CC(=O)c2c(cccc2)C1=O	1
CHEMBL84010	O=C1c2c(cccc2)C(=O)C=C1Nc1ccccc1	1
CHEMBL465250	O1[C@H](COC(=O)\C=C/c2ccc(OC)cc2)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1OC=C[C@]2(O)[C@H]1[C@@](O)(C[C@H]2O)C	1
CHEMBL2391366	O=C(N1CC[NH+](CC1)CC(=O)NC(CC)CC)CC	1
CHEMBL2334456	O=C1c2c(cccc2)C(=O)C=C1NC(C)C	1
CHEMBL404140	O1C([C@@H]2CC(=O)[C@@]3([C@H](CC[C@@]4([C@@]35O[C@@H]5C(O[C@H]4c3ccoc3)=O)C)[C@]2(C=CC1=O)C)C)(C)C	1
CHEMBL464644	O(C)c1cc(CO)c(N2C=Nc3c(cc(OC)cc3)C2=O)cc1	1
CHEMBL2391540	O=C(N(C)C1CCCC1)C[NH+]1CC[NH2+]CC1	1
CHEMBL257169	O1[C@H]([C@]2(C(=C(C)[C@@H](O)CC2)C1=O)C)c1ccoc1	1
CHEMBL1813360	O1c2c(CCC1(C)C)c(-c1onc(c1)-c1ccc(OC)cc1)c(O)c(C)c2C	1
CHEMBL1951846	Oc1c2c(ccc1C(=O)\C=C\c1cc(O)c(O)cc1)cccc2	1
CHEMBL479683	O1c2c(C(=O)C=C1CCc1ccccc1)c(O)ccc2	1
CHEMBL1951840	O1c2c(cc(C)c(c2)C)C(=O)C(O)=C1c1ccc(N2CCCC2)cc1	1

CHEMBL2425177	S(=O)(=O)(n1c2c(c3c1cccc3)cccc2)c1ccc(cc1)CC	1
CHEMBL32644	S1SCCC1CCCCC(=O)NCCc1ccc(NC(=[NH2+])c2sccc2)cc1	1
CHEMBL240319	O=C1c2c(cccc2)C(=O)C=C1NC	1
CHEMBL2152550	Oc1cc2C[NH+]3C(N(c2cc1)C)CCC3	1
CHEMBL481658	O1c2c(C[C@H](OC(=O)\C=C(\C)/C)C1(C)C)cc1C=CC(Oc1c2)=O	1
CHEMBL2391357	O=C(NC1CCCCC1)C[NH+]1CCC[NH+](CC1)C	1
CHEMBL2069530	O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@H](/C(=N/OC(=O)C5CC[NH2+]CC5)/C)[C@]4(CC3)C)CCC2=C1)C	1
CHEMBL2387145	FC(F)(F)C(=O)N(\N=C\c1cc(O)ccc1)c1ccc(cc1C)C	1
CHEMBL2334455	O=C1c2c(cccc2)C(=O)C=C1NCC	1
CHEMBL1951853	O(C)c1cc(nc2c1cccc2)-c1cc(O)c(O)cc1	1
CHEMBL1165331	O1c2c(CCC1(C)C)c(-c1nnn(c1)Cc1cc(O)c(O)cc1)c(O)c(C)c2C	1
CHEMBL2334463	O=C1c2c(cccc2)C(=O)C=C1NCCc1ccccc1	1
CHEMBL2391364	O=C(N(CCCC)CCC)C[NH+]1CC[NH2+]CC1	1
CHEMBL1813357	O1c2c(CCC1(C)C)c(-c1onc(c1)-c1ccccc1)c(O)c(C)c2C	1
CHEMBL2334465	O=C1c2c(cccc2)C(=O)C=C1NCc1cccnc1	1
CHEMBL2334470	O(C)c1ccc(cc1)CNC1=CC(=O)c2c(cccc2)C1=O	1
CHEMBL2391377	O=C(N1CC[NH+](CC1)C(C(=O)NC1CCCC1)C)CC	1
CHEMBL1813362	O1c2c(CCC1(C)C)c(-c1noc(c1)-c1c3c(OC(CC3)(C)C)c(C)c(C)c1O)c(O)c(C)c2C	1
CHEMBL466928	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@H]([C@@H](O)c1cc(OC)c(O)c(OC)c1)CO	1
CHEMBL2069519	O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@H](/C(=N/OC(=O)[C@@H]([NH3+])C(C)C)/C)[C@]4(CC3)C)CCC2=C1)C	1
CHEMBL593382	S1SCCC1CCCCCn1nnc(c1)Cc1c2c(OC(CC2)(C)C)c(C)c(C)c1O	1
CHEMBL1641655	Oc1ccc(cc1C(C)(C)C)\C=C\c1cc(O)cc(O)c1	1
CHEMBL461923	Fc1c(F)cc(cc1F)C(=O)\C=C\c1cccc(OC)c1O	1
CHEMBL415711	O=C1c2c(cccc2)C(=O)C=C1N	1
CHEMBL1164853	O1c2c(CCC1(C)C)c(CC(=O)\C=C\c1cc(O)c(O)cc1)c(O)c(C)c2C	1
CHEMBL2425180	S(=O)(=O)(n1c2cc(ccc2c2c1cccc2)-c1ccccc1)c1ccc(cc1)C	1
CHEMBL500570	O1c2c(C(=O)C(O[C@@H]3O[C@H](CO)[C@H](O)[C@H](O)[C@H]3O[C@@H]3O[C@H](COC(=O)\C=C\c4cc(OC)c(O)cc4)[C@@H](O)[C@H](O)[C@H]3O)=C1c1cc(O)c(O)cc1)c(O)cc(O)c2	1
CHEMBL445512	Oc1ccc(cc1)C(O[C@H]1[C@H]2[C@](CC[C@@H]3[C@@]2(CC[C@H](O)C3(C)C)C)(C)[C@]2([C@@H]([C@@H]3[C@@](C[C@@H]2O)(CC[C@H]3C(C)=C)C)C1)C)=O	1
CHEMBL595013	S1SCCC1CCCCC(=O)NCc1c2c(OC(CC2)(C)C)c(C)c(C)c1O	1

CHEMBL2152541	Oc1cc2C[NH+]3C(N(c2cc1)C)c1c(CCC3)cccc1	1
CHEMBL594076	S1SCCC1CCCCCc1nc(on1)C1(Oc2c(CC1)c(C)c(O)c(C)c2C)C	1
CHEMBL465507	O(C)c1cc(CO)c(N2Cc3cc(OC)ccc3N(C2)C=O)cc1	1
CHEMBL590	O=C1c2c(cccc2)C(=O)C=C1C	1
CHEMBL464888	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1OC=C[C@]2(O)[C@H]1[C@@](OC(=O)\C=C/c1ccccc1)(C[C@H]2O)C	1
CHEMBL2152543	O(C(=O)NCCCCCCC)c1cc2C[NH+]3C(N(c2cc1)C)c1c(CCC3)cccc1	1
CHEMBL2391354	O=C(NC1CCCCC1)C[NH+]1CC2[NH+](CCCC2)CC1	1
CHEMBL1165154	O1c2c(CCC1(C)C)c(Cn1nnc(c1)-c1cc(O)c(O)cc1)c(O)c(C)c2C	1
CHEMBL32450	S1SCCC1CCCCC(=O)Nc1ccc(NC(=[NH2+])c2sccc2)cc1	1
CHEMBL575601	O1C[C@]23[C@@H](CC(=O)[C@]4([C@@]56O[C@@H]5C(=O)C[C@H]([C@@]6(CC[C@H]24)C)c2occc2)C)C(O[C@@H]3CC1=O)(C)C	1
CHEMBL444904	O(C)c1cc(ccc1O)C(O[C@H]1C[C@@]2([C@@H]([C@H]3C[C@@H](OC(=O)c4cc(OC)c(O)cc4)[C@H]4[C@](CC[C@@H]5[C@@]4(CC[C@H](O)C5(C)C)C)(C)[C@]13C)[C@@H](CC2)C(C)=C)C)=O	1
CHEMBL2391362	O=C(N(CCCC)CCC)C[NH+]1C[C@@H]([NH2+]C[C@H]1C)C	1
CHEMBL1813355	O1c2c(CCC1(C)C)c(-c1noc(c1)-c1ccc(O)cc1)c(O)c(C)c2C	1
CHEMBL2391360	O=C(N1CC[NH+](CC1)CC(=O)NCC(CC)C)CC	1
CHEMBL1641653	Oc1ccc(cc1C(CC)CC)\C=C\c1cc(O)cc(O)c1	1
CHEMBL1951842	O1c2c(cc(C)c(c2)C)C(=O)C(O)=C1c1cc(O)c(N2CCCC2)cc1	1
CHEMBL1641666	O(C)c1cc(cc(O)c1)\C=C\c1cc(C(C)(C)C)c(O)c(c1)C(C)(C)C	1
CHEMBL1164286	O1c2c(CCC1(C)c1onc(n1)Cc1cc(OC)c(OC)cc1)c(C)c(O)c(C)c2C	1
CHEMBL31574	O1c2c(ccc(O)c2)C(=O)C(O)=C1c1cc(O)c(O)cc1	1
CHEMBL2334461	O=C1c2c(cccc2)C(=O)C=C1NCc1ccccc1	1
CHEMBL2334469	O=C1c2c(cccc2)C(=O)C=C1NCc1ccc(cc1)C	1
CHEMBL1165069	O1c2c(CCC1(C)C)c(Cc1nc(on1)CCc1cc(O)c(O)cc1)c(O)c(C)c2C	1
CHEMBL1165407	O1c2c(CCC1(C)C)c(Cc1nc(on1)\C=C\c1cc(O)c(O)cc1)c(O)c(C)c2C	1
CHEMBL594858	S1SCCC1CCCCc1nnnn1Cc1c2c(OC(CC2)(C)C)c(C)c(C)c1O	1
CHEMBL1096007	OC1=CC(=CC=C(C[NH+]2CC[NH+](CC2)Cc2ccc([N+](=O)[O-])cc2)C1=O)C(C)C	1
Decoy001	O(c1ccc(cc1)C(=O)NC1=CNC(=O)NC1=O)c1ccc(cc1)C(=O)NC1=CNC(=O)NC1=O	0
Decoy002	Br[C@H](C(C)(C)C)CC[C@@H]1C[C@H](CCC1)C	0
Decoy003	[S-]c1ccc(cc1)C#N	0
Decoy004	FC(F)(C(=O)[O-])C(F)F	0
Decoy005	ClC=1CS(=O)(=O)CC=1	0
Decoy006	BrC\C=C\C#N	0

Decoy007	Clc1ccc(Cl)cc1[C@H](Cl)c1c2c(cccc2)c(F)cc1	0
Decoy008	s1cccc1[C@@H](N1N=C(CC1)C)C#N	0
Decoy009	SCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCO	0
Decoy010	N#CC1CC2CC(CC2C1)C#N	0
Decoy011	Brc1cc(ccc1)C1CC([NH2+]C)C1	0
Decoy012	S=C1O[C@H]2[C@H](O1)CC1CC(C1)C2	0
Decoy013	s1c(ccc1CO)-c1cc(C)c(cc1)C	0
Decoy014	FC1(F)OC(F)(F)C[NH2+]C1	0
Decoy015	N(NC(c1ccccc1)(c1ccccc1)c1ccccc1)c1ccccc1	0
Decoy016	O=Cc1c2CCCCc2[nH]c1	0
Decoy017	O\N=C(/C)\[C@@H]1[C@H]2C=C[C@@H](C1)C2	0
Decoy018	Brc1cc([N+](=O)[O-])c(SC2CCCCC2)cc1	0
Decoy019	o1c(ccc1\C=C(\C#N)/C#N)C	0
Decoy020	O=C(N(C)C)[C@H]([NH2+][C@H](CC#N)C)C	0
Decoy021	ClCCC#Cc1cncnc1	0
Decoy022	S(C(C)(C)C)C(=O)C	0
Decoy023	O=C[C@H]1C=CCC[C@@H]1C	0
Decoy024	Cl\C(\Cl)=C\1/CCCC/1=O	0
Decoy025	ClC(Cl)(Cl)C(OC)=[N-]	0
Decoy026	S(=O)(=O)(NCCNC(=O)NCC(=O)[O-])C	0
Decoy027	O=C1NC2C=C[C@H]3[C@H](C13)C=C2	0
Decoy028	O=C1CC(CC([O-])=C1\C=N\CC(C)(C)C)(C)C	0
Decoy029	S1C(C=C(N=C1SSSC=1SC(C=C(N=1)C)(C)C)C)(C)C	0
Decoy030	O=C([O-])C1C[C@H]2C[C@@H](C1)C2([NH3+])C(=O)[O-]	0
Decoy031	N#C[C@@H](C(C)C)c1ccc(cc1)-c1ccc(cc1)C(C)C	0
Decoy032	O1[C@@H](CCC[C@H]1OC)C	0
Decoy033	Brc1cc(F)c(cc1)-c1oc(nn1)C	0
Decoy034	FC(F)(F)[C@H](O)CC#N	0
Decoy035	NC=1C(C#N)(C#N)[C@@H]([C@@H]2C(=CCCCC2)C=1C#N)c1c(cc(cc1C)C)C	0
Decoy036	[nH+]1c(nc(N(C)C)cc1C)C1CN(C1)c1nc[nH+]c(c1)C	0
Decoy037	[O-][N+](C)(C)C12CC3CC(C1)CC(C2)C3	0
Decoy038	Clc1cc(cc(OCC)c1OCc1ccc(F)cc1)C[NH2+]CCC[NH2+]CC	0
Decoy039	P(O[C@@H]1[C@H](O)[C@H](C)[C@@H](C)[C@H](O)[C@@H]1O)(=O)([O-])[O-]	0
Decoy040	S1CCSC[C@@H]1C#N	0
Decoy041	Clc1oc(C)c(c1)[C@@H](C(C)C)C(=O)[O-]	0

Decoy042	Brc1cc(cc([O-])c1)C#N	0
Decoy043	Brc1ccc(cc1)C(=O)CSc1nc2c(cccc2C)c(c1)C	0
Decoy044	ClC[C@@H]1ON=C(C1)C1CC1	0
Decoy045	s1cc(nc1N[C@H](C(=O)[O-])C)C	0
Decoy046	O=C([O-])\C=C\C(=C\C)\CC	0
Decoy047	[S-]C1(CCCCC1)C=O	0
Decoy048	O=C(Nc1ccccc1C(C)(C)C)N[C@H]1C[C@@H]1C	0
Decoy049	Clc1sc(cc1)CNC#N	0
Decoy050	BrC=1CC=NC2=NC=NC=12	0
Decoy051	Fc1c(ccc(F)c1F)C1(O)CCCCCC1	0
Decoy052	Clc1sc(cc1)C(=O)NC1(CCCC1)/C(=N\O)/N	0
Decoy053	O=C1N(C(=O)C[C@H]1C)c1cc(ccc1)C#C	0
Decoy054	O1[C@@H]2[C@@H](OC[C@@H]1C(=O)N(CC1CC1)C)C=CC=C2	0
Decoy055	O(CC(C)=C)c1c2N[C@H]([C@H]3[C@H](C=CC3)c2ccc1)c1cc2c(cc1)cccc2	0
Decoy056	ClC1(Cl)[C@H]2[C@@H]1COC(OC2)C	0
Decoy057	S1(=O)c2c(cccc2F)[C@@H]([NH2+]C)[C@@H]1C	0
Decoy058	[O-]\C=C\[NH+]1[C@H](CCC[C@@H]1C)C	0
Decoy059	s1cc(nc1/C(=C\Nc1ccc(S(=O)([O-])=NC(=[NH2+])N)cc1)/C#N)-c1cc([N+](=O)[O-])ccc1	0
Decoy060	N#CC1=CCC2(CC=C(C#N)C12C)C	0
Decoy061	ClC1=C[CH-]C(=[C+](=C=Nc2ccc(cc2)C)[C-]2CC=C(Cl)C=C2)C=C1	0
Decoy062	S(CC(C(=O)[O-])=C)c1cc(F)c(F)cc1	0
Decoy063	S([C@H](OC(=O)C)[C@H](OC(=O)C)[C@H](OC(=O)C)[C@H](OC(=O)C)[C@H](OC(=O)C)COC(=O)C)CC	0
Decoy064	OC(=N)/C(=N\[O-])/C([O-])=N	0
Decoy065	[NH2+](CC#C)[C@@H]1CCCC[C@@H]1C#N	0
Decoy066	O1[C@@]23[C@]45OO[C@@]4(C12C(CCCC3(C)C)(C)C)C(CCCC5(C)C)(C)C	0
Decoy067	S1(=O)C[C@]2(CCC[NH2+]CC2)CCC1	0
Decoy068	S1[C@@H]([NH+](C)C)C(=CC1=N)CC	0
Decoy069	S([C@H]([C@@H](O)C(OC(C)C)=O)c1cc(ccc1)C)c1ccccc1N	0
Decoy070	Brc1ccc(cc1)[C@H]([NH2+]Cc1ccc(F)cc1)C(=O)N	0
Decoy071	P(=O)([O-])(Cc1nc([O-])c2cc(F)ccc2n1)CO	0
Decoy072	O=C([O-])C[C@H](C1CCC1)c1cc(ccc1)C	0
Decoy073	O=C(C12CC3CC(C1)CC(C2)C3)c1nccnc1	0
Decoy074	S(CCCOc1ccccc1C)c1nnc(n1N)C1CCOCC1	0

Decoy075	S1SC[C@H]2NC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@@H](NC(=O)[C@H](NC2=O)C1)C(C)C)[C@@H](CC)C)[C@@H](CC)C	0
Decoy076	Brc1cc(ccc1F)[C@H]([NH+]1CCCCCC1)C#N	0
Decoy077	Cl\C(\Cl)=C\[C@@H]1[C@H](C(=O)n2c3c(nc2SC)cccc3)C1(C)C	0
Decoy078	O=C([O-])CCC=1C2=[NH+]C(=Cc3[nH]c(C=C4[NH+]=C(C=c5[nH]c(=C2)c(C)c5CCC(=O)[O-])C(C)=C4CCC(=O)[O-])c(C)c3CCC(=O)[O-])C=1C	0
Decoy079	O=C1[C@H]2CC[C@H](C2)C(=O)[C@H]2CC[C@@H]1C2	0
Decoy080	O1C(OC(OC1[C@@H]1CCC=CC1)[C@@H]1CCC=CC1)[C@@H]1CCC=CC1	0
Decoy081	O1C[C@]2([C@H]([C@H]3OC(=O)[C@H]([C@@H]3[C@@H](O)C2)C)C(=C)C1=O)C=C	0
Decoy082	O(C)C1=NCC2(C1)CCCCC2	0
Decoy083	S([C@@H]([C@H]([NH3+])CC)C(F)(F)F)c1ccc(cc1)C(C)C	0
Decoy084	S(=O)(=O)([C@H](C#N)C)[C@H]1C[C@@H](CCC1)C	0
Decoy085	ClCC1=C/C(/N=[N+](C)C1=O)=C\1/C=CNC=C/1	0
Decoy086	O=C([O-])C([NH2+]CC#C)(C)C	0
Decoy087	Clc1ccc(S[C@@H]2C[C@@H](CC[C@H]2C#N)CCC)cc1	0
Decoy088	S=C(\N=C(/NC1CCCCC1)\Nc1nc(cc(n1)C)C)Nc1ccc(F)cc1	0
Decoy089	O=C([O-])C1C(C(=O)[O-])C(C(=O)[O-])C1C(=O)[O-]	0
Decoy090	O=C([O-])[C@H]1[C@@H](C1(C)C)c1ccncc1	0
Decoy091	S1CC(Nc2cccc(C)c2C)C1	0
Decoy092	Clc1cc(N([C@H](C(C)C)C)C)c(cc1)C#N	0
Decoy093	o1c2c(cccc2C)c(C(C)C)c1C[NH2+]C(C)C	0
Decoy094	OC[C@@]1(N(CC[C@@H]1c1ccccc1)\C=C\[N+](=O)[O-])c1ccccc1	0
Decoy095	O(CC1(CCCCC1)C#N)c1cc2CCCCc2cc1	0
Decoy096	O=C([O-])C[C@H]([NH3+])C(=O)[C@@H]([NH3+])C	0
Decoy097	Brc1cnc(nc1)CNC(OC(C)(C)C)=O	0
Decoy098	S1C(=CP(=O)(N[C@H](CC)CO)C=C1c1ccccc1)c1ccccc1	0
Decoy099	Clc1cc(C(OCC)=O)c(OP(SCCC)(=S)Oc2ccc(SC)cc2)cc1	0
Decoy100	Brc1sc(cc1)[C@H](N(Cc1occc1)C1CC1)[C@H]([NH3+])CC	0
Decoy101	O=Cc1c(C)c(Cc2c(C)c(C=O)c(cc2C)C)c(cc1C)C	0
Decoy102	Brc1cc(N[C@H](C#N)c2cc3OCOc3cc2)ccc1	0
Decoy103	O[C@H](Cc1nc(cc(c1)C)C)C	0
Decoy104	ClC(=O)[C@@H]1OC=CCC1	0
Decoy105	S(\C(=C(/C#N)\C#N)\c1nc2c(nc1C)cccc2)C	0
Decoy106	P(OCC(C)C)(OCC(C)C)(OCCCCOP(OCC(C)C)(OCC(C)C)=O)=O	0

Decoy107	O1[C@H]2[C@@H]1C[C@@]13[C@@](CCC1)(C3)C2	0
Decoy108	O1CC[C@H](C#N)[C@H]1C(C)(C)C	0
Decoy109	[O-]C1=[NH+]\C(\N=C(C1)C(C)(C)C)=C/1\N=C[NH+]=N\1	0
Decoy110	O=C(N=C=O)c1cc2CCCc2cc1	0
Decoy111	Clc1cccc(C(F)(F)F)c1NC(=O)COC(=O)C12CC3(O)C[C@H](C1)C[C@H](C2)C3	0
Decoy112	c1cccc(\C=C(\c2ccccc2)/c2ccccc2)c1C=C	0
Decoy113	O=C(N1C2C[C@@H]3CC(C[C@H](C2)C3)C1)c1cc[n+]([O-])cc1	0
Decoy114	IC1=C/C(/C=C(OCC)C1=O)=C/NNc1cc(Br)ccc1	0
Decoy115	S(C)c1ccc(NC(=O)C2(CCCCCC2)C#N)cc1	0
Decoy116	o1nc(c2c1c(C)c([O-])cc2)CC	0
Decoy117	S1[C@@H](C)[C@@H](C(OC)=O)[C@H](C(OC)=O)C12C1CC3CC2CC(C1)C3	0
Decoy118	S(C)C1=NC(=O)C[C@@H](CC)[C@@H]1C#N	0
Decoy119	FC(F)(F)c1ccccc1[C@@H]1C2C(=NC(=C)C1C#N)CCCC2=O	0
Decoy120	Brc1sc(Br)cc1[C@@H](Cl)[C@H]1C[C@@H]1C	0
Decoy121	S1[C@@H]2C(CCC2)=C(C#N)C1=O	0
Decoy122	Clc1cc(F)c2c(c1)CC[NH2+][C@@H]2[C@@H](Cl)C	0
Decoy123	S=C(Nc1c(cccc1C)CC)[N-]N(C(=S)Nc1c(cccc1C)CC)C	0
Decoy124	s1ccnc1C1(CCCC1)C#N	0
Decoy125	ClCc1[nH+]c([nH]c1)C12CC3CC(C1)CC(C2)C3	0
Decoy126	BrC(=C)[C@H]1CC(OC1)=O	0
Decoy127	S1[C@H]2C(CC(OC2)(C)C)=CC1=N	0
Decoy128	ClC(Cl)(Cl)C=O	0
Decoy129	N#C[C@H]1CC=CC[C@@H]1C#N	0
Decoy130	s1cc(cc1)[C@H](O)c1cc[nH+]cc1	0
Decoy131	Ic1ccc(OC)nc1OC	0
Decoy132	Fc1cc(N)c(N[C@@H](C)C23CC4CC(C2)CC(C3)C4)cc1	0
Decoy133	S(=O)(=O)(N1C[C@@H](O[C@H](C1)C)C)c1cc(F)ccc1F	0
Decoy134	O=C(Nc1cc(ccc1)C#N)c1ccccc1-c1ccccc1C#N	0
Decoy135	Brc1cc(sc1)N=C=O	0
Decoy136	O1[C@H](CC)[C@](O)(C)[C@H](O)[C@@H](C)\C(=N\O)\[C@@H](C[C@](O)(C)[C@H](O[C@H]2O[C@H](C[C@@H]([NH+](C)C)[C@H]2O)C)[C@@H](C)[C@H](O[C@H]2O[C@@H](C)[C@@H](O)[C@](OC)(C2)C)[C@@H](C)C1=O)C	0
Decoy137	Clc1ccc(cc1)C(=O)\C(\C#N)=C\1/OCCN/1	0
Decoy138	FC(F)(F)Oc1ccc(cc1)-c1ccc([nH+]c1)C(=O)[O-]	0

Decoy139	[S-]c1onc(n1)C1CC1	0
Decoy140	FC1(F)CCC(CC1)C#N	0
Decoy141	[S-]CCOc1ccc(OCC)cc1	0
Decoy142	Clc1c(OCl)c(OCl)ccc1Cl	0
Decoy143	s1ccnc1[C@H]1[NH2+]CCc2c1cc(O)c(O)c2O	0
Decoy144	O=C([O-])[C@@]1(CC[NH+](C1)CC#CC)C	0
Decoy145	S1[C@@H]([NH2+][C@H](SC1CC(C)C)C)C	0
Decoy146	s1c(SCC(=O)NN)nnc1SCC(=O)NN	0
Decoy147	s1nnc(c1)\C=C\c1nc(ccc1)C	0
Decoy148	Cl[C@]1(CCC=C[C@H]1OC(=O)C)C#N	0
Decoy149	ClC1=NNC(=S)C=C1	0
Decoy150	O=C([O-])C[C@H](CCC[C@@H](CCC[C@H](CCCC(C)C)C)C)C	0
Decoy151	[NH+]=1[C@@H](C(CC)CC)C(=[NH2+])N(CC=C)C=1C1CCCC1	0
Decoy152	s1cc(nc1)[C@@H]1c2c(CCOC1)coc2C=O	0
Decoy153	O=C(N[N-]C(=O)N)C12CC3(C[C@H](C1)C[C@H](C2)C3)C	0
Decoy154	FC(F)(F)c1nc(CC(C)C)c([n-]1)C#N	0
Decoy155	[S-]c1nc(nc(c1)COC)C	0
Decoy156	O=C(C)c1ccc(NC(=O)\C=C(/C(=O)Nc2ccc([NH+](CC)CC)cc2C)\C)cc1	0
Decoy157	O([C@H]([C@H]([NH3+])C)c1cn(nc1)C)C(C)C	0
Decoy158	P(Oc1ccccc1)(Oc1ccccc1)(=O)\[NH+]=C(\Nc1ccccc1)/c1ccccc1	0
Decoy159	Ic1ccc(cc1)[C@H]([NH3+])c1ccc(cc1)CCC	0
Decoy160	S1C(NC(=O)COc2ccccc2[N+](=O)[O-])=C(C2=C(C[C@@H](CC2)C)C1=S)C#N	0
Decoy161	O1CCOC12CCC([NH2+]CCO)CC2	0
Decoy162	Clc1cc(ccc1C)C1=NNc2cc(Cl)c(Cl)cc2N1O	0
Decoy163	Brc1ccc(nc1)N(C(=O)[C@H]1CCC=CC1)C	0
Decoy164	[NH2+](Cc1c[nH]nc1C(C)(C)C)[C@@H]1[C@@H]2[C@H](CCC2)[C@H]1c1ccccc1	0
Decoy165	Brc1cc/2c(OCCC\C\2=N/O)cc1	0
Decoy166	s1cccc1[C@@H](CNC(=O)N(Cc1ccsc1)C)c1c2c([nH]c1)cccc2	0
Decoy167	O=C(N\N=C\c1ccc(N(C)C)cc1)C(=O)N\N=C(\N[N+](=O)[O-])/N	0
Decoy168	P1(O[C@H]2CCC[C@@H]2C)(=O)CC=CC1	0
Decoy169	s1cc(cc1[N+](=O)[O-])C[NH2+]C(C#C)(C)C	0
Decoy170	O=C([O-])[C@@]12CC([C@@H](C1)CCC2)=C	0
Decoy171	Br[C@H]([C@H](CCC)C)c1cc(F)ccc1F	0
Decoy172	Clc1cc2c(Sc3c(N=C2C)cc(cc3)C(=O)N[C@@H](CC)C)cc1	0
Decoy173	Clc1sc(cc1)-c1oc(C(F)(F)F)c(c1)CC#N	0

Decoy174	S(=O)(=O)([O-])c1cc(NC(=O)C)c(O)c(N)c1	0
Decoy175	O1CC(=[NH+]c2cc(N)ccc12)NC12CC3CC(C1)CC(C2)C3	0
Decoy176	Brc1cc(C)c(cc1C)[C@H](Cl)[C@@H]1OCCCC1	0
Decoy177	S([C@@H](C(=O)C=1C[NH+]=C2C=1C=CC=C2)c1ccccc1)c1nc([nH]n1)\C=C\c1ccc(F)cc1	0
Decoy178	O=C(NNC(=O)\C=C\C(=O)[O-])\C=C\C(=O)[O-]	0
Decoy179	Fc1ccccc1C1(CC1)/C(/[O-])=N\OC	0
Decoy180	s1c2c(cccc2)c(OC(=O)N(C)C)c1\C=C\C=1CCCCC=1	0
Decoy181	S=C1NC=CN1c1cc(ccc1)C#N	0
Decoy182	Brc1cc(Cl)c(cc1)-c1oc(cc1)C[NH2+]C[C@@H](O)c1ccccc1	0
Decoy183	Fc1cc(ccc1)[C@H]1C[C@@H]([NH2+][C@@H]1CC)C	0
Decoy184	S[C@@H]1CCCC[C@H]1[NH2+]C(C)(C)C	0
Decoy185	Cl[C@H](CC(C)(C)C)c1cc2OC[C@@H](COc2cc1)C	0
Decoy186	FC(F)(F)c1oc(c2c1C(=O)CCC2)C(=O)[O-]	0
Decoy187	O=C1NC(=NC2=C1CCN(C2)C(=O)C1(CC1)C(=O)N)c1ccc(cc1)C(=O)N	0
Decoy188	n1c(cccc1\N=C\c1ccc(cc1)C#Cc1ccccc1)C	0
Decoy189	FC1(F)COCC1(F)F	0
Decoy190	Fc1ccc(cc1)-c1[nH+]c(c2n1C=CC=C2)CCC(=O)[O-]	0
Decoy191	Clc1cccc(N2C[C@@H](OC[C@@H]2CC)C)c1C#N	0
Decoy192	Fc1c(cncc1F)C(F)(F)F	0
Decoy193	O(C[C@]([NH2+]C(C)C)(C#N)C)c1ccc(cc1C)C(C)(C)C	0
Decoy194	Brc1cc(C(=O)NC(=S)NC[C@@H](O)C)c(OCCC(C)C)cc1	0
Decoy195	O=C1CCCC=2[C@H]3[C@H](N(C1=2)CCC#N)C=CC(=C3)C	0
Decoy196	O1CCC[C@@H]1[C@H](O)C=1CCCCC=1	0
Decoy197	Clc1ccc(NC(=O)N\C(=C(/N)\C#N)\C#N)cc1	0
Decoy198	n1n(c/2c(CCC\C\2=C/c2ccccc2)c1-c1ccccc1)-c1ccccc1	0
Decoy199	Clc1cc(Cl)c(Cl)cc1NC(=S)Nc1ccc(OC(F)F)cc1	0
Decoy200	O=Cc1[n-]c(cc1C)C=O	0
Decoy201	FC(F)(F)C=1C=C/C(/N(C=1)C)=C(/C#N)\C#N	0
Decoy202	s1ccc(C)c1[C@H]([NH3+])c1ccc(cc1)C1CCCCC1	0
Decoy203	S(S[C@@H](Cc1ccc(OCCc2[nH+]cc(cc2)CC)cc1)C(=O)[O-])[C@@H](Cc1ccc(OCCc2ncc(cc2)CC)cc1)C(=O)[O-]	0
Decoy204	S1C[C@]12CC[C@@]1([C@H](C2)CC[C@@H]2[C@@H]1CCC1=C2CCC1(C)C)C	0
Decoy205	Br\C(=C/c1ccccc1)\[C@@H]1OC(c2c(N1)cccc2)(c1ccccc1)c1ccccc1	0
Decoy206	O[C@@H]1C[C@H](CC1)c1nccnc1	0
Decoy207	O1CCC(Nc2ccc(NC(=O)[C@@H]3C[C@@H]3c3ccc(cc3)C(C)C)cc2)CC1	0

Decoy208	Fc1cc(cc2c1[nH]cc2)C#N	0
Decoy209	Oc1cc(ccc1O)[C@@H]1c2cc(O)c(O)cc2C=C(C(O[C@H](Cc2cc(O)c(O)cc2)C(=O)[O-])=O)[C@H]1C(O[C@@H](Cc1cc(O)c(O)cc1)C(=O)[O-])=O	0
Decoy210	S1[C@@H]2[C@@H](CCCC2)[C@@](O)(C[C@@H]1C)C#C	0
Decoy211	O(C1CCC(CC1)C)c1nnc(cc1)C[NH2+]C	0
Decoy212	S1\C(\NC=C1C)=N\C(=O)N[C@H]1C[C@@H]1c1ccccc1	0
Decoy213	S\1[C@@H](N=N/C/1=N/C(OCC(C)C)=O)C12CC3CC(C1)CC(C2)C3	0
Decoy214	O=C([O-])C1(CC(C1)(C)C)C(C)C	0
Decoy215	o1cccc1[C@@H](N(C(=O)N[C@H]1C[C@H](OCC)C12CCCC2)C)C	0
Decoy216	O=C1NC[C@H](C1)C(=O)[O-]	0
Decoy217	O(Cc1ccccc1Nc1cccc(N)c1C)C	0
Decoy218	o1cc(c2c3c(ccc12)cccc3)CC(=O)N[C@H](C)c1ccc[nH+]c1	0
Decoy219	S=C(NC)[N-]\N=C(\[C@H](O)[C@H](O)[C@H](O)CO)/C=N/[N-]C(=S)NC	0
Decoy220	s1cccc1[C@@H](N(C(=O)c1snc(C(=O)N)c1N)c1cc(F)ccc1)C(=O)NCC(OCC)=O	0
Decoy221	s1c(ccc1S(=O)C)C=O	0
Decoy222	S1(=O)(=O)C[C@H](CC1)C(=O)Nc1n(nc(c1)C(C)(C)C)C	0
Decoy223	BrC=1COC(=N)C=1C1CCS(=O)CC1	0
Decoy224	Brc1ccc(SCCNC(=O)NC23CC4CC(C2)CC(C3)C4)cc1	0
Decoy225	O1C[C@]2(C[C@@H]2C(=O)[O-])CCC1	0
Decoy226	Br[C@H](C(OC)=O)C	0
Decoy227	OCC1(CCCCC1)C=O	0
Decoy228	S(CCCC)c1nc([O-])c2c(n1)N=C(C)/C(=C(\OCC=C)/[O-])/[C@H]2c1cc(F)ccc1	0
Decoy229	O=C(N[C@](C(=O)[O-])(C)C1CC1)c1cc2nn[n-]c2cc1	0
Decoy230	Fc1c2[nH+]c(n(c2ccc1)[C@@H](C)c1oc(cc1)C)N	0
Decoy231	Clc1nc(S(=O)C)nc(Cl)c1	0
Decoy232	O=C1C(=C(N[C@@H]2CCC[C@H](C)[C@@H]2C)C1=O)c1cc(C)c(cc1C)C	0
Decoy233	s1c(ccc1[C@](O)(C(F)(F)F)C)C	0
Decoy234	Fc1ccc(NC(=O)[C@@H]2[NH+]=C3C(C=C(OC)C=C3)=C2)cc1	0
Decoy235	O=C1Nc2c(cc(cc2CC)[C@H](O)C(C)(C)C)C1(C)C	0
Decoy236	S([C@H]/1[C@H]2CC[C@H](C2)\C\1=N/O)c1ncccn1	0
Decoy237	[nH+]1cc(C)c(NC(C#C)(C)C)cc1	0
Decoy238	O=C([O-])[C@@H]1[C@@H]2C=C[C@@H](C2)[C@@H]1C	0
Decoy239	O=C([C@@]1(C#N)[C@H](C#N)C12CCC(CC2)C(C)(C)C)c1ccccc1	0

Decoy240	ICC1(N=[N+]=[N-])CCC(CC1)C(C)(C)C	0
Decoy241	S(C)c1cc(SC)cnc1	0
Decoy242	Brc1cc(sc1)C([NH2+]C)(C)C	0
Decoy243	Clc1ccccc1[C@@H](N(C(=O)C[C@H](NC(=O)N)c1ccccc1)C)C	0
Decoy244	S(C[C@@]([NH2+]CC)(C#N)C1CC1)c1nc(ccn1)C	0
Decoy245	Brc1ccc(cc1)C1=NN=C(C=C(C1)c1ccccc1)c1ccccc1	0
Decoy246	[O-]c1nc(cnc1)-c1ccncc1	0
Decoy247	Clc1nc(nc(c1)C(C)(C)C)[C@@H]1[C@H]2O[C@@H](C1)CC2	0
Decoy248	S1[C@@H]2C(=CC1=N)CCc1cc(F)ccc12	0
Decoy249	S(C)C=1NC2=C([C@@H](C)C=1C#N)C(=O)CC(C2)(C)C	0
Decoy250	O(C(=O)[C@@H](NC(=O)N[C@H]([C@H](O)C)C(=O)[O-])C)C	0
Decoy251	FC(F)(C(F)(F)C(F)(F)F)C#C\C(\C(F)(F)F)=C\1/CCCC/1	0
Decoy252	O=C([O-])c1cnc(nc1C1CC1)[C@H]1C[C@H](CCC1)C	0
Decoy253	S1[C@@H](SC)[C@H]([C@H]2N=NC=C2)C(C)=C1C#N	0
Decoy254	Brc1cc(oc1Br)[C@H]1SC[C@H]([NH2+]1)C(=O)[O-]	0
Decoy255	Clc1sc(cc1)[C@@H](Oc1ccc(cc1)CCOC)[C@H]([NH3+])C	0
Decoy256	[NH+]1(CCC([C@@H]2[C@H](NCCC2(C)C)C1)(C)C)C	0
Decoy257	O=C1N[C@@H](CC[C@@H](C1)C)C(C)C	0
Decoy258	O([C@@H]1C[C@H](CCC1)CC)c1ccc(cc1)CC\C(=N\O)\C	0
Decoy259	Brc1cc([C@H]([NH2+]C2CCCCCCC2)CC)c([O-])cc1	0
Decoy260	O=C(N\N=C/1\[C@H]2[C@H](C\1)CC=C2)CCCCC(=O)N\N=C/1\[C@@H]2[C@@H](C\1)CC=C2	0
Decoy261	O=C=N[C@]1(CC=2[C@H](C=C(CC=2)C(C)(C)C)C1)[C@@H]1CC=CC=C1	0
Decoy262	P1(OCC(CO1)C(C)(C)C)O	0
Decoy263	O(C)c1cc(cc(OC)c1)CNc1ccc(cc1)C(C)C	0
Decoy264	Clc1cc(cc(c1)C(=O)C)-c1ccc(cc1)C#N	0
Decoy265	S=C1OC(=CN1)C(C)(C)C	0
Decoy266	O1[C@H](C)C(=O)[C@@H](/C(=N/c2cc(C)c(cc2)C)/C)C1=O	0
Decoy267	[nH+]1c2c(ccc1C)cccc2N[C@@H]1[C@@H]2[C@H](C1)CC=C2	0
Decoy268	Brc1cc(C)c(O)c(N=Nc2cc(cc(c2)C)C)c1	0
Decoy269	S(=O)(=O)(\C(=C\N\N=C\C(C)(C)C)\C#N)C(C)(C)C	0
Decoy270	Brc1cc(N[C@H](C[C@@H](C)c2ccccc2)CO)ccc1	0
Decoy271	S1C=Cn2c1nc(C)c2C[NH2+][C@H](C)c1c(noc1C)C	0
Decoy272	O(C(C)(C)C)C(=O)C[NH+](CC(OC(C)(C)C)=O)C[C@H]([NH+](CC(OC(C)(C)C)=O)CC(OC(C)(C)C)=O)C[NH3+]	0
Decoy273	O[C@@H]1C[C@H](O)[C@H](C\C=C/CCCC(OC(C)C)=O)[C@H]1CC[C	0

	@@H](OC=O)CCc1ccccc1	
Decoy274	Brc1ccc(cc1)-c1c2c(sc1)ncnc2Nc1c(Cl)cc(Cl)cc1Cl	0
Decoy275	S=C(N)c1ccc(cc1N[C@@H](C)[C@@H]1OCCC1)C	0
Decoy276	ClCC=1N2CCN=C2SC=1	0
Decoy277	S1(=O)(=O)CC[C@@H]2OC(C[C@H]([C@H]2C1)CC(=O)[O-])(C)C	0
Decoy278	O=C([O-])[C@@H]([NH3+])c1[n+]([O-])cc[nH]1	0
Decoy279	Brc1nsc2nc(cc(c12)C(F)(F)F)-c1ccc(OCC)cc1	0
Decoy280	Clc1ccc(cc1)CO[C@H]1[C@H](N=[N+]=[N-])[C@@H](Sc2ccc(cc2)C)O[C@@H](COCc2ccc(Cl)cc2)[C@H]1OCc1ccc(Cl)cc1	0
Decoy281	O1CCN=C1N1CC2CCC(CC2)C1	0
Decoy282	O=C1C[C@@]2(C[C@]1(CCC2)C)C=O	0
Decoy283	Clc1sc(Cl)cc1S(=O)(=O)NC(CC)(CC)C(=S)N	0
Decoy284	Clc1ccc(cc1)[C@H]1CC(=O)C2=C(N=C(C)C(C(OCC(C)C)=O)[C@@H]2c2ccc(O)cc2)C1	0
Decoy285	S=C(N[C@@H]1[C@H]2[C@H]3[C@H]([C@@H](C1)C2)CC=C3)[N-]\N=C\c1ccccc1O	0
Decoy286	BrCc1c2CCCCc3ccc(CCCCc(c1)cc2)cc3	0
Decoy287	s1c(ccc1C)[C@@H]1C[C@@H]1C(=O)[O-]	0
Decoy288	FC(F)(F)COc1ncc(N\C=C(\C#N)/C#N)cc1	0
Decoy289	S1C[C@]2(O[C@H]1C)C1CC[N+]([O-])(C2)CC1	0
Decoy290	Clc1cc(N([C@@H]([C@@H](C)c2ccccc2)C(=O)NC(C)(C)C)C(=O)c2occc2)ccc1	0
Decoy291	N(c1ccc(cc1C)C#N)C1CC1	0
Decoy292	O1c2c(OC[C@@H]1\C(\[O-])=N\N=C\c1cc(n(c1C)-c1cc(ccc1)C)C)cccc2	0
Decoy293	O1[C@@H]2[C@@H]3[C@H]([C@H]([C@@H](C3)C2)C(=O)Nc2ccc(Oc3ccc(cc3)-c3ccccc3)cc2)C1=O	0
Decoy294	O=C(N\N=C(\Cc1ccccc1)/CC)[C@H](Nc1cc2c(cc1)cccc2)C	0
Decoy295	Clc1cc(cc(Cl)c1)-c1nn(nn1)CC	0
Decoy296	N=C1[C@@H](C#N)/C(/C[C@](CC)(C)C1(C#N)C#N)=C\C	0
Decoy297	O=Cc1n(c2c(N(C[C@H]2C(C)C)C)c1)C	0
Decoy298	Clc1cc(ccc1F)[C@@H](O)CC#CC	0
Decoy299	O=C([C@H]1C[C@H](CCC1)CC)c1nccc(c1)C	0
Decoy300	Clc1ccc(cc1)C(CNC(=O)Nc1cc(ccc1)C1=NNC(=O)C=C1)(C)C	0
Decoy301	O\N=C/1\C[C@H]2C[C@@H]([C@]\1(n1ccnc1)C)C2(C)C	0
Decoy302	O1N=C(N[C@H]1C(=O)N[C@@H](Cc1ccccc1)CO)C=1C=CC=2[C@H](N=CC=2)C=1	0

Decoy303	S(CC(=O)N[C@H]1N=C(CCSC)[C@H](C)[C@@H]1C#N)c1[nH+]c(C)c([nH]1)CC(C)C	0
Decoy304	o1c2c(C[C@H](CC2)C)c(C#N)c1C1CC1	0
Decoy305	s1cccc1\C=N\N=C(/[O-])\C(F)(F)F	0
Decoy306	IC1=C(I)C(=O)NC1=O	0
Decoy307	O(CC)[C@H]1C[C@@H]([O-])C1(C)C	0
Decoy308	S1CCc2c(nc(nc2CC#N)C)C1	0
Decoy309	Fc1c2OCC(=Cc2ccc1)C#N	0
Decoy310	s1c(cnc1Cc1c(cc(cc1C)C)C)C=O	0
Decoy311	O=C1[C@@H](C[C@H](C(C)(C)C)C(=O)C1=[N+]=[N-])C(C)(C)C	0
Decoy312	s1cc(nc1-c1ccccc1)Cc1[nH]nc(n1)C1CC1	0
Decoy313	Clc1cc(c2[NH2+][C@H]([C@@H]3[C@H]4CC[C@@H]([C@H]3c2c1)C4)C(CC)CC)C(=O)[O-]	0
Decoy314	Brc1cc(ccc1F)CNc1ccccc1SC(F)(F)F	0
Decoy315	O=C(N(CC)C12CC3CC(C1)CC(C2)C3)[C@H]1CCC=CC1	0
Decoy316	O=C1c2c(nc(nc2C)Nc2nc(c3cc(ccc3n2)C)C)C[C@H](C1)c1cc(ccc1)C	0
Decoy317	Brc1cnc(O[C@@H]2CCOC2)nc1	0
Decoy318	s1c(ccc1P(=S)(N(CC)CC)N(CC)CC)\C=N\[N-]C(=S)N	0
Decoy319	Brc1ccc(O[C@H](CC)C(=O)Nc2nocc2)cc1	0
Decoy320	s1cccc1C=1OC(=O)/C(/N=1)=C\c1oc(cc1)-c1cc(ccc1)C(=O)[O-]	0
Decoy321	O=C1NC([O-])=CC(=C1)C(=O)N[C@H](CCC(=O)N)C(=O)[O-]	0
Decoy322	S(C\C=C\CCC1(CC[C@@H](CCOCOC)C1=O)CC\C=C\CSc1ccccc1)c1ccccc1	0
Decoy323	O=C1NC(=O)C[C@@H]1[NH2+]C(C)(C)C	0
Decoy324	FC(F)(F)C1=NN([C@@H]2CCCCC[C@@H]2O)C(=O)C1	0
Decoy325	s1c2c(cc1)[C@@H](N(CC2)C(=O)c1occc1)C1CC1	0
Decoy326	S1\C(=C\2/c3cc(ccc3NC/2=O)C)\C(=O)N(NC(=O)C)C1=S	0
Decoy327	s1cc(cc1)-c1nc2cc(F)ccc2cc1C[NH2+]CCC=1[C@H](N=NC=1C)C	0
Decoy328	s1nc(nc1N1CCC[NH+](CC1)CC(F)F)C	0
Decoy329	O[C@@H](c1cc(ccc1C)C)C=1CCCCC=1	0
Decoy330	FC(F)(F)C[C@H]([NH3+])c1ncoc1	0
Decoy331	O(CC[NH+](C)C)c1ccc(cc1)[C@@](O)([C@@H](CCO)c1ccccc1)c1ccccc1	0
Decoy332	Br[C@H]1C[C@@H](CCCC1)c1ccc(Cl)cc1	0
Decoy333	Ic1c2nc(C)c(C(C)C)c(Cl)c2ccc1	0
Decoy334	Br[C@@H](CC(F)(F)F)c1ccc(cc1)C(C)C	0
Decoy335	Clc1c(C(OCc2c(Cl)c(Cl)ccc2Cl)=O)c(Cl)ccc1Cl	0
Decoy336	Clc1ccc(SCc2cc(\C=C(\C#N)/C#N)c(cc2C)C)cc1	0

Decoy337	Clc1cc(SC(C)(C)C)cc(SC(C)(C)C)c1	0
Decoy338	s1c2c(CC[C@@H](C2)C(C)(C)C)c(C#N)c1\N=C/c1sccc1	0
Decoy339	BrCC1(O[C@H]2C[C@H](CCC2)CC)CCCCCC1	0
Decoy340	S(=O)(C)c1ccc(cc1)C(=O)N1CCCc2c1cc(cc2C)C	0
Decoy341	Clc1cc(\N=C(/Nc2ccc(F)cc2)\N2SC(=CC2=N)C)c(OC)cc1OC	0
Decoy342	ClC=1C[C@H]2[C@H](CC=1)C(=O)N(CC[NH+](C)C)C2=O	0
Decoy343	Clc1cccc(F)c1C[C@@H](CNc1[nH+]cc(cc1)C)CO	0
Decoy344	S1C[C@H](C#N)[C@H](C1)C#N	0
Decoy345	N#CCC=1C[C@H]2[C@@H](C=1)C=CC2	0
Decoy346	BrC=1C(=O)CCCC=1[O-]	0
Decoy347	O(\C=C\1/C[C@@](CCC/1)(C#N)C)C	0
Decoy348	Fc1ccc(cc1)[C@H]1[NH2+][C@H]([C@H]([N+](=O)[O-])C(C)(C)[C@@H]1[N+](=O)[O-])c1ccc(F)cc1	0
Decoy349	Clc1ccc(nc1C[NH+](C)[C@H]1CCCC[C@@H]1C)NN	0
Decoy350	S(=O)(=O)(\N=C(/[O-])\Cc1cc2CCCCc2cc1)C	0
Decoy351	s1nncc1C(=O)N[C@@H]1CCc2c1cccc2F	0
Decoy352	Brc1cc(\C=N\NC(=O)C23CC4CC(C2)CC(C3)C4)c(F)cc1	0
Decoy353	O1[C@@H](C(=O)[O-])[C@@H](O)[C@@H](O)[C@H](O)[C@H]1Oc1cc(ccc1)[C@@H](O[C@H]1O[C@@H](C(=O)[O-])[C@@H](O)[C@@H](O)[C@H]1O)C[NH2+]C	0
Decoy354	Brc1ccc(cc1)-c1oc(N2C[C@@H]3C=4N(C[C@@H](C3)C2)C(=O)C=CC=4)c([P+](c2ccccc2)(c2ccccc2)c2ccccc2)n1	0
Decoy355	Fc1cc2cc([nH]c2cc1)[C@H](O)[C@@H]([NH3+])C(=O)[O-]	0
Decoy356	Oc1ccccc1\C=N\[C@H]([C@H](\[NH+]=C\c1ccccc1O)c1ccccc1O)c1ccccc1O	0
Decoy357	O([C@@H](C(=O)c1c2c([nH]c1)cccc2)c1ccccc1)C(=O)c1ccccc1C(=O)c1ccccc1	0
Decoy358	S([C@H](C(=O)NC[C@H](C)c1ccccc1)C)c1nc(c(nn1)-c1ccccc1)-c1ccccc1	0
Decoy359	O=C(N(CC=C)CC=C)N[C@@H](C(C)(C)C)c1ccccc1)C	0
Decoy360	P(O[C@@H]1C[C@@H](CC[C@@H]1C(C)C)C)(O[C@@H]1C[C@H](CC[C@@H]1C(C)C)C)(=O)[C@@H](C[N+](=O)[O-])c1ccc(N(C)C)cc1	0
Decoy361	Clc1cccc(Cl)c1C[C@@H](C[NH3+])c1ccc(cc1)C(C)C	0
Decoy362	O1[C@H]2[C@@]13CC[C@@H](CC(=O)[C@H]1[C@H](CCC1)[C@@H]2OC)C3	0
Decoy363	S1[C@H]2C[C@H](CCC2=C2C1=NC(=NC2=O)C)C	0
Decoy364	O=C1C[NH2+]C[C@@H]1CC(C)(C)C	0

Decoy365	S(=O)(=O)(C(C(=O)N[C@@H]1C[C@@](OC)(C)C1(C)C)(C)C)C	0
Decoy366	Brc1ccc(cc1)C=1OC(=O)C(C#N)=C(SC)C=1	0
Decoy367	Br\C(=C(/Cl)\C(=O)[O-])\C=O	0
Decoy368	o1cccc1[C@@H](NC1=NC=CN(CC(C)C)C1=O)C	0
Decoy369	Oc1cc(ccc1)[C@H]1[C@H](N2[C@H](C=Cc3c2cccc3)C1(C#N)C#N)C(=O)c1ccccc1	0
Decoy370	Clc1c(OC(=O)\C(=N/OC)\c2occc2)c(Cl)c(Cl)c(Cl)c1Cl	0
Decoy371	Clc1c2c(S(=O)(=O)CC[C@@H]2[NH2+]C2CC2)c(Cl)cc1	0
Decoy372	BrC12CC3(C[C@@H](C1)C[C@H](C3)C2)C(=O)N1CCC(O)CC1	0
Decoy373	O1CC2(COC1CCC)[C@@H](CC(=C[C@@H]2C)C)C	0
Decoy374	FC(F)(C(F)(F)O[C@](F)(C(F)(F)O[C@](F)(/C(/[O-])=N/c1ccc(cc1)C#N)C(F)(F)F)C(F)(F)F)C(F)(F)F	0
Decoy375	Ic1ccc(NC2CCC(CC2)c2ccccc2)cc1	0
Decoy376	Clc1ccc(cc1)[C@@H]1C(C#N)=C(OC(N)=C1S(=O)(=O)CCC)c1ccccc1	0
Decoy377	Brc1cc(ccc1)C1=NN=C[C@H]1C[NH+]1CCC[C@H]1[C@H]1NOC(=C1)C(C)C	0
Decoy378	S1C[C@H](N(C(=O)C)[C@H]1[C@H](O)[C@H](O)[C@H](O)[C@H](O)CO)CO	0
Decoy379	OCC#Cc1ccc(nc1)C(=O)N(CC(=O)N)CC(=O)N	0
Decoy380	S=C(N(Cc1ccccc1OC)CCC1=C2C=C(C=CC2=[NH+][C@H]1C)C)NCC	0
Decoy381	S(CCS(=O)(=O)[O-])C(NC(=[NH2+])N)=N	0
Decoy382	S(=O)(=O)(N(C(C)C)C)N[C@H](C)c1oc(cc1)C	0
Decoy383	s1c2cc(ccc2nc1N[C@H](P(Oc1ccccc1)(Oc1ccccc1)=O)CCC)C	0
Decoy384	Brc1sc(cc1)CNC(=O)C(CCC)(CCC)C(=S)N	0
Decoy385	O(CC=C)c1c(cc(cc1OCC)\C=N/NC(=O)CC[C@@H](O)c1ccc(OCC)cc1)CC=C	0
Decoy386	o1nc(nc1C1CCC(CC1)C(C)(C)C)[C@]([NH3+])(CC)C	0
Decoy387	s1c2c(nc1CC1(CCCC1)C(=O)Nc1cc3NC(=O)Nc3cc1)cccc2	0
Decoy388	Brc1cc(C(=O)N[C@H](C(=O)NC)C)c(nc1)NN	0
Decoy389	s1c(cnc1N1CC(O[C@@H](C1)C)(C)C)CO	0
Decoy390	O(C)c1ncc(n1C1CC1)C[NH3+]	0
Decoy391	Clc1cc(cc(OC)c1OC)-c1[nH]cc(n1)CCl	0
Decoy392	Clc1sc(cc1)C[NH+](CC1=CC(Oc2c1ccc(O)c2C)=O)CC=C	0
Decoy393	O([C@@H]([C@@H](O)[C@H](\C=C(\[C@@H](O)[C@H](C(=O)CCC[C@@H](CC(=O)N)CC(=O)[O-])C)/C)C)\C=C\CC\C=C\C(=O)[O-])C	0
Decoy394	O=C1NC(=CC=C1C[NH3+])c1c(cc(cc1C)C)C	0
Decoy395	Clc1cccc(NC(=O)[C@H](C(=O)[C@@H]2C[C@@H]2C)C#N)c1C	0

Decoy396	O1[C@H]2[C@H]3[C@H]4[C@@H]([C@H](C3)[C@H]2O)C(=O)N(C(C)C)[C@@]14C=C	0
Decoy397	S(C)C1=NC(=O)[C@@H]2C(NC(=O)C[C@@H]2c2ccc(F)cc2)=N1	0
Decoy398	Ic1cc(I)cc(\C=N\c2sc3c(CCCC3)c2C#N)c1OCc1ccc(Cl)cc1Cl	0
Decoy399	Clc1cccc(N[C@H](CC(C)C)C(OC)=O)c1C(=S)N	0
Decoy400	O=C1C2(C[NH+]3CC1(C[NH+](C2)C3)C)CCC	0
Decoy401	s1cc2c(OC[C@H]2c2n[nH]cc2C)c1C=O	0
Decoy402	O1c2c(cc(cc2)C(C)C)[C@@]([NH3+])(CC12CCCCC2)C	0
Decoy403	O(C)[C@H]1CCCC[C@@H]1Nc1ccc(cc1)-c1[nH+]c[nH]c1	0
Decoy404	O(CC)c1cc(ccc1OCC)[C@H]1[C@@H]2C(=CC[C@@H](C2)C(C)(C)C)[C@@H](C#N)C(=N)C1(C#N)C#N	0
Decoy405	S1c2nc(cn2N=C1Sc1ccccc1)C	0
Decoy406	o1cc2c([C@@H]3[C@@H](C2)[C@H]([NH2+]C3)C(=O)[O-])c1C	0
Decoy407	S(C)c1ccc(NC(=O)[C@@H](SCc2cc(ccc2)C(=O)N)C)cc1	0
Decoy408	O1CC[NH2+][C@H](C)[C@@H]1C(C)(C)C	0
Decoy409	Clc1cc(cc2OCCOc12)[C@H]1C[C@H]1C(=O)[O-]	0
Decoy410	S(c1cc2c(cc1)cccc2)c1ncnc2c1oc1c2cccc1	0
Decoy411	FC(F)(F)Oc1ccc(cc1)[C@@H]1c2c(OC(N)=C1C#N)[nH]nc2CCC	0
Decoy412	S(Cc1nccnc1)c1ccc([nH+]c1)N	0
Decoy413	Clc1cc(N[C@@H]2[C@@H]3[C@@H](C2)CC=C3)ccc1NC(=O)C	0
Decoy414	Brc1cc(O[C@@H]([C@@H]([NH3+])CC)c2cc(ccc2)C)cnc1	0
Decoy415	[NH2+]1CCC2=C(CCCC2)[C@H]1c1cc(ccc1)C	0
Decoy416	S(c1ncc(cc1C)C=O)C1CCCCC1	0
Decoy417	ClC=1N[C@@H](SCC(OCC)=O)C(CC)(CC)[C@](C(=O)N)(C#N)C=1C#N	0
Decoy418	S1CC[NH2+]C[C@H]1c1c(C)c(cc(C)c1C)C	0
Decoy419	s1c2c(cc1)c(OC[C@H](CCCC)CC)c1sccc1c2OC[C@H](CCCC)CC	0
Decoy420	Clc1cccc(F)c1C/C(/[O-])=N/c1sc2cc([N+](=O)[O-])ccc2n1	0
Decoy421	S=C1Nc2c(cccc2)C(=O)N1Cc1cc(O[C@@H](CC)C#N)ccc1	0
Decoy422	O1CC=C[C@]1(CC)C(=O)[O-]	0
Decoy423	S(=O)([O-])(=N[C@@H]([C@@H](O)C)C(=O)[O-])C(F)F	0
Decoy424	ClC1=CC(Cl)=Cn2c1nc(c2)CS(=O)(=O)C	0
Decoy425	O([C@H]1CCCC[C@@H]1O)C1CCC1	0
Decoy426	FC(F)(F)C=1C=C(NC(=O)N[C@@H]2CCCC[C@@H]2C(C)(C)C)C(=O)NC=1	0
Decoy427	FC(F)(F)C(=O)NC(C(=O)[O-])(C)C	0
Decoy428	s1c(c(-c2ccccc2)c(C(OCC)=O)c1NC(=O)Nc1ccccc1)-c1ccccc1	0
Decoy429	Brc1nnc(cc1)C#N	0

Decoy430	OCC=1c2n(C=CC=1)c(N)c(n2)-c1ccc(cc1)[C@H](CC)C	0
Decoy431	Brc1ccc(\N=C\c2ccc(OC(=O)c3ccc(OCCCCC)cc3)cc2)cc1	0
Decoy432	O(CCC(C)C)c1ccc(NC(=O)N([C@@H](C)c2cc[nH+]cc2)C)cc1	0
Decoy433	O=C(C(=O)[O-])[C@]1(CCC(=C)C1(C)C)C	0
Decoy434	Cl[C@@H]1C[C@](CCC1)(C(=O)[O-])C	0
Decoy435	O=C(NCC)[C@@H](NC(=O)N[C@H](Cc1[nH]c[nH+]c1)C(=O)[O-])C	0
Decoy436	Clc1ccc(cc1)[C@@H]1N(CCC1)C(=O)Nc1c(F)cccc1F	0
Decoy437	Fc1ccc(cc1C)[C@@H]1N(C)C(=O)CCC[C@H]1C(=O)[O-]	0
Decoy438	ICSC(=O)[C@]1(OC(=O)CC)[C@@]2([C@H]([C@@H]3C[C@H](F)C4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C2)C[C@H]1C)C	0
Decoy439	O=C([O-])CC[C@@H](Nc1[nH+]ccc2c1ccc(C)c2N)C(=O)[O-]	0
Decoy440	Clc1ccc(cc1)C1(NC(=O)Nc2nn(cc2)CCCOC)CC1	0
Decoy441	P(OC[C@H]1O[C@@H](N2C=[NH+]C(=NC2=O)N)[C@@H](O)[C@H]1O)(=O)([O-])[O-]	0
Decoy442	OCCC#Cc1c(C)c(C)c(C)c(C)c1C	0
Decoy443	SCc1cc2nc[nH]c2cc1	0
Decoy444	[NH2+](CC)C[C@@H](C)c1nc([nH]n1)C	0
Decoy445	S=C(N)[N-]\N=C/1\C=C(C(C)(C)C)C(=O)C(=C\1)C(C)(C)C	0
Decoy446	S1CC(=CC1=N)c1oc(nc1C)C	0
Decoy447	S(C(=S)N1CCCCC1)c1nc(SC(=S)N2CCCCC2)nc(SC(=S)N2CCCCC2)n1	0
Decoy448	P(=NC1=N[N-]C(=O)NC1=O)(N(CCCC)CCCC)(N(CCCC)CCCC)N(CCCC)CCCC	0
Decoy449	O=C(c1c2CCc3c2c(cc1)c(cc3)C(=O)c1ccccc1)c1ccccc1	0
Decoy450	BrC1=NC=CN(C1=O)C1CC1	0
Decoy451	S(Oc1cc2onc(c2cc1)-c1cc(F)c(F)c(F)c1)(=O)(=O)Cc1ccccc1	0
Decoy452	S(=O)([O-])(=Nc1ccc(S(=O)(=O)\N=C/2\NCCCCC\2)cc1)c1cc(OC(F)(F)F)ccc1	0
Decoy453	S[C@@H]1c2n(CC1)cnc2C(C)C	0
Decoy454	S1c2c(Nc3c1cccc3)cc(cc2)/C(=N/Nc1ccc(cc1C)C)/C	0
Decoy455	s1cc2O[C@H]3[C@@H](c2c1C=O)C[NH+](C3)C	0
Decoy456	Clc1cc(F)ccc1CSCC(=O)N[N-]C(=S)Nc1ccc(cc1)C(=O)C	0
Decoy457	ClC=1c2cc(Cl)ccc2OCC=1\C=N\OC[C@@H](O)C[NH2+]Cc1ccc(cc1)C(F)(F)F	0
Decoy458	Brc1cc(cc(Br)c1OC)C[NH2+]CCNc1ccc([N+](=O)[O-])cc1Cl	0
Decoy459	Fc1ccc(cc1)[C@H]1C[C@@H]1CC(=O)[O-]	0
Decoy460	S(CC)C=1O[C@@H]2[C@@H](CCCC2)C2(N=1)CCCCC2	0
Decoy461	Brc1ccc(cc1)-c1ccc(cc1)/C(=N/[N-]C(=S)N)/C	0

Decoy462	s1cccc1[C@@H]([O-])C(C#N)=C	0
Decoy463	S(=O)([O-])(=Nc1cc(ccc1)-c1nnc(OCC(C)C)cc1)C	0
Decoy464	o1c2cc(ccc2nc1[O-])[C@@H]([NH3+])c1ccc(cc1)C(C)C	0
Decoy465	Brc1cc(oc1Br)\C=C\[N+](=O)[O-]	0
Decoy466	Clc1ccc(Cl)cc1[C@H](O)c1ccc(SC(F)(F)F)cc1	0
Decoy467	O=C1CCC[NH2+]C[C@H]1Cc1cn[nH]c1	0
Decoy468	s1c(C(=O)\C(=C(/[O-])\c2occc2C)\C#N)c(nc1[C@H](OC)C)C	0
Decoy469	O1c2c(CC(C(=O)N[C@@H](C)c3cc(ccc3)C#N)=C1C)cccc2	0
Decoy470	S([C@@H]1CCCC1=O)c1cn(nc1)C	0
Decoy471	S(c1ccc(F)cc1)c1nc2c(cccc2)c(c1)C(=O)NCC[NH+](C)C	0
Decoy472	S1\C(=C/c2cc(OCCC(=O)[O-])ccc2)\C(=O)N(CCCCCCCCCC(=O)[O-])C1=S	0
Decoy473	S(=O)(=O)(N1CC(C1)C(=O)[O-])C1=CNC(=O)N=C1[O-]	0
Decoy474	S=C1N(C(C)C)C(=N[N-]1)c1cc(oc1C1CC1)C(C)C	0
Decoy475	Brc1cc(F)c(cc1)C(=O)N[C@@](CC)(C#N)C	0
Decoy476	FC(F)(F)CNC(=O)[C@H](ONC(=O)Cc1c2c(ccc1)cccc2)C	0
Decoy477	n1(-c2c(cccc2C)CC)c(C)c(cc1C)\C=N\c1cc(C)c(cc1)C	0
Decoy478	Brc1sc(cc1)CNc1ccc([NH+](C)C)cc1C	0
Decoy479	Fc1ccc(cc1)COCC12[NH+](COC1)COC2	0
Decoy480	ClCCSc1nc([O-])ccn1	0
Decoy481	FC(F)(F)COc1ccc(cc1)C[NH2+][C@H](C)c1cc2NC(=O)Nc2cc1	0
Decoy482	O=C(N)c1ccc(N)cc1NCC(=O)[O-]	0
Decoy483	S=C(N)c1ccccc1Oc1ccccc1[C@@H](CC)C	0
Decoy484	S1C[C@](SC(C)C)(CC1)C(=O)[O-]	0
Decoy485	[NH+]1=NC=2[C@@H]([NH+]=C3C=2C=CC=C3)N=C1N\N=C\C=C\C	0
Decoy486	Fc1cccc(F)c1C1(CC1)C#N	0
Decoy487	ClC1(Cl)SC(=O)C(=O)N1C	0
Decoy488	Fc1c(N=O)c(F)c(F)c(F)c1F	0
Decoy489	S=C(\[NH+]=C(/Nc1ccccc1)\c1ccccc1)Nc1ccccc1	0
Decoy490	Brc1cc(c2OCC(C)(C)C(=O)N(c2c1)C)CC	0
Decoy491	[NH+]1(CCCC1)Cc1ccccc1N\C=C(\C#N)/C#N	0
Decoy492	Clc1c2SC[C@@H](C)[C@H]([NH2+]C)c2ccc1	0
Decoy493	ClCc1cc(ccc1)-c1oc2c(n1)cccc2	0
Decoy494	S1CC2([NH+]=C1NC1CC1)CCCC2	0
Decoy495	O[C@H]1C[C@@H]2[C@@H]([C@@H]3CC[C@@H]([C@H](CC(=O)C[NH2+]CCCNC(=O)[C@@H](O)[C@H](O)[C@H](O)C(O)O)C)[C@@]13C)CC[C@H]1C[C@H](O)CC[C@@]12C	0

Decoy496	Brc1ccc(N[C@@H]2O[C@@H](C)[C@H](O)[C@H](O)[C@@H]2O)cc1	0
Decoy497	Brc1cc(N2C(=O)[C@H](SC23CCC(CC3)C(C)(C)C)C)ccc1	0
Decoy498	O=C(N(C)c1cc(ccc1)C#N)c1ccc(cc1)-c1[nH]nc(n1)C	0
Decoy499	Fc1ccccc1[C@@H](N(C(=O)[C@@H]1OCCC1)C)C#N	0
Decoy500	O\N=C/1\C2CC[NH+](C\1)CC2	0
Decoy501	O[C@H](CNc1nc[nH+]cc1)C1CC1	0
Decoy502	o1cccc1[C@@H]([NH+](C)C)CNCc1ccc(cc1)C#N	0
Decoy503	Clc1cc(NC(=[NH2+])NC(C)(C)C)c(F)cc1	0
Decoy504	s1c2cc(ccc2nc1C1=CC(=O)CCC1)C#N	0
Decoy505	FC(F)(F)c1noc([N-]C(=O)C(=O)N2CCC[C@H](C)[C@H]2C)c1	0
Decoy506	[NH2+]([C@H](C)c1ccccc1N(C)[C@@H]1C[C@H](CCC1)C)C	0
Decoy507	N(Cc1ccccc1C)c1ccc(cc1N)C#N	0
Decoy508	Cl[C@H]1c2c([nH]nc2CC)CC1	0
Decoy509	O=C(N(CC)C[C@H](C#N)C)[C@H]1CC=CC[C@@H]1C(=O)[O-]	0
Decoy510	S(=O)(=O)(C)[C@H]1C[C@@H](Nc2nc(ccn2)C)CCC1	0
Decoy511	Clc1cc(Cl)cc(\C=[NH+]\[C@@H]2[C@@H]3[C@H](OCC3)C2(C)C)c1[O-]	0
Decoy512	Clc1cc(c2NC(=O)[C@](O)(c2c1)[C@H](\C(=N\[N-]C(OC)=O)\c1ccc(OC)cc1)c1ccc(OC)cc1)C	0
Decoy513	s1cc(cc1CCC)C(=O)N[N-]C(=S)N[C@@H](C)c1ccccc1	0
Decoy514	Clc1cc(Cl)ccc1[C@H](N(C(=O)[C@]([NH3+])(C)C1CC1)C)C	0
Decoy515	Clc1cc(c2OCOCc2c1)CSc1nc(ccn1)C(F)(F)F	0
Decoy516	FC(F)(F)C1(N=C(N=C(C)[C@@H]1C#N)C)C(F)(F)F	0
Decoy517	Brc1cc(nc(Cl)c1)C(OC)=O	0
Decoy518	O=C1N(C(C)C)C(=CC=C1C(=O)C)C	0
Decoy519	n1ccn([C@H]2CCCCC[C@@H]2C#N)c1C	0
Decoy520	N#CC12CCC(CC1)(CC2)C#N	0
Decoy521	Clc1cc(Cl)cc2CC3(Nc12)CC3	0
Decoy522	Fc1cc(ccc1OC[C@@H]1CC=CC[C@@H]1C)C#N	0
Decoy523	Brc1ccc(NC=2NC(=O)C(CCSCc3ccccc3)=C(N=2)C)cc1	0
Decoy524	O1CCCc2cc(ccc12)[C@@H]1[NH+]2[C@H](CCCC2)C[NH2+]C1	0
Decoy525	[S-]c1[nH+]cn(C)c1C[C@@H]([NH3+])C(=O)[O-]	0
Decoy526	Clc1cc2c(n(CC)c(Cl)c2C(=O)C)cc1Cl	0
Decoy527	Clc1snnc1CSc1[n+]([O-])cccc1	0
Decoy528	Clc1cc(cc(Cl)c1)C(=O)N[C@@H](C)c1ncccc1	0
Decoy529	Cl\C(=C/[C@H]1C(C#N)C(=NC(C)=C1C#N)C)\c1ccc(cc1)CC	0
Decoy530	Brc1cc(oc1Br)\C=N\c1ccc(Cl)cc1Cl	0
Decoy531	Clc1sc(nn1)[C@H]1C[C@@H]1C	0

Decoy532	s1c2c(nc1S[C@@H](C[C@@]([NH2+]C(C)C)(CO)C)C)cccc2	0
Decoy533	ClCC(=O)c1cc([O-])c(SC)cc1	0
Decoy534	o1c2c(cc(cc2)C(C)C)c(C2CC2)c1C(=O)C	0
Decoy535	Fc1ccc(F)cc1[C@@H]([NH2+]C)C#N	0
Decoy536	[O-]c1nc(N(C)C)ccc1C#N	0
Decoy537	Clc1ccc(cc1)C(=O)N1N=C(CC1(C)C)C	0
Decoy538	O=C(N([C@@H](C(=O)NC(CC(C)(C)C)(C)C)c1ccc(cc1C)C)CCC)CCC1CCCCC1	0
Decoy539	o1ccc(CC[NH3+])c1-c1cnc(nc1)C	0
Decoy540	O([C@@H]1CC(C[C@@H](C1)C)(C)C)c1cc(N)ccc1C(=O)NC	0
Decoy541	Clc1cc(C)c(cc1C)[C@H]([NH2+]C)c1cc2c(COC2)cc1	0
Decoy542	O=C1C=C2N([O-])/C(/NC2=C[C@H]1[O-])=N/C(OC)=O	0
Decoy543	o1nc(C)c(C(=O)NC[C@H](OC)C(C)(C)C)c1C	0
Decoy544	s1ccc(C)c1[C@@H](O)[C@@H]1C[C@H](CCC1)C	0
Decoy545	O=C([O-])[C@@H]([NH3+])c1n2N=C3C(CCC3)=C([O-])c2nn1	0
Decoy546	S1CCC(NS(=O)(=O)[O-])CC1	0
Decoy547	FC=1C=CC2=NC(=C[C@H]2C=1)C(=O)[O-]	0
Decoy548	Brc1ccc(cc1)C#Cc1ccc(Br)cc1	0
Decoy549	Br[C@H]1CC[C@@H](C[C@H]1CCc1ccsc1)CC	0
Decoy550	S1[C@H](C)[C@H](N=C1C)C	0
Decoy551	o1cccc1/C=C(/C(/[O-])=N/c1cnc(nc1)-c1ccccc1)\C#N	0
Decoy552	S(Cc1ccccc1)c1nc(nc2Oc3c(Cc12)c(c[nH+]c3C)CO)-c1ccc(cc1)CC	0
Decoy553	Ic1ccc(N2C([NH+]=C([NH+]=C2N)N)(C)C)cc1	0
Decoy554	O[C@@H](c1cccc(C)c1C)c1c2[nH+]cccc2ccc1	0
Decoy555	Brc1ccc(cc1)[C@H]1[C@]2(C#N)[C@@]1(C#N)C1(OCCO1)[NH+]=C2N	0
Decoy556	Clc1ccc(N2C(=O)C([C@@H]3[NH+](CCc4c3c(OC)c3OCOc3c4)C)=C([O-])N(C)C2=O)cc1	0
Decoy557	Ic1cc(Cl)c(N[C@@H](CCC(C)C)C)cc1	0
Decoy558	Brc1cc(Cl)c(cc1)[C@H]([NH2+]C)c1cc2CCCCc2cc1	0
Decoy559	Fc1cc(ccc1)CN(C(=O)[C@@H](Nc1ccc(Oc2ccc(cc2)C#N)cc1)C)C	0
Decoy560	Clc1sc(cc1)[C@@H](O)CNC(=O)[C@@H](CSC(F)(F)F)C	0
Decoy561	[NH+]1(CC=C2[C@@H](C1)[C@H](C(C#N)(C#N)C(N)=C2C#N)c1cccnc1)CC	0
Decoy562	Clc1sc(cc1)[C@H]1SCC[NH2+]1	0
Decoy563	S1C[C@@H](NC(=O)[C@H]1C(C)C)C(=O)[O-]	0
Decoy564	s1nncc1S(=O)C1CCCCC1	0
Decoy565	O=C([O-])[C@@H]1CC[C@H](C[C@H]1[NH+](C)C)CC	0

Decoy566	Clc1ccc(NC(=S)N[C@H](NC(=O)C(C)C)C(Cl)(Cl)Cl)cc1	0
Decoy567	Fc1cc(F)cc2[NH2+]CC[C@@H](Oc12)C	0
Decoy568	O(C)[C@H]1C[C@H]([NH2+]CCC2CCCCC2)CCC1	0
Decoy569	O=C(NC)c1cc(C)c(NC(=O)N[C@H](C)c2cc3CCCCc3cc2)cc1	0
Decoy570	ClCC[C@@H]1OCCC1	0
Decoy571	s1cc(nc1-c1cc(ccc1)C)CNC(=S)Nc1ccc(cc1)[C@@H](CC)C	0
Decoy572	S(=O)([C@H](C(=O)NC(=O)N)C)c1oc2cc(N)ccc2n1	0
Decoy573	S1[C@H]2[C@H](N=C1C)C=C(O[C@H]1C[C@H]([NH2+]C1)C(OC)=O)C=C2	0
Decoy574	S=C(N)c1ccc(NCCC2CCCC2)cc1C(F)(F)F	0
Decoy575	s1cccc1[C@H](Nc1cccc(N)c1C)CCC	0
Decoy576	Clc1cc(ccc1S(=O)(=O)C=C)C#N	0
Decoy577	N12[C@H]3[C@@H]4N(CC1)C=CC=C4C=CC3=CC=C2	0
Decoy578	O=C([O-])[C@@H]1CCC[C@H]1n1cccc1	0
Decoy579	s1cc(nc1N)-c1c2C[C@@H](CCc2oc1CCC)C	0
Decoy580	[NH2+]([C@@H](C)C1CC1)[C@H](C)c1n2c(nn1)C=CC=C2	0
Decoy581	Ic1cc(Br)cc(\C=N\Nc2nc(cc(COC)c2C#N)C)c1[O-]	0
Decoy582	S1N(C(=S)C2=C1C(Nc1c2cc(cc1)C)(C)C)c1ccc(cc1)CCCC	0
Decoy583	o1cc2c([C@@H](COC2)C(C)C)c1C=O	0
Decoy584	s1nc(C)c(C#N)c1NC	0
Decoy585	Clc1cc(Cl)ccc1[C@H]1C[NH2+]C[C@H]1C	0
Decoy586	O=C1N=C(NC2=[NH+]CC(=N[C@@H]12)[C@@H](O)[C@H](O)C)[NH-]	0
Decoy587	s1c2c(nc(nc2[O-])[C@H]([NH3+])C(=O)N)cc1	0
Decoy588	FC(F)(F)[C@]1(CC12CCCC2)C(=O)[O-]	0
Decoy589	o1c(ccc1C)[C@H]1Nc2c(NC3=C1C(=O)C[C@H](C3)c1ccccc1)cccc2	0
Decoy590	Clc1ccccc1CN1C(=O)[C@@H]2[C@@H]([C@H]([NH2+][C@@]23c2c(NC3=O)cccc2)CCC(=O)N)C1=O	0
Decoy591	S(CC[C@@H](NC(OC(C)(C)C)=O)C(=O)Nc1ccc(cc1)C(C)C)C	0
Decoy592	O(C(=O)[C@@H]([NH2+]CC(C)C)c1cc2c(nccc2)cc1)C	0
Decoy593	ClCC(=O)c1scc(c1)C(=O)[O-]	0
Decoy594	Brc1cc(ccc1)[C@@H](Nc1ccc(cc1)C(C)C)C	0
Decoy595	Brc1cc(OCCO)ccc1C[NH2+][C@@H](C)c1cnn(C)c1C	0
Decoy596	Clc1ccc(\N=C(/[O-])\[C@H]([NH+]2CCCNCC2)C)cc1N	0
Decoy597	Clc1ccc(nc1C(=O)[O-])N(C)[C@H]1CCSC1	0
Decoy598	S1c2c(N(c3c1cccc3)C[C@@H](O)CNc1ccc(cc1)C(C)C)cccc2	0
Decoy599	BrC[C@H]1OC(=O)N(C1)c1ccc(F)cc1	0
Decoy600	Fc1ccc(cc1)C(=O)Nc1ccc(cc1)[C@@H](NC(=O)CCc1ccc(cc1)C#N)C	0

Decoy601	O=C(N)c1cc(ncc1)NC(C(=O)[O-])(C)C	0
Decoy602	Brc1ccccc1SCCCC[C@]([NH2+]CCC)(CO)C	0
Decoy603	P(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)(=O)([O-])[O-]	0
Decoy604	Brc1cc(n(c1)C)C#N	0
Decoy605	[NH+]1(C)[C@H](C#N)C(=CC[C@@H]1C)CC	0
Decoy606	S(=O)(=O)(N1CC[C@H]2[NH2+][C@H](CC2)C1)CC	0
Decoy607	Brc1sc(Br)c(C(OC)=O)c1-c1c(C(OC)=O)c(Br)sc1Br	0
Decoy608	FC(F)(F)[C@@H]1C[C@@]([NH3+])(CCC1)Cc1cc(cc(c1)C)C	0
Decoy609	O(C)c1c(OC)c2c(cc1OC)C1(CCCCC1)C[NH2+]C2	0
Decoy610	n12c3CCCCc3nc1N=C(CC2)C	0
Decoy611	O=C1CC(Cc2n([C@@H]3CCC[C@@H]3OC)c(cc12)C)(C)C	0
Decoy612	Ic1ccc(cc1)[C@@H]1NC(=S)NC(C)=C1C(OCC(C)C)=O	0
Decoy613	Brc1cc(Cl)cc(S(=O)(=O)N=[N+]=[N-])c1OC	0
Decoy614	Fc1cccc(F)c1C1(CCCC1)CN/C(=[NH+]\C1CCOCC1)/NC1CC1	0
Decoy615	N1c2c(N(C[C@@H]1C)Cc1cc(ccc1)C#N)cccc2	0
Decoy616	Brc1ccc(cc1)C1=NC(=S)C=2CCCCC=2N1c1ccc(cc1)C	0
Decoy617	O=C1[NH+]=C(C)C(CC(=O)[O-])=C(N1[C@@H]([C@H](CC)C)C)C	0
Decoy618	S(CC(=O)N1c2c(ccc(c2)C)C(=CC1(C)C)C)C#N	0
Decoy619	S(=O)([O-])(=Nc1cccc(C)c1C)C1CC1	0
Decoy620	FC=1C2=[NH+][C@@H](C)C(=C2C=CC=1)CC(=O)N[C@@H](C)C1=CNN([C@@H]1C)c1cc(F)ccc1	0
Decoy621	Clc1ccc(cc1)C(CC=1C(OC(=CC=1[O-])C)=O)CC=1C(OC(=CC=1[O-])C)=O	0
Decoy622	s1cc(nc1N)/C(=N\OC)/C(=O)N[C@H]1[C@@H]2SCC(C)=C(N2C1=O)C(OCOC(=O)C(C)(C)C)=O	0
Decoy623	n1n(ccc1)-c1cc(N[C@H](CCCCC)C)ccc1	0
Decoy624	Oc1c(cccc1CC=C)C1Nc2c3c(ccc2)cccc3N1	0
Decoy625	Clc1sc(cc1)[C@@H]([NH2+][C@H](C)c1ccc(cc1O)C)C	0
Decoy626	S1C[C@H]2N([C@H]3[C@H](C2)C[NH2+]C3)C1	0
Decoy627	Clc1nccc(c1)C(=O)N[C@@]1(CCSC1)C#N	0
Decoy628	S1CC[C@@H](NC(=O)C=2OCCOC=2)c2c1cccc2	0
Decoy629	S(CC[C@H](NC(=O)N)C(=O)N[N-]C(=O)NCC1CC1)C	0
Decoy630	FC(F)Oc1ccccc1[C@@H]1C[C@@H]1C(=O)N[C@@H]1[C@@H]2CC[C@@H](C2)[C@@H]1C(=O)N	0
Decoy631	Clc1ccc(Cl)nc1COC(=O)c1cc(N2N=C(O)C=CC2=O)ccc1	0
Decoy632	S1[C@H]2[NH2+][C@H](S)N(C[C@H]3N=NC=C3)C(=O)[C@@H]2C=C	0

	1CC	
Decoy633	Brc1sc(cc1)C[NH2+]C[C@@H](O)COc1nsnc1	0
Decoy634	FC1(F)C2C[C@@H]3CC1(C[C@H](C2)C3)CCO	0
Decoy635	O=C([O-])CC[C@@H](NC(=O)N(C[C@H](C#N)C)C)C(=O)[O-]	0
Decoy636	Clc1nc2c(CCCC2)c(-c2ccccc2F)c1C#N	0
Decoy637	O1[C@@](OC[C@H]1C)(C)C1CC1	0
Decoy638	Clc1ccc(cc1)-c1nc(nc(c1)C(F)F)-n1nc(cc1)C(=O)[O-]	0
Decoy639	S\1[C@@](NC(=O)N(/C/1=C/C)c1ccccc1)(C(F)(F)F)c1ccccc1	0
Decoy640	S1CCN=C1NC(=O)C1=NO[C@@H](C1)c1ccccc1	0
Decoy641	O1CCOC12C[C@@]1([C@H](CC2)CCCC1)C#N	0
Decoy642	s1nccc1-c1cc2n(c1)C=CC=C2C=O	0
Decoy643	[NH+]([C@H](C#N)c1cc2c(nccc2)cc1)(C)C	0
Decoy644	O(C(=O)CCCOc1ccc(cc1)C(CC)(C)C)c1ccc(cc1)-c1ccc(cc1)C	0
Decoy645	BrCc1c2CCCc2nnc1[O-]	0
Decoy646	S1CCC(=O)Nc2cc(ccc12)C(=O)NC[C@H](C=1C[NH+]=C2C=1C=CC=C2)c1ccccc1	0
Decoy647	Clc1nc(Oc2cccc(F)c2C#N)ccn1	0
Decoy648	n1c(cc(nc1N\\N=C/1\[C@H]2[C@@H](C\1)C=CC2)C)C	0
Decoy649	Clc1c2c(NC(OC2=O)=O)cc(Cl)c1	0
Decoy650	S=C(NC=1CS(=O)(=O)CC=1)N[C@@H]1CS(=O)(=O)C[C@H]1NC(=S)NC=1CS(=O)(=O)CC=1	0
Decoy651	Clc1cc(Cl)c(Cl)cc1OCC(=O)N([C@H]1CCS(=O)(=O)C1)c1ccccc1	0
Decoy652	Clc1ccccc1-c1noc(C)c1C(=O)Nc1sc2c(CCCC2)c1C(OC(C)C)=O	0
Decoy653	O=C(N[C@H]1C[C@H]1CCC)c1cc2nc(C)c(nc2cc1)C	0
Decoy654	O=C(NNC(=O)[C@@H]1[C@H](\C=C(\C)/C)C1(C)C)c1cc(N(C)C)ccc1	0
Decoy655	Clc1ccc(cc1)C(=O)NN\C(=C\C(=O)NC12CC3CC(C1)CC(C2)C3)\C	0
Decoy656	Clc1cc2c(SC[C@H]2[NH2+]CC)cc1	0
Decoy657	n1c2c([n-]c1[C@@H]1C[C@H]1C)cncc2	0
Decoy658	Fc1ccc(cc1)[C@@H](C(=O)[C@H]1OCCOC1)C#N	0
Decoy659	O=Cc1n[n-]nc1C(C)(C)C	0
Decoy660	O(c1ccccc1Nc1nccc(C)c1N)c1ccccc1	0
Decoy661	Clc1cc2nc(sc2cc1)S[C@H]1C[C@H](OC1=O)C	0
Decoy662	Clc1ccc(cc1[N+](=O)[O-])[C@@H]1C2=C(N(C(N)=C1C#N)c1cc(Cl)cc(Cl)c1)C[C@H](CC2=O)c1ccccc1	0
Decoy663	Clc1c2[nH]c(CO)c(c2ccc1)-c1nc(oc1)N	0
Decoy664	s1cc(nc1C1(NC(OC(C)(C)C)=O)CCCC1)C	0

Decoy665	Clc1ccsc1\C=C(\C#N)/C#N	0
Decoy666	O=C1N[C@@H](CC1)C(=O)N1[C@@H]2[C@@H](C[C@@H]1C(OC)=O)CCCC2	0
Decoy667	[NH2+](CC#C)C12CC3CC(C1)CC(C2)C3	0
Decoy668	Clc1cc(Cl)ccc1[C@H](P(O[C@@H]1C[C@@H](CC[C@H]1C(C)C)C)(O[C@@H]1C[C@@H](CC[C@@H]1C(C)C)C)=O)O	0
Decoy669	O1[C@H](CO[C@H]2OC[C@](O)(CO)[C@H]2O)[C@@H](O)[C@H](O)[C@@H](O[C@H]2OC[C@](O)(CO)[C@H]2O)[C@@H]1O[C@@H](CCc1ccc(O)cc1)CCCCc1ccc(O)cc1	0
Decoy670	Clc1cc2c([nH]nc2C([NH3+])(C)C)cc1	0
Decoy671	S1c2c(N(CC[C@@H]1C)C(=O)CSc1oc(nn1)-c1ccc(F)cc1)cccc2	0
Decoy672	FC(F)(F)[C@]1([NH+]=N1)c1ccc(cc1)C(=O)NC(CO[C@H]1[C@@H](O)[C@@H](O)[C@H](O[C@H]1CO)O)CO[C@H]1[C@@H](O)[C@@H](O)[C@H](O[C@H]1CO)O	0
Decoy673	S(C)c1ccc(S(=O)(=O)NCC(O[C@H](C(C)C)C(=O)NC(=O)N)=O)cc1[N+](=O)[O-]	0
Decoy674	S=C(N(Cc1ccc(N(C)C)cc1)C1CC([NH2+]C(C1)(C)C)(C)C)Nc1cccc(C)c1C	0
Decoy675	O=Cc1ccc(cc1[O-])C#N	0
Decoy676	Br[C@H]([C@H](C(C)C)C)c1ccc(Cl)cc1Cl	0
Decoy677	Clc1ccccc1\C=N/N=C/c1ccccc1Cl	0
Decoy678	O=C(Nc1ccccc1)NC[C@@H](C)c1ccccc1	0
Decoy679	S(C)c1ccc(cc1)[C@@H]1NC(=O)CC[C@H]1[N+](=O)[O-]	0
Decoy680	O(C\C=C(\[C@@H](O)C[C@@H](O)[C@@](O)(CC\C=C(\C)/C)C)/C)C[C@H](O)[C@H](O)[C@H](O)[C@H](O)CO	0
Decoy681	Clc1cc(Cl)ccc1O[C@H]1[C@H]2O[C@H]2CCC1	0
Decoy682	Clc1oc(cc1)C[NH2+]C1C2CC3CC1CC(C2)C3	0
Decoy683	s1cccc1C=1CCN(CC=1)c1nnc([O-])cc1	0
Decoy684	s1cccc1S(=O)(=O)\C(=C\c1[nH]cnc1)\C#N	0
Decoy685	O=[N+]([O-])c1c(ccnc1N1C[C@@H]2[C@H](C1)C[NH+](C)[C@@H]2c1ccccc1)C	0
Decoy686	O([C@H](C(=O)Nc1cc(NC(=O)C)ccc1)C)c1ccc(cc1)C(=O)CC	0
Decoy687	OC[C@@H](O)[C@@H](O)Cc1ncc(nc1)[C@@H](O)[C@H](O)[C@H](O)CO	0
Decoy688	s1c2nc(nc(N(C)C)c2cc1C)CC	0
Decoy689	S(c1nc(F)c(N2CC[NH2+]CC2)c([O-])c1F)c1cc(C(C)(C)C)c(F)c(c1)C(C)(C)C	0
Decoy690	s1c2c(nc1N=C=O)CCSC2	0

Decoy691	Clc1ccc(cc1)C(O\N=C(/N)\COc1ccc(cc1)C1SCCS1)=O	0
Decoy692	Brc1ccc(cc1)CSc1cc2c(cc1)cccc2	0
Decoy693	S(CC#N)c1cc(F)c(F)cc1	0
Decoy694	Clc1sc(cc1)/C(=N/[N-]C=1SCC(=O)N=1)/C	0
Decoy695	Clc1sc(cc1)C(=O)COC(=O)c1[nH]c2c(c1C)C(=O)CCC2	0
Decoy696	S=C1N=C(N)C2=C(N1)NC1=C([C@H]2c2ccccc2)C(=O)CCC1	0
Decoy697	O=C1C[C@]2([C@@H](CC1)CCCC2)C(=O)[O-]	0
Decoy698	Clc1ccc(cc1)[C@](OC)(C(=O)[O-])C	0
Decoy699	s1c2c(nc1Cc1ccc(F)cc1)CC(C[C@@H]2[NH2+]C)(C)C	0
Decoy700	Brc1cc2c(cc1)c(\C=N\c1c3nsnc3ccc1)c(O)cc2	0
Decoy701	FC(F)(F)c1nn(cc1)Cc1onc(c1)C[NH2+]C	0
Decoy702	S(=O)(=O)(NCCO)c1cc2c(-c3c(cc(S(=O)(=O)NCCO)cc3)C2=C(C#N)C#N)cc1	0
Decoy703	[nH+]1c[nH]cc1-c1cc(\N=C\c2c3c([nH]c2)cccc3)ccc1	0
Decoy704	ClC=1C(O[C@H](O[C@@H]2C[C@@H](CC[C@@H]2C(C)C)C)C=1Cl)=O	0
Decoy705	OC1(CCC(CC1)CCCCC)C1(O)CCC(CC1)CCCCC	0
Decoy706	s1cc2O[C@H]3[C@H](c2c1C=O)CCC3	0
Decoy707	N1C[C@H](Cc2cc(C)c(cc12)C)CC	0
Decoy708	Clc1c(OCC(C)=C)c(Cl)c(nc1C)C	0
Decoy709	O(C(=O)c1ccccc1C(OCCCCCCC(C)C)=O)CCCCCCC(C)C	0
Decoy710	BrC=1C=C(c2n(C=1)c(CC#N)c(n2)C(C)(C)C)C	0
Decoy711	FC(F)(F)C1CCC(Nc2c3[nH]ncc3ccc2)CC1	0
Decoy712	s1nc(cc1C=O)[C@H]1C[C@@H](OCC1)C	0
Decoy713	S1[C@H]2N=CC=C2N(C[C@H]1C(C)C)C	0
Decoy714	[S-]c1n(nc(c1)C(C)(C)C)CCC#N	0
Decoy715	Brc1c2c(cccc2)c(cc1)CC(=O)N\N=C\c1oc(cc1)-c1ccc(Br)cc1	0
Decoy716	S(CC(=O)c1[nH]c(C)c(C(=O)C)c1C)c1[nH]c2c(n1)cccc2	0
Decoy717	s1cccc1[C@H](NC(=O)N[C@@H](Cc1cc(cc(c1)C)C)C)CCO	0
Decoy718	Clc1ccccc1[C@H](N(C)c1cc([nH+]cc1)C(=S)N)C	0
Decoy719	Clc1ccc([nH+]c1CN1C=CC(=O)C=C1)N	0
Decoy720	s1ncc(-c2n(C)c(C(=O)[O-])c(c2)CC)c1C	0
Decoy721	[NH+]=1CCCNC=1c1ccccc1Cn1nnc2c1cccc2	0
Decoy722	Clc1ccc(cc1)/C(=C/c1ccc(Cl)cc1)/c1ccc(OCC[NH+](CC)CC)cc1	0
Decoy723	O=C(N(C)c1cc(ccc1)C#N)[C@]1([NH2+]CCC1)C	0
Decoy724	Clc1ccccc1COc1nc2c(cc1C[NH2+]CC1(COC1)C)cc(cc2)C	0
Decoy725	Clc1cc(NC(=O)NC=2SC(=S)C3=C(CC[C@@H](C3)C)C=2C#N)ccc1	0

Decoy726	S(S\C(=C\C)\C[C@H](O)N(Cc1cnc(nc1N)C)C=O)\C(=C/C)\C[C@@H](O)N(Cc1cnc(nc1N)C)C=O	0
Decoy727	S(=O)(=O)(CNC(=O)[C@H](N(CCC)C(=O)\C=C\CCCCC)C(CC)CC)c1ccc(cc1)C	0
Decoy728	O1CCC[C@@H]1CNc1nc([nH+]c(N)c1[N+](=O)[O-])NCC(=O)[O-]	0
Decoy729	s1cc(nc1[C@@H]([NH3+])[C@H]1CCOC1)C	0
Decoy730	O=Cc1[nH]c(C)c(C)c1CC	0
Decoy731	Fc1cc(ccc1)[C@@H]1O[C@@H](C[NH2+]1)C	0
Decoy732	O=CN[C@H]1[C@H]2CC[C@H](C2)C1(C)C	0
Decoy733	Ic1ccc(cc1)C1CCC(CC1)CCCC	0
Decoy734	Clc1c(cccc1Cl)-c1oc(cc1)\C=C(/C#N)\c1n[nH]c(N)c1C#N	0
Decoy735	Clc1cc(Cl)cc([C@H]2Nc3c([C@@H]4[C@@H]2CC=C4)cc(OCCOC)cc3)c1O	0
Decoy736	s1ncc(c1)[C@@H]1[NH2+][C@H](CCC1)C(=O)[O-]	0
Decoy737	S(C(F)(F)F)c1ccc(N[C@H](C(=O)Nc2ccccc2C#N)C)cc1	0
Decoy738	Clc1cc([C@]2(O)CCCC[C@H]2C2CCCCC2)c(nc1)N	0
Decoy739	N(=Nc1ccccc1)c1c2c(ccc1N)cc1c(c2)cccc1	0
Decoy740	Fc1ccccc1[C@@H]1O[C@@H](CO1)CC#N	0
Decoy741	O=C1N([C@@H](CC#N)C)C(=O)CC2(C1)CCCCC2	0
Decoy742	c12cc(ccc1-c1c(cc(cc1)C#CC)C2(C[C@@H](CCCC)CC)C[C@H](CCCC)CC)C#CC	0
Decoy743	O=C(C)c1c(C)c([nH]c1C)C(=O)N([C@H](C)c1cc[nH+]cc1)C	0
Decoy744	O(CC=1N=C2N(C=CC(=C2)C)C(=O)C=1)c1ncnc2c1cc(cc2)C	0
Decoy745	Clc1cc(cc2OCOc12)-c1scc(n1)C[NH2+]C(C)C	0
Decoy746	Clc1ccc(cc1)C(=O)CSC1=NC=2[C@@H]([C@H]([C@@H]1C#N)c1occc1)C(=O)CCC=2	0
Decoy747	O=C([O-])[C@@](CC)(C#N)[C@H]1CCCC=C1	0
Decoy748	O=C1N=NC(=C1)c1ccc(N[C@H]2[C@@H]3CC[C@H](C2)C3)cc1	0
Decoy749	S(CC#N)c1cc(ccc1)C(=O)N[C@H](C1CCCCC1)c1ccc[nH+]c1	0
Decoy750	S1\C(=C\C=2C(C)=C(C#N)C(=O)N(C)C=2N2C[C@@H](C[C@H](C2)C)C)\C(=O)N(C2CCCCC2)C1=S	0
Decoy751	Clc1cc2S(=O)(=O)N[C@@H](Nc2cc1)C(=O)Nc1cc(ccc1)C(C)C	0
Decoy752	Brc1ccc(Oc2ccc(\N=C\3/SSC4=C/3c3cc(ccc3NC4(C)C)C)cc2)cc1	0
Decoy753	o1nc(cc1COc1ccccc1)CC1([NH2+]C2CCCCC2)COC1	0
Decoy754	IC=1N[C@@]2(NC(=O)[C@](C#N)(C=1C#N)C2(C)C)C	0
Decoy755	O1CCC[NH+](C[C@H]1C)[C@@H]1C[C@H](CC[C@@H]1C(=O)[O-])C	0
Decoy756	O=C(N[C@H]1[C@@H]2CC[C@@H](C2)[C@@H]1C(=O)[O-	0

	])C1([NH3+])CCCC1	
Decoy757	O1CCC(=O)C[C@@](O)(C(=O)[O-])[C@H]1C(=O)[O-]	0
Decoy758	FC(F)(F)C[NH+]1CCC2(OCCO2)CC1	0
Decoy759	Ic1cc(NCc2cc(Br)cc(Br)c2OCC)ccc1	0
Decoy760	S(Cc1cc(ccc1)C)[C@@H]1O[C@H](NN1)[C@@H](NC(OC(C)(C)C)=O)CC=1C[NH+]=C2C=1C=CC=C2	0
Decoy761	Brc1oc(cc1)C(=O)NC=1C(=O)NC(SCC(=O)Nc2scc(n2)C)=NC=1N	0
Decoy762	O=C([O-])C1([NH2+]CC#C)CCCC1	0
Decoy763	Clc1sc(cc1)\C=C(/C(=O)Nc1ccccc1)\C#N	0
Decoy764	N(C)(C)c1ccc(cc1)\C=C\C=1CC(C\C(\C=1)=C(/C#N)\C#N)(C)C	0
Decoy765	s1c(cc(C(=S)N)c1CC)-c1cc(C)c(F)cc1	0
Decoy766	Clc1ncnc(C2CC2)c1C=O	0
Decoy767	n1cc(ccc1)[C@H]1Nc2c([C@@H]3[C@@H]1CC=C3)cc(cc2)C#N	0
Decoy768	FC(F)(F)C(Oc1nc(nc(n1)N\N=C\c1cccc([N+](=O)[O-])c1O)N(c1ccccc1)c1ccccc1)C(F)(F)F	0
Decoy769	Brc1cc2CN(COc2cc1)c1ccc(cc1)C	0
Decoy770	Brc1ncc(NC(=O)NC(C)(C)c2cc(ccc2)C(C)=C)cc1	0
Decoy771	O=C([O-])C[NH+](Cc1cnc(nc1N)N)C	0
Decoy772	O=C1N(N=C(CC)C(CC)=C1C#N)C[C@H](O)c1cc(C)c(cc1)C	0
Decoy773	O1C[C@@H](CC1)C(=O)Nc1ccc(nc1)N(CC)CC	0
Decoy774	s1cc(nc1)C[NH2+][C@H](C(C)(C)C)Cn1ccnc1	0
Decoy775	s1cc(nc1-c1ccc(cc1)C(=O)N)CSCC(=O)N(CC(C)=C)CC	0
Decoy776	Clc1cc(N\C=C\2/N=C(OC/2=O)c2ccc(cc2)CCCC)ccc1C	0
Decoy777	Clc1cc(cc(Cl)c1)-c1nc(cc(n1)N)COC	0
Decoy778	Brc1cc([C@@H]2Nc3c(C4=C2C(=O)C[C@@H](C4)c2ccccc2)c2c(nccc2)cc3)c(OC)cc1	0
Decoy779	S1c2c(N(c3c1cccc3)C(=O)COC(=O)C(O)(c1ccccc1)c1ccccc1)cccc2	0
Decoy780	S1c2c(C=3OC(N)=C(C(OCC)=O)[C@@H](C=3C1=O)c1ccccc1C(F)(F)F)cccc2	0
Decoy781	O1C(NNC(=O)CNNCC(=O)NNC=2OC(=CC(=O)C=2C(=O)C)C)=C(C(=O)C)C(=O)C=C1C	0
Decoy782	S(C)c1nccc(c1)C(=O)N1[C@@H](COC[C@H]1C)C	0
Decoy783	O(CCCC)c1cc(ccc1)[C@H]1n2nnnc2NC2=C1C(=O)CC(C2)(C)C	0
Decoy784	O=C(Nc1cc2c(nc1)cccc2)C(=O)NCc1cc(NC(=O)C)ccc1	0
Decoy785	Clc1c2c(sc1C(=O)NNC(=O)c1ccccc1OCCCCC)cccc2	0
Decoy786	O1Cc2cc(ccc2C1)C(=O)N(C[C@H](C#N)C)C	0
Decoy787	Ic1nc([nH]c1)C	0

Decoy788	Clc1ccc(\[NH+]=C\2/N=C(SCC(=O)[O-])N(C/23CCCCC3)c2ccc(cc2)C(=O)[O-])cc1	0
Decoy789	Fc1cc(ccc1F)[C@@H]1[NH2+][C@H](CC(=O)C1)C(=O)[O-]	0
Decoy790	O([C@H]1CC[NH2+]C1)C1CCC1	0
Decoy791	S=C1N[C@@H]2[N-]\C(=N/[N+](=O)[O-])\[N-][C@H]2N[N-]1	0
Decoy792	s1cccc1[C@@H](\[NH+]=C(/NC(C)C)\NC[C@@H](O)c1cc(F)c(F)cc1)C	0
Decoy793	O1CCCN(c2ccc(cc2)C(=O)Nc2c3c(ccc2)cncc3)C1=O	0
Decoy794	O(C(=O)[C@@H]1CCCc2[nH]c([nH+]c12)C(C)(C)C)C	0
Decoy795	S=C(Nc1cc(ccc1)C#N)N[C@@H]1[C@H]2OC[C@H](Nc3nc(ccn3)-c3ccc(cc3)-c3ccccc3)[C@H]2OC1	0
Decoy796	O=C1C(=C\C(\C=C1C(C)(C)C)=C\C=C/1\C=CN(C=C\1)CCCCCCCCCCCCO)C(C)(C)C	0
Decoy797	O=C(Nc1cc2CCCc2cc1)c1cc([N+](=O)[O-])ccc1	0
Decoy798	Clc1ccc(cc1)[C@H](NC(=O)N[C@H](CS(=O)(=O)C)C)CC(C)C	0
Decoy799	Brc1cc(ccc1F)CN1c2c(C=CC1=O)cccc2	0
Decoy800	S=C1[NH+](N[C@@]2(N1)C[C@@H](CCC2)C)CCC(C)C	0

Table S2. Structures of the 260 Compounds (in SMILE format) from the Test set together with Their activities (1 or 0) for glutamate-induced models.

Name	Structure	Activity
CHEMBL2152545	O(C(=O)NCCCCCCC)c1cc2C[NH+]3C(N(c2cc1)C)c1c(CC3)cccc1	1
CHEMBL2069520	O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@H](/C(=N/OC(=O)[C@H]5[NH2+]CCC5)/C)[C@]4(CC3)C)CCC2=C1)C	1
CHEMBL33601	S1SCCC1CCCCC(=O)NCc1ccc(NC(=[NH2+])c2sccc2)cc1	1
CHEMBL33692	S1SCCC1CC(=O)NCCc1ccc(NC(=[NH2+])c2sccc2)cc1	1
CHEMBL478507	FC(F)(F)c1ccc(cc1)C[NH+](Cc1c2c(nccc2)c(O)cc1)Cc1c2c(nccc2)c(O)cc1	1
CHEMBL2151788	Clc1cc2[nH+]c3c(CCCC3)c(NCCCNC(=O)\C=C\c3cc(O)c(O)cc3)c2cc1	1
CHEMBL2151789	Clc1cc2[nH+]c3c(CCCC3)c(NCCCCCCCNC(=O)\C=C\c3cc(O)c(O)cc3)c2cc1	1
CHEMBL595697	S1SCCC1CCCCCNC(=O)C1(Oc2c(CC1)c(C)c(O)c(C)c2C)C	1
CHEMBL1165728	O1c2c(CCC1(C)C)c(-c1onc(c1)-c1cc(O)c(O)cc1)c(O)c(C)c2C	1
CHEMBL1641656	Oc1c(cc(cc1C(C)(C)C)\C=C\c1cc(O)cc(O)c1)C(C)(C)C	1
CHEMBL1641657	Oc1ccc(cc1C(CC)CC)\C=C\C=C\c1cc(O)cc(O)c1	1
CHEMBL1641658	Oc1c(cc(cc1C(CC)CC)\C=C\C=C\c1cc(O)cc(O)c1)C(CC)CC	1
CHEMBL1641659	Oc1ccc(cc1C(C)(C)C)\C=C\C=C\c1cc(O)cc(O)c1	1
CHEMBL1641660	Oc1c(cc(cc1C(C)(C)C)\C=C\C=C\c1cc(O)cc(O)c1)C(C)(C)C	1
CHEMBL1641663	Oc1c(cc(cc1C(C)(C)C)\C=C\c1cc(C(C)(C)C)c(O)c(c1)C(C)(C)C)C(C)(C)C	1
CHEMBL1641665	O(C)c1c(cc(cc1C(C)(C)C)\C=C\C=C\c1cc(O)cc(O)c1)C(C)(C)C	1
CHEMBL165	Oc1cc(cc(O)c1)\C=C\c1ccc(O)cc1	1
CHEMBL1813354	O1c2c(CCC1(C)C)c(-c1noc(c1)-c1ccc(OC)cc1)c(O)c(C)c2C	1
CHEMBL1813361	O1c2c(CCC1(C)C)c(-c1onc(c1)-c1ccc(O)cc1)c(O)c(C)c2C	1
CHEMBL1096008	O1c2c(CCC1(C(=O)N1CC[NH+](CC1)CC1=CC=C(C=C(O)C1=O)C(C)C)C)c(C)c(O)c(C)c2C	1
CHEMBL2425176	S(=O)(=O)(n1c2c(c3c1cccc3)cccc2)c1ccc(cc1)C	1
CHEMBL2425184	S(=O)(=O)(n1c2c(c3c1cccc3)ccc1c2cccc1)c1ccc(cc1)C	1
CHEMBL461922	Fc1cc(ccc1OC)C(=O)\C=C\c1cccc(OC)c1O	1
CHEMBL512570	Fc1cc(ccc1OC)C(=O)\C=C\c1cc(O)c(OC)cc1	1

CHEMBL523763	O1C(C(O)COC(=O)CCCCCNC(=O)CCCCCCC\C=C/C\C=C/CCCCC)C([O-])=C(O)C1=O	1
CHEMBL1215857	OC1(CC[NH+](CC1)C[C@@H]1C[C@@]1(C(OC)=O)c1ccc(cc1)C)c1ccccc1	1
CHEMBL122701	O1c2c(cccc2)C(=O)C(O)=C1c1cc(O)c(O)cc1	1
CHEMBL1951837	O1c2c(ccc3c2cccc3)C(=O)C(O)=C1c1ccc(N(C)C)cc1	1
CHEMBL31574	O1c2c(ccc(O)c2)C(=O)C(O)=C1c1cc(O)c(O)cc1	1
CHEMBL2334464	O=C1c2c(cccc2)C(=O)C=C1NCc1ccncc1	1
CHEMBL2334467	Clc1ccc(cc1)CNC1=CC(=O)c2c(cccc2)C1=O	1
CHEMBL2334468	Clc1cc(ccc1)CNC1=CC(=O)c2c(cccc2)C1=O	1
CHEMBL447012	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1OC=C([C@@H]2[C@H]1C(=C[C@H]2OC(=O)\C=C\c1ccc(OC)cc1)CO)C(OC)=O	1
CHEMBL500233	O1c2c(C(=O)C(O[C@@H]3O[C@H](CO)[C@H](O)[C@H](O)[C@H]3O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)=C1c1ccc(O)cc1)c(O)cc(O)c2	1
CHEMBL501132	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1OC=C([C@@H]2[C@H]1C(=C[C@H]2OC(=O)\C=C/c1ccc(OC)cc1)CO)C(OC)=O	1
CHEMBL503795	O1c2c(C(=O)C(O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O[C@@H]3O[C@H](COC(=O)\C=C\c4cc(OC)c(O)cc4)[C@@H](O)[C@H](O)[C@H]3O)=C1c1cc(O)c(O)cc1)c(O)cc(O)c2	1
CHEMBL505056	O1c2c(C(=O)C(O[C@@H]3O[C@H](CO)[C@H](O)[C@H](O)[C@H]3O[C@@H]3O[C@H](COC(=O)\C=C\c4cc(OC)c(O)cc4)[C@@H](O)[C@H](O)[C@H]3O)=C1c1ccc(O)cc1)c(O)cc(O)c2	1
CHEMBL506966	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1OC=C([C@@H]2[C@H]1C(=C[C@H]2OC(=O)\C=C\c1ccc(O)cc1)CO)C(OC)=O	1
CHEMBL500710	O(C)c1cc(ccc1O)C(O[C@H]1[C@H]2[C@](CC[C@@H]3[C@@]2(CC[C@H](O)C3(C)C)C)(C)[C@]2([C@@H]([C@@H]3[C@@](C[C@@H]2OC(=O)c2ccccc2)(CC[C@H]3C(C)=C)C)C1)C)=O	1
CHEMBL508571	O(C)c1cc(ccc1O)C(O[C@H]1[C@H]2[C@](CC[C@@H]3[C@@]2(CC[C@H](O)C3(C)C)C)(C)[C@]2([C@@H]([C@@H]3[C@@](C[C@@H]2OC(=O)c2ccc(O)cc2)(CC[C@H]3C(C)=C)C)C1)C)=O	1

CHEMBL457074	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1OC=C[C@]2(O)[C@H]1[C@@](OC(=O)\C=C\c1ccc(OC)cc1)(C[C@H]2O)C	1
CHEMBL464666	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1OC=C[C@]2(O)[C@H]1[C@@](OC(=O)\C=C/c1ccc(OC)cc1)(C[C@H]2O)C	1
CHEMBL516702	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1OC=C[C@]2(O)[C@H]1[C@@](OC(=O)\C=C\c1ccccc1)(C[C@H]2O)C	1
CHEMBL518566	O1[C@H](COC(=O)\C=C\c2ccc(OC)cc2)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1OC=C[C@]2(O)[C@H]1[C@@](O)(C[C@H]2O)C	1
CHEMBL284237	[NH2+]1[C@@H]2Cc3c(cccc3)[C@]1(c1c2cccc1)C	1
CHEMBL28862	P(=O)([O-])([O-])CCCC([NH3+])C(=O)[O-]	1
CHEMBL479696	O1c2c(C[C@H](OC(=O)\C(=C\CO)\C)C1(C)C)cc1C=CC(Oc1c2)=O	1
CHEMBL481656	O1c2c(C[C@H](OC(=O)[C@@]3(O[C@@H]3C)C)C1(C)C)cc1C=CC(Oc1c2)=O	1
CHEMBL404868	O1[C@H]([C@]2(C([C@@H](O)C1=O)=C(C)[C@@H](O)CC2)C)c1ccoc1	1
CHEMBL437025	O1[C@H]([C@]2(C(=C(C)[C@H](O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)CC2)C1=O)C)c1ccoc1	1
CHEMBL466729	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@H]([C@H](O)c1cc(OC)c(O)cc1)CO	1
CHEMBL468549	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@H]([C@@H](O)c1cc(OC)c(O)cc1)CO	1
Decoy801	o1cccc1[C@@H]([NH+]1CCC(CC1)C)C#N	0
Decoy802	N#CC[C@@H]1CCCC[C@@H]1CC#N	0
Decoy803	Clc1cc(N(C(=O)[C@H]2[C@@H]3C=C[C@H]([C@@H]2C)C23CC2)C=O)ccc1	0
Decoy804	s1ccc(C)c1[C@@H]1[C@@H]2C(=NC(C)=C1C(=O)Nc1[nH+]cc(cc1)C)CC(CC2=O)(C)C	0
Decoy805	[NH2+](C(C#C)(C)C)[C@@H]1CC(C[C@H](C1)C)(C)C	0
Decoy806	S=P1(OCC(CO1)(C)C)[C@H](Nc1ccc(OCC)cc1)c1ccccc1	0

Decoy807	s1cccc1[C@H]([NH2+]Cc1nc(on1)-c1ccccc1)c1ccc(F)cc1	0
Decoy808	FC(F)(F)c1ccccc1C[C@@H](NC(=O)NC[C@H]1C[C@@H](O)CCC1)CC	0
Decoy809	Cl[C@H]1N=C(C=CN1[S-])C	0
Decoy810	Brc1ccc(cc1)-c1nnc(SCc2c(F)cccc2Cl)cc1	0
Decoy811	Clc1cc(OC)c(N[C@H]([C@H](CC)C)C)cc1OC	0
Decoy812	S(C(C)(C)C)c1cc(Nc2ccccc2)ccc1N[C@@H](CC(C)C)C	0
Decoy813	s1c(ccc1C(=O)C)-c1noc(c1)C	0
Decoy814	S1c2sccc2[NH2+]C[C@H]1C(C)C	0
Decoy815	s1c(CC)c(cc1C(=O)NNC(=O)C[NH+](C)[C@@H]1CCC[C@@H]1SC)C	0
Decoy816	O=C1C[C@H](C\C(=[NH+]/CCc2c3cc(ccc3[nH]c2C)C)\[C@H]1C(=O)CCC)c1ccccc1	0
Decoy817	O=C(NC12CC3CC(C1)CC(C2)C3)[N-]\N=C\c1cn[nH]c1-c1ccccc1	0
Decoy818	Brc1ccc(NC=2C[C@](O)(C)[C@H](C(=O)C)[C@@H](C=2C(=O)C)c2ccc(Cl)cc2)cc1	0
Decoy819	Brc1n(c2C[C@H](C[C@@H]3[NH2+]Cc1c23)CC)C	0
Decoy820	S1C=C(n2c1c([NH3+])c(C(C)(C)C)c2C(=O)[O-])C	0
Decoy821	Brc1cc(ccc1)\C=C(/C#N)\c1ccc(Cl)cc1	0
Decoy822	Brc1cc(ccc1)\C=C(\C#N)/c1nc(nc(n1)N)Nc1ccccc1	0
Decoy823	Brc1sc(cc1)C=1N(\N=C\c2ccc(OCCCC)cc2)/C(/SC=1)=N/CC=C	0
Decoy824	S1\C(=C/c2ccncc2)\C([O-])=NC1=S	0
Decoy825	O1[C@@H]2[C@@H](OC1(C)C)[C@H]1OC(O[C@H]1O[C@@H]2COc1ccccc1C)(C)C	0
Decoy826	s1nnc(c1)-c1ccc(cc1)CSc1[nH+]c(C)c([nH]1)C	0
Decoy827	O=C([O-])[C@@H](C(C)C)c1cc(ccc1)C#N	0
Decoy828	n1c(Nc2cc3CCCNc3cc2)c(C#N)c(cc1C)C	0
Decoy829	s1c2c(nc1-c1ccn3c1OCC3)C[NH2+][C@H]2C	0
Decoy830	S([C@H](CC)C(=O)Nc1ccc(O)cc1)C=1NC(=O)C=C(N=1)CSC(C)C	0
Decoy831	Fc1cc(F)c(F)cc1NC(=O)N(CC)C[C@@H](C#N)C	0
Decoy832	O(C)c1cc(C)c(cc1OC)[C@@H](Nc1ncc(cc1)C(=O)NC1CC1)C	0
Decoy833	ClC=1C=CC=2N(C=1)C(=O)C=C(N=2)C(F)(F)F	0
Decoy834	O1[C@H](C=CC1=N)[C@H]1CCCOC1	0

Decoy835	Brc1cc2[nH]c(nc2nc1)[C@H](OC(=O)CC1CCCC1)C	0
Decoy836	S(CCNC(=O)C)C[C@@H]([NH3+])C(=O)[O-]	0
Decoy837	O1C[C@H](CC1)COc1cc([nH+]cc1)CNC(C)(C)C	0
Decoy838	F[C@H]1CC(CN(C1)C(OC(C)(C)C)=O)(C)C	0
Decoy839	S\1CC(=NN(C)/C/1=N/[C@H](CC)C)C12CC3CC(C1)CC(C2)C3	0
Decoy840	Brc1cc2c(oc(C(=O)c3cc(ccc3)C#N)c2C)cc1	0
Decoy841	Clc1ccc(cc1)[C@H]\1[NH+]=C([O-])N=C(C)/C/1=C(/OC)\[O-]	0
Decoy842	O(CCCCn1c2c(nc1\C=C\c1ccccc1)cccc2)c1ccc(cc1)[C@H](CC)C	0
Decoy843	O1CC[C@@H](O)C[C@@H]1C1CC1	0
Decoy844	S([C@H]1CCOC1=O)c1oc(nn1)-c1c(cc(cc1C)C)C	0
Decoy845	Clc1cccc(Cl)c1CSC1=NN[C@H](N1N)[C@@H]1N=NC2=C1CCC2	0
Decoy846	Clc1ccc(cc1)[C@@H](NC(=O)N)CC(OCC(=O)\C(=C(\N)/C)\C#N)=O	0
Decoy847	Clc1nsnc1N1CCCC1(C)C	0
Decoy848	s1c2c(nc1SCCC/C(/O)=N/c1nc3c(n1CCC)cccc3)cccc2	0
Decoy849	S=C1N=C(NC(C)=C1C#N)C	0
Decoy850	S1CCc2nc(C=O)c(cc12)C#N	0
Decoy851	o1c2CCCCc2nc1C(=O)[O-]	0
Decoy852	O(CCNC(=O)\C=C\C(C)(C)C)c1ccc(cc1)C(C)C	0
Decoy853	O(C)[C@@]1(C[C@@H](Nc2nc([nH+]cc2)C)C1(C)C)C	0
Decoy854	Clc1cc(ccc1)C(=O)NNC(=O)c1oc2c(\C(=N\NS(=O)(=O)c3ccc(F)cc3)\CCC2)c1C	0
Decoy855	O=C([O-])c1nnc(nc1[O-])N	0
Decoy856	Clc1c(c2c(occ2CC(=O)N(C)C)cc1C)C	0
Decoy857	S=C1NC(=S)N(N=C(C1)C)C	0
Decoy858	O1[C@@H]([NH+](C)C)C(=N)C=C1C	0
Decoy859	S1C=2C[C@H](CCC=2n2c1ncc2C=O)C	0
Decoy860	ClCc1ccc(O[C@@H]2CCCC[C@H]2C)nc1	0
Decoy861	ClCc1[nH]c2c(n1)cc1OCCCOc1c2	0
Decoy862	O(NC(=O)c1n[n-]nc1)CC(=O)[O-]	0
Decoy863	s1c(C)c(cc1C)[C@@H](NC(=O)C[C@H](NC(OC(C)(C)C)=O)C)C	0
Decoy864	O1c2n(C=C1[C@@H]([NH3+])CCC)ccn2	0
Decoy865	Brc1ccc(cc1)/C(/[O-	0

	])=C/1\[C@H](N(C(=O)C\1=O)c1[nH+]cccc1)c1ccccc1	
Decoy866	S1C[C@H](N(CC1)C(=O)c1cc(ccc1F)C#CCO)C	0
Decoy867	Clc1nc(nc2sc3CCCc3c12)NCCOC	0
Decoy868	Clc1sc(cc1)C[NH+](CC=C)CC(=O)Nc1ccc(NC(=O)C)cc1	0
Decoy869	S(C)c1nnc(N2CCS(=O)[C@@H](C)[C@H]2C)cc1	0
Decoy870	O(C[C@H](O)C[NH2+]CCNC(=O)Nc1ccc(O)cc1)c1ccc(OCCOCC2CC2)cc1C#N	0
Decoy871	Brc1cc([C@@H]2N3NC=NC3=[NH+][C@H](C2)c2ccc(F)cc2)c(OC(F)F)cc1	0
Decoy872	O1c2cc(ccc2OC1)CNc1nc[nH+]c(N2[C@H]3CC(C[C@](C3)(C2)C)(C)C)c1N	0
Decoy873	Brc1cc(ccc1)[C@@H]([NH+]1C[C@H](C[C@H](C1)C)C)C=1Sc2n(nc(n2)C)C=1O	0
Decoy874	O=C1n2c(nnc2N)N=C1[C@@H](C(=O)C)CCCCC[C@H](C(=O)C)C1=Nc2n(C1=O)c(nn2)N	0
Decoy875	S=C(N)[N-]N[C@H]1[C@@H]2O[C@@H](OC2)\C(=N/[N-]C(=S)N)\C1	0
Decoy876	s1cc(nc1[C@@H](Nc1oc2c(n1)cccc2)C1CC1)C	0
Decoy877	S1(=O)C[C@H]([NH3+])[C@H](OCC)CC1	0
Decoy878	O(C(=O)[C@@H]1CCCN(C1)C(=O)N(C)C)c1cccc(C)c1C	0
Decoy879	Brc1cc(ccc1)C1CC([NH2+]C2CCC(CC2)C(=O)N)C1	0
Decoy880	Clc1cc([O-])cnc1Cl	0
Decoy881	n1cc(cc(C)c1NC)C=C	0
Decoy882	S(C[C@H]1OCCC1)c1nc(nc(C)c1C#N)C	0
Decoy883	FC(F)(F)CNC(=O)c1[nH+]ccn1C	0
Decoy884	S=C(N)C=1C=C2C(OC=1Nc1cc(ccc1)C)=CC(=O)C=C2	0
Decoy885	S(C)c1cc(NCCCc2ccc([NH+](CC)CC)cc2)ccc1	0
Decoy886	S=C(NCc1ccccc1)[N-]\N=C\c1c2c(n(c1)CCOc1cc(ccc1)C)cccc2	0
Decoy887	S(\C(\Sc1ccccc1)=C\C(=O)N\N=C\c1c2c([nH]c1)cccc2)c1ccccc1	0
Decoy888	Clc1cc(C#N)c(Nc2ccc(N)cc2)cc1	0
Decoy889	Brc1cccc(C#N)c1N=C=O	0
Decoy890	O=C(N1C[C@H](CC[C@@H]1C)C)c1nc(ncc1)C1CC1	0
Decoy891	Clc1ccccc1N1C(=O)[C@H]2N(CSC2)C1=S	0
Decoy892	FC(F)(F)[C@H]1OC(OC1)=O	0

Decoy893	S1[C@H](C[NH+](C[C@@H]1C)CCC#N)C	0
Decoy894	FC(F)(F)[C@@]1(O)CC[NH+](C1)C(C)C	0
Decoy895	O1[C@@H](CC[C@H]1C[NH2+]CC(C)C)Cn1ccnc1	0
Decoy896	S(Oc1ccccc1[N+](=O)[O-])(=O)(=O)C=1CCc2c(C=1)cccc2	0
Decoy897	O1c2c(Nc3c1cccc3)cc1nc3c([n+](c1c2)-c1ccccc1)cc(Nc1ccccc1)cc3	0
Decoy898	O1c2c(cc3c(oc(C)c3-c3ccccc3)c2C)C(C)=C(CCC(=O)N[C@@H](CC(C)C)C(=O)[O-])C1=O	0
Decoy899	Clc1cc2nc3c(nc2cc1Cl)[C@@]1(CC[C@@]3(C(=O)NNC(=O)c2ccc(F)cc2)C1(C)C)C	0
Decoy900	[NH2+](C)[C@@H]1C[C@@H](CC1)[C@@H]1C[C@H](CCC1)C	0
Decoy901	S(=O)(=O)(C)c1ccc(N2Cc3c(cc(F)cc3)C2=[NH2+])cc1	0
Decoy902	Brc1c2c(ccc1)[C@@H](NC(=O)[C@H]1NC(=O)CC1)CC2	0
Decoy903	Clc1cccc(Oc2ccccc2Cl)c1/C(=N\O)/N	0
Decoy904	FC(F)(F)c1[nH]c2cc(ccc2n1)[C@H](NC(=O)CC(C)(C)C)c1ccccc1	0
Decoy905	O[C@@H]1CC[C@H](C[C@H]1[NH+]([C@H](C(C)C)C)C)C(C)C	0
Decoy906	S(N=O)C([C@H](NC(=O)C)C(=O)N[C@@H]1[C@H](O)[C@H](O)[C@@H](O[C@@H]1O)CO)(C)C	0
Decoy907	Clc1cc(NC(=O)C2=CC=3CCCCC=3NC2=O)ccc1N(C)C	0
Decoy908	Clc1cc(cc(OC)c1OC)C(=O)Nc1sc(cc1C#N)CC	0
Decoy909	ClCC(=O)[C@@H](NC(=O)[C@H]1N(CCC1)C(=O)[C@H]([NH3+])Cc1ccccc1)CCC\[NH+]=C(\N)/N	0
Decoy910	Brc1cnc(nc1)N1CC[C@H](CCC1)C(C)(C)C	0
Decoy911	S1[C@@H](Cc2c3c(sc2[C@@H]1c1ccccc1)[nH+]c(SCCC(OC)=O)nc3N)c1ccccc1	0
Decoy912	O(CC1CCCCC1)c1cc(ccc1)CNC(=O)c1[nH]c(c2c1CCC2)-c1ccccc1	0
Decoy913	O=C1N(C=NC(=C1)C)C[C@@H]([NH2+]CCC)C(C)(C)C	0
Decoy914	OCC(\N=C/1\C=C2[N+]=3[C@@]4(N=C2C=C\1)[C@H](CCCC4)C[C@H]1C=3CCCC1)(C)C	0
Decoy915	s1cc(c2c1ncnc2N[C@@H](C(=O)[O-])CO)C(=O)[O-]	0

Decoy916	Clc1ccc(cc1)[C@H](N/C(=[NH+]\CC)/NCc1ccccc1NC(=O)C)C	0
Decoy917	Brc1ccc(cc1)-c1n(-c2ccc(F)cc2)c(SCC(C)C)nc1	0
Decoy918	O=C1c2c(N(C=C1C)CC(=O)[O-])cc(cc2C)C	0
Decoy919	s1ccc(C)c1[C@@H]1Nc2c([C@H]3[C@H]1CC=C3)cc(NC(=O)c1ccccc1)cc2	0
Decoy920	Fc1cc2[n+]([O-])c3n(CCCC3)c2cc1	0
Decoy921	S(=O)(=O)(N([C@@H](C[NH3+])C)C)C(C)C	0
Decoy922	Brc1cc2OCCCOc2cc1[C@@H]([NH3+])[C@@H]1CCOC1	0
Decoy923	O=C([C@@H](NC(=O)[C@H](N(C(=O)[C@@H](NC(=O)[C@@H]([NH2+]C)CC(C)C)C(C)C)C)[C@H](O)[C@@H](C\C=C\C)C)[C@H](O)C)CCCC	0
Decoy924	S(Cc1[nH]c2[n+](c1)cccn2)c1nc(cc(n1)C)C	0
Decoy925	s1c2cc(cnc2cc1)[C@@H](Nc1cc2CCOc2cc1)C	0
Decoy926	S(CC(=O)N)c1ccccc1C(=O)NCCSCc1ccccc1F	0
Decoy927	Brc1cc(sc1)[C@H]1[NH2+][C@H](COC1)C	0
Decoy928	O=C1N=C[NH+]=C2C1=CC1=[NH+]C=NC(=O)C1=C2	0
Decoy929	Clc1sc(cc1)[C@H]([NH2+]Cc1cn[nH]c1C)c1sccc1	0
Decoy930	S(=O)(=O)(C)c1[n-]c(cc1)CC(F)(F)F	0
Decoy931	[S-]/C(=[NH+]\C=[N+](\C)/C)/Nc1cc(F)ccc1	0
Decoy932	Clc1c2c(sc1C(Oc1ccccc1Cl)=O)cccc2	0
Decoy933	FC(F)(F)[C@H](n1ncnc1)[C@H]([NH3+])C	0
Decoy934	Clc1nnc(N[C@@H](C)c2cc[nH+]cc2)cc1	0
Decoy935	o1c2c(cc1[C@H](NC(=O)NC)c1ccccc1)cccc2	0
Decoy936	O([C@@H]1CC(C[C@@H](C1)C)(C)C)c1cc(ncc1)C#N	0
Decoy937	S\1c2c(N/C/1=C(\C(=O)CSc1nnnn1-c1ccccc1)/C#N)cccc2	0
Decoy938	S1(=O)(=O)C[C@H]([NH+](C)[C@@H]2C[C@@H](CC[C@@H]2C#N)C)CC1	0
Decoy939	O=C1N(C[NH+](C(c2ccccc2)c2ccccc2)C)C(=O)N[C@H]1CC(C)C	0
Decoy940	s1nnc(C[NH+](C)C2CCOCC2)c1NCC	0
Decoy941	O[C@@H]1CC[C@H](C[C@H]1CC1CCCC1)C	0
Decoy942	Ic1oc2cc(Br)cnc2c1	0
Decoy943	Cl[C@@H]1C[C@@H](CC[C@@H]1C(Cc1c2c(sc1)cccc2)(C)C)C	0
Decoy944	ClC(=O)Cc1cc(sc1C)-c1ccc(cc1)C(C)C	0
Decoy945	Clc1sc(cn1)C(Cl)=O	0

Decoy946	Clc1nc(nc(C)c1C)CC	0
Decoy947	O=C(N[C@@](C(=O)[O-])(C)C1CC1)C=C	0
Decoy948	s1c(nnc1NC(=O)C(=O)NC[C@@](O)(C)c1ccsc1)C(C)(C)C	0
Decoy949	s1cc(cc1)[C@@H]1C=2[C@H](OC(N)=C1C#N)N=NC=2C	0
Decoy950	Clc1cnccc1C(O[C@H](C)c1ccc[nH+]c1)=O	0
Decoy951	Clc1snnc1COC(=O)C=1COc2c(C=1)cc(Cl)cc2	0
Decoy952	Ic1ccccc1OCc1oc([N+](=O)[O-])cc1	0
Decoy953	o1c(ccc1CNc1onc(n1)C1CC1)[C@H]1C[C@@H]1C	0
Decoy954	S([C@H]1CCN(C)C1=O)c1ccc([nH+]c1)N	0
Decoy955	S1[C@@H](C[NH+](C[C@@H]1C)C[C@@H]1C[C@@H](CC[C@@H]1O)C)C	0
Decoy956	Clc1ncc(cc1)CN(C(=O)Nc1cc2oc(nc2cc1)C)C	0
Decoy957	S\1C=C(N/C/1=N\c1ccc(OCC)cc1)[C@@]1(OC(=O)[C@]2(C1)C[C@H](OC2=O)C)C	0
Decoy958	O=Cc1nc2c(cc1)cccc2C#N	0
Decoy959	Clc1ccccc1CC[NH2+]Cc1c2c([nH]c1C(=O)[O-])cc(cc2)C	0
Decoy960	Clc1ccc(cc1)C(=O)Nc1ccc(cc1)C(=O)N[C@@H](C)[C@@H]1Oc2c(OC1)cccc2	0
Decoy961	s1cc(nc1[C@H]([NH3+])c1ccc(OC(F)(F)F)cc1)C(C)C	0
Decoy962	S1C[C@](NC(=O)CC(F)(F)F)(CC1)C(=O)[O-]	0
Decoy963	O(C)c1ncc(N[C@H](CC(C)(C)c2ccccc2)C)cc1	0
Decoy964	O=C(C(C(C)=C)(CCc1nc(nc(n1)N)N)N)CCc1nc(nc(n1)N)N)C	0
Decoy965	FC(F)(F)c1nc(N2C[C@H]3[C@H](CC=CC3)C2)c(cc1)C#N	0
Decoy966	FC(F)(F)/C(/[O-])=N/[C@@H](CC)C#N	0
Decoy967	S(Cc1nc(oc1C)-c1ccc(cc1)C(=O)N[C@H](CC)C)c1ccc(cc1)C	0
Decoy968	Fc1ccccc1C(=O)NC1=Nc2c(N=C(C)[C@@H]1c1ccc(F)cc1)cccc2	0
Decoy969	Clc1cc(NC(=O)N([O-])[C@H]2N(N)C(SC2(C)C)=S)ccc1Cl	0
Decoy970	O(C)c1ccc(cc1[N+](=O)[O-])[C@@H]1Nc2c([C@H]3[C@@H]1CC=C3)cc(OC)cc2OC	0
Decoy971	S(=O)(=O)(C(CC)(CC)CNC(=O)C(=O)Nc1cc2c([nH]cc2)cc1)C	0
Decoy972	Clc1ccccc1-c1oc(cc1)[C@H]1Oc2nc(SC)nnc2-c2c(N1)cccc2	0
Decoy973	Brc1cc(N2N=C([C@H](C2)c2ccccc2)c2sccc2)ccc1	0
Decoy974	S1C=C(N(CC(=O)NNC(=O)c2ccc(NS(=O)(=O)c3ccc(OCC)cc3)cc2)C1=O)C	0

Decoy975	Fc1c(F)c(F)ccc1C(Oc1ccc(NC(OC)=O)cc1)=O	0
Decoy976	s1cc(nc1)[C@H](NC)c1[nH+]ccn1C	0
Decoy977	Fc1ccc(F)cc1-c1nc([nH]c1)[C@]([NH3+])(CCC)C	0
Decoy978	s1cc(nc1-c1ccsc1)C(=O)N(C)C	0
Decoy979	Ic1ccc(cc1)C(=O)Nc1sc(cn1)Cc1ccc(SC(F)F)cc1	0
Decoy980	S=C(Nc1ccc(Oc2ccccc2)cc1)NC(=O)C12CC3CC(C1)CC(C2)C3	0
Decoy981	Clc1cc(\N=C/2\S[C@H](CN\2)C)ccc1C#N	0
Decoy982	s1cncc1[C@@H]1[NH2+][C@H](CCC)C(=O)NC1	0
Decoy983	S1[C@H]([C@H]([N+](=O)[O-])[C@H](C(C#N)=C1N)c1ccc(cc1)C)c1ccccc1	0
Decoy984	Fc1ccc(cc1)C=1N=C(C)[C@@H](C=1)C(=O)N1C[C@@H](C[C@H](C1)C)C	0
Decoy985	FC(F)(F)COCc1cc(oc1C(C)(C)C)C(=O)Nc1cc2oc3c(c2cc1)cccc3	0
Decoy986	n1ccccc1N1[C@@H](C=C(C=C1c1ccccc1)c1ccccc1)c1ccccc1	0
Decoy987	Brc1ccc(S[C@@H]2C[C@H](CC[C@@H]2C#N)C(CC)(C)C)nc1	0
Decoy988	S1(=O)(=O)N(CCC1)c1ccccc1C#CCCO	0
Decoy989	O=C(N[C@@]1(C[C@@H](CCC1)C)C(=O)[O-])c1ncc([O-])nc1	0
Decoy990	Oc1c2c(ccc1)[C@H]([C@H]1C(C2=O)=C([O-])[C@@H]2[C@H]([C@H]([NH+](C)C)C([O-])=C(C(=O)N)C2=O)[C@@H]1O)C	0
Decoy991	O=C(NCc1[nH+]cccc1)N1CCC(=CC1)c1ccccc1	0
Decoy992	Brc1c(n(nc1C)CC=O)C	0
Decoy993	S1[C@H](C=CC1=N)c1scc(n1)C	0
Decoy994	S(=O)(=O)(N(CC(C)=C)CC)c1c(n[nH]c1C)C	0
Decoy995	Clc1ncccc1C(=O)N[C@@H](C(C)C)C(OC)=O	0
Decoy996	S=C(N)c1c(C)c(nnc1NC1CCC(CC1)CC)C	0
Decoy997	Brc1cc(C)c(N2NCCCC2=O)cc1	0
Decoy998	Clc1cc(N\C(=[NH+]\c2nc(cc(n2)N)[C@H]([C@@H](C(=O)C)C(OCC)=O)C(=O)C)\N)c(OC)cc1	0
Decoy999	Clc1ccc(cc1)C=1[C@H](N=NC=1C)NC=1CC(CC(=O)C=1)(C)C	0
Decoy1000	s1c2c(cc1CNC(=O)N1CCS(=O)[C@@H](C)[C@H]1C)cc(F)cc2	0
Decoy1001	O[C@H]1C[C@H]2[C@@H]([C@@H]3CC[C@H]([C@@H](CCC(=O)[O-])C)[C@@]13C)C1(N=N1)C[C@@H]1C[C@H](O)CC[C@@]12C	0

Decoy1002	s1nc([O-])c2c1nc(C)c(C)c2C	0
Decoy1003	O(CCCC[C@]([NH2+]C)(C(OCC)=O)C)CCOCCCC	0
Decoy1004	S(C[C@@H](O)COc1ccc(cc1)C#N)c1[nH+]c(Cc2ccccc2)c([nH]1)C	0
Decoy1005	FC(F)(F)Oc1ccc(cc1)[C@H]1[NH+]2[C@H](C[C@H]([NH2+]C3CC3)C1)c1[nH]c3c(c1C[C@H]2C(OC)=O)cccc3	0
Decoy1006	O1CCCC[C@H]1O[C@@H]/1CCCC\C\1=C\C(C)C	0
Decoy1007	Clc1cccc(NC2=NN=C(SCc3ccc(F)cc3)N(CC=C)C2=O)c1C	0
Decoy1008	S(=O)(CC[C@H](NC(=O)[C@H]([NH3+])Cc1ccc(O)cc1)C(=O)NCC(=O)N[C@@H](Cc1ccc(F)cc1)C(=O)N)C	0

Table S3. Structures of the 700 Compounds (in SMILE format) from the Training set together with their activities (1 or 0) for H_2O_2-induced models.

Name	Structure	Activity
Lentinan	O1C(CO)C(O)C(OC2OC(COC3OC(CO)C(O)C(O)C3O)C(O)C(OC3OC(CO)C(O)C(OC4OC(COC5OC(CO)C(O)C(O)C5O)C(O)C(OC5OC(CO)C(O)C(OC)C5O)C4O)C3O)C2O)C(O)C1C	1
1	Clc1cc2sc(cc2cc1)CC(=O)N[C@@H](CCC(=O)NCCC1CC[NH+](CC1)Cc1ccccc1)C(OCCCCCC)=O	1
2	o1[n+]([O-])c(C)c(n1)\C=[N+](/[O-])\C(C)(C)C	1
CHEMBL1080631	O(CCCCCC)C(=O)[C@@H](NC(=O)c1ccccc1)CCC(=O)NCCC1CC[NH+](CC1)Cc1ccccc1	1
CHEMBL1080813	s1cccc1C(=O)N[C@@H](CCC(=O)NCCC1CC[NH+](CC1)Cc1ccccc1)C(OCCCCCC)=O	1
CHEMBL1080814	Brc1cc(sc1)C(=O)N[C@@H](CCC(=O)NCCC1CC[NH+](CC1)Cc1ccccc1)C(OCCCCCC)=O	1
CHEMBL1082081	O(CCCCCC)C(=O)[C@@H](NC(OC(C)(C)C)=O)CCC(=O)NCCC1CC[NH+](CC1)Cc1ccccc1	1
CHEMBL1099213	Clc1cccc(Cl)c1\C=C\C=1OC(=O)C=C(OC)C=1COC	1
CHEMBL1163570	Clc1ccc(cc1)-c1nc(SC)nnc1-c1ccc(Cl)cc1	1
CHEMBL1163571	Clc1ccc(cc1)-c1nc(SCC)nnc1-c1ccc(Cl)cc1	1
CHEMBL1163577	Clc1ccc(cc1)-c1nc(SCCCC)nnc1-c1ccc(Cl)cc1	1
CHEMBL1163600	S(C)c1nc(c(nn1)-c1ccccc1)-c1ccccc1	1
CHEMBL1163601	S(CC)c1nc(c(nn1)-c1ccccc1)-c1ccccc1	1
CHEMBL1214705	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1C2=C(Oc3c(c(O)c(-c4cc(O)c5Oc6c(C(=O)c5c4O)c(O)cc(O)c6)c(O)c3)C2=O)[C@H](O)CC1	1
CHEMBL1214706	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1Oc1c2c(Oc3c(c(O)c(-c4cc(O)c5Oc6c(C(=O)c5c4O)c(O)cc(O)c6)c(O)c3)C2=O)c(O)cc1	1
CHEMBL1214707	O1[C@H]([C@H](O)[C@@H](O)[C@H](O)[C@H]1CO)c1c(O)c(c2Oc3c(cc(O)c(O)c3)C(=O)c2c1O)-c1cc(O)c2Oc3c(C(=O)c2c1O)c(O)cc(O)c3	1

CHEMBL127028	Oc1cc(ccc1O)\C=C\C(=O)CCc1ccccc1	1
CHEMBL13210	[O-]\[N+](=C/c1ccccc1)\C(C)(C)C	1
CHEMBL1428	O(C(=O)C=1C(C(C(OCCOC)=O)=C(NC=1C)C)c1cc([N+](=O)[O-])ccc1)C(C)C	1
CHEMBL153	O1c2c(CCC1(C(=O)[O-])C)c(C)c(O)c(C)c2C	1
CHEMBL1629795	Clc1cc2Sc3c(N(NC(=O)CC[NH+](C)C)c2cc1)cccc3	1
CHEMBL1629796	Clc1cc2Sc3c(N(NC(=O)C[NH+]4CC[NH+](CC4)C)c2cc1)cccc3	1
CHEMBL1688934	O1C[C@H]2[C@H](CO[C@@H]2c2cc3OCOc3cc2)[C@H]1c1cc(O)c(O)cc1	1
CHEMBL1782110	O1c2c(OC1)cc1c(-c3c(cc(OC)c(OC)c3OC)C(=O)[C@@H](C)[C@H](C)[C@@H]1OC(=O)C)c2OC	1
CHEMBL1782120	O1c2c(OC1)cc1c(-c3c(cc(OC)c(OC)c3OC)[C@H](OC(=O)\C(=C\C)\C)[C@@H](C)[C@@H](C)[C@H]1OC(=O)C)c2OC	1
CHEMBL1782124	O1c2c(OC1)cc1c(-c3c(cc(OC)c(OC)c3OC)C[C@H](C)[C@H](C)[C@H]1O)c2OC	1
CHEMBL1938397	Clc1cc2Sc3c(N(NC(=O)CC[NH+]4CC[NH+](CC4)C)c2cc1)cccc3	1
CHEMBL1938453	Clc1cc2Sc3c(N(NC(=O)C[NH+](C)C)c2cc1)cccc3	1
CHEMBL1938456	Clc1cc2N(NC(=O)C[NH+]3CCCCC3)c3c(Sc2cc1)cccc3	1
CHEMBL1938461	Clc1cc2Sc3c(N(NC(=O)C)c2cc1)cccc3	1
CHEMBL1938462	S1c2c(N(NC(=O)CC[NH+]3CCCC3)c3c1cccc3)cccc2	1
CHEMBL1938463	Clc1cc2Sc3c(N(NC(=O)CC[NH+]4CCCC4)c2cc1)cccc3	1
CHEMBL1938466	S1c2cc(OC)ccc2N(NC(=O)CC[NH+]2CC[NH+](CC2)C)c2c1cccc2	1
CHEMBL1938467	S1c2cc([N+](=O)[O-])ccc2N(NC(=O)CC[NH+]2CC[NH+](CC2)C)c2c1cccc2	1
CHEMBL1957559	O(C)c1ccccc1\C=C\C(=O)[C@H]1CC[C@H]2[C@H]3[C@H](CC[C@]12C)[C@@]1(C(C[C@@H](O)CC1)=CC3)C	1
CHEMBL1983100	O=C(NC1CCCCC1)C[NH+]1CC[NH2+]CC1	1
CHEMBL2036258	S(C(=O)C)CCC(=O)NCCCNc1c2CCCCc2[nH+]c2c1cccc2	1
CHEMBL2036259	SCCC(=O)NCCCNc1c2CCCCc2[nH+]c2c1cccc2	1
CHEMBL2036262	Clc1cc2[nH+]c3c(CCCC3)c(NCCCCCCNC(=O)CCSC(=O)C)c2cc1	1
CHEMBL2036263	Clc1cc2[nH+]c3c(CCCC3)c(NCCCCCCNC(=O)CCS)c2cc1	1
CHEMBL2151787	Clc1cc2[nH+]c3c(CCCC3)c(NCCNC(=O)\C=C\c3cc(O)c(O)cc3)c2c	1

	c1	
CHEMBL2180482	O[C@@H]1C[C@@](C[C@@H]2CC=C3[C@H](CCCC3(C)C)[C@@]12C)([C@@H](O)CO)C	1
CHEMBL2180483	O[C@@H]1C[C@@H]2[C@]3(C[C@@]1(C=C3)CO)[C@@H](O)C[C@H]1[C@]2(CCCC1(C)C)C	1
CHEMBL2180484	O[C@]1(C[C@@H](O)[C@H]2[C@](CCC[C@@]2(CO)C)(C)[C@@H]1CCC(C=C)=C)C	1
CHEMBL218693	O1[C@@H]2c3c([C@@]4([C@@H](C2)C(CCC4)(C)C)C1=O)c(O)c(O)c(c3)C(C)C	1
CHEMBL2312737	O1c2c(c(O)c(O)c(O[C@@H]3O[C@H](CO)[C@H](O)[C@H](O)[C@H]3O)c2)C(=O)C=C1c1ccc(O)cc1	1
CHEMBL2331619	O1[C@]2(O)CCCC[C@]2(C)C(=CC1=O)c1ccoc1	1
CHEMBL2333074	OC1=C2[C@](CCCC2(C)C)(c2c(c(C3=C4C=C(O)C(=O)C=C4[C@@]4([C@@H](C3=O)C(CCC4)(C)C)C)c(O)c(O)c2)C1=O)C	1
CHEMBL2336882	SCCNC(=[NH2+])NCC[NH3+]	1
CHEMBL2336883	SCCNC(=[NH2+])NCCC[NH3+]	1
CHEMBL2337285	SCCNC(=[NH2+])NCCCCCO	1
CHEMBL2337286	SCCNC(=[NH2+])NCCCOC(=O)c1cc(OC)c(O)c(OC)c1	1
CHEMBL2337715	o1cccc1[C@@H]1CC(=O)[C@]2(O)CCCC[C@]12C	1
CHEMBL2337716	o1cccc1C1=CC(=O)[C@]2(O)CCCC[C@]12C	1
CHEMBL2337718	o1cc(cc1)C1=CC(=O)[C@@H]2CCCC[C@]12C	1
CHEMBL2376099	Oc1c(cc2c([C@@]3([C@@H](CC2)C(CCC3)(C)C)C=O)c1O)C(C)C	1
CHEMBL2391354	O=C(NC1CCCCC1)C[NH+]1CC2[NH+](CCCC2)CC1	1
CHEMBL2391355	O=C(NC1CCCCC1)C[NH+]1[C@H]2C[C@H]([NH2+]C2)C1	1
CHEMBL2391356	O=C(NC(C)C)C[NH+]1CC[NH2+]CC1	1
CHEMBL2391357	O=C(NC1CCCCC1)C[NH+]1CCC[NH+](CC1)C	1
CHEMBL2391358	O=C(NC1CCCCC1)C([NH+]1CC[NH+](CC1)C1CCCC1)CC	1
CHEMBL2391359	O=C(N(C)C1CCCC1)C[NH+]1CC([NH+](CC1)CC)C	1
CHEMBL2391361	O=C(NC(CC)CC)C[NH+]1CCC[NH+](CC1)C	1
CHEMBL2391363	O=C(N1CC[NH+](CC1)CCC(=O)NC1CCCCC1)C1CC1	1
CHEMBL2391364	O=C(N(CCCC)CCC)C[NH+]1CC[NH2+]CC1	1
CHEMBL2391366	O=C(N1CC[NH+](CC1)CC(=O)NC(CC)CC)CC	1
CHEMBL2391367	O=C(N1CC[NH+](CC1)CC(=O)NC1CCCCC1)CC	1

CHEMBL2391369	O=C(NCCC1CCCCCCC1)C([NH+]1CC[NH2+]CC1)C	1
CHEMBL2391381	O=C(N1CCC[NH+](CC1)CCC(=O)NC1CCCCCC1)C	1
CHEMBL2391540	O=C(N(C)C1CCCC1)C[NH+]1CC[NH2+]CC1	1
CHEMBL2397172	Clc1cc(ccc1)CCC(=O)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2397175	O(C)c1cc(ccc1O)CCC(=O)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2397177	Oc1cc(ccc1O)\C=C\C(=O)CCCCc1ccccc1	1
CHEMBL2397178	O(C(=O)C)c1cc(ccc1OC(=O)C)\C=C\C(=O)CCc1ccccc1	1
CHEMBL2397179	Clc1cc(ccc1)CCC(=O)\C=C\c1cc(OC(=O)C)c(OC(=O)C)cc1	1
CHEMBL2397181	O(C(=O)C)c1cc(ccc1OC(=O)C)\C=C\C(=O)CCc1ccc(OC)cc1OC	1
CHEMBL2397182	O(C(=O)C)c1cc(ccc1OC(=O)C)\C=C\C(=O)CCc1cc(OC)c(O)cc1	1
CHEMBL2397184	O(C(=O)C)c1cc(ccc1OC(=O)C)\C=C\C(=O)CCCCc1ccccc1	1
CHEMBL2409143	O=C1NC2=C(C=C1)[C@@]1([NH3+])C[C@@H](C[C@@H](C2)[C@H]1C=C)C	1
CHEMBL2413094	S(=O)(=O)(NCc1ccccc1)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2414564	S(=O)(=O)(NCCc1ccccc1)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2414566	S(=O)(=O)(NCCCCc1ccccc1)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2414569	S(=O)(=O)(NCc1ccc(F)cc1)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2414571	S(=O)(=O)(NCc1ccc(OC)cc1)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2414572	Clc1ccc(cc1)CCNS(=O)(=O)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2414573	S(=O)(=O)(N(CCc1ccccc1)C)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2414575	S(=O)(=O)(NCCc1ccccc1)\C=C\c1cc(OC(=O)C)c(OC(=O)C)cc1	1
CHEMBL2414577	S(=O)(=O)(NCCCCc1ccccc1)\C=C\c1cc(OC(=O)C)c(OC(=O)C)cc1	1
CHEMBL2414578	Clc1ccc(cc1)CNS(=O)(=O)\C=C\c1cc(OC(=O)C)c(OC(=O)C)cc1	1
CHEMBL2414579	S(=O)(=O)(NCc1ccc(cc1)C(F)(F)F)\C=C\c1cc(OC(=O)C)c(OC(=O)C)cc1	1
CHEMBL2414582	S(=O)(=O)(NCc1ccc(OC)cc1)\C=C\c1cc(OC(=O)C)c(OC(=O)C)cc1	1
CHEMBL2414583	Clc1ccc(cc1)CCNS(=O)(=O)\C=C\c1cc(OC(=O)C)c(OC(=O)C)cc1	1
CHEMBL2414584	S(=O)(=O)(N(CCc1ccccc1)C)\C=C\c1cc(OC(=O)C)c(OC(=O)C)cc1	1
CHEMBL252696	OC[C@H](NC(=O)[C@@H](NC(=O)[C@H]1N(CCC1)C(=O)[C@@H](NC(=O)[C@@H]([NH3+])CC(=O)N[O-])C)C(C)C)C(=O)N[C@@H]([C@H](CC)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(=O)N)C(=O)N[O-]	1
CHEMBL290916	O=C1N(N=C(C1)C)c1ccccc1	1
CHEMBL38464	O1c2cc(ccc2OC(CO)C1c1cc(OC)c(O)cc1)C=1Oc2c(C(=O)C=1O)c(	1

	O)cc(O)c2	
CHEMBL443973	s1nc(nc1\C=[N+](/[O-])\C1CCCCC1)-c1ccccc1	1
CHEMBL450611	O(C(=O)C=1C(C(C#N)=C(NC=1C)N)c1ccncc1)CC	1
CHEMBL451743	O=C1C2=C(NC(N)=C(C#N)C2c2ccncc2)CC(C1)(C)C	1
CHEMBL452007	O(C)c1ccc(cc1)C1C2=C(NC(N)=C1C#N)CC(CC2=O)(C)C	1
CHEMBL453572	Fc1ccc(cc1)C1C2=C(NC(N)=C1C#N)CC(CC2=O)(C)C	1
CHEMBL455640	O=C1C2=C(NC(N)=C(C#N)C2c2ccccc2)CC(C1)(C)C	1
CHEMBL456967	O(C1Cc2c(cc(OC)c(OC)c2)C1=O)c1ccc(cc1)C(=O)CC[NH+](CC)CC	1
CHEMBL461076	Fc1ccc(cc1)C1C(C(OCC)=O)=C(NC(N)=C1C#N)C	1
CHEMBL461077	FC(F)(F)c1ccccc1C1C(C(OCC)=O)=C(NC(N)=C1C#N)C	1
CHEMBL468000	Fc1ccc(cc1)C1C2=C(Nc3[nH+]c4c(CCCC4)c(N)c13)CC(CC2=O)(C)C	1
CHEMBL468001	O(C)c1ccc(cc1)C1C2=C(Nc3[nH+]c4c(CCCC4)c(N)c13)CC(CC2=O)(C)C	1
CHEMBL482408	[O-]\[N+](=C/c1nc(C)c(nc1C)C)\C(C)(C)C	1
CHEMBL487805	O1c2c(c(O)c(O)c(O[C@@H]3O[C@H](C(=O)[O-])[C@@H](O)[C@H](O)[C@H]3O)c2)C(=O)C=C1c1ccc(O)cc1	1
CHEMBL493072	s1nc(nc1\C=[N+](/[O-])\Cc1ccccc1)-c1ccccc1	1
CHEMBL493073	Clc1ccc(cc1)-c1nc(sn1)\C=[N+](/[O-])\C(C)(C)C	1
CHEMBL493279	s1nc(nc1\C=[N+](/[O-])\C(C)(C)C)-c1ccc(OC)cc1	1
CHEMBL494097	s1nc(nc1\C=[N+](/[O-])\C(C)(C)C)-c1cc(C(C)(C)C)c(O)c(c1)C(C)(C)C	1
CHEMBL494100	o1[n+]([O-])c2cc(ccc2n1)\C=[N+](/[O-])\C(C)(C)C	1
CHEMBL50	O1c2c(C(=O)C(O)=C1c1cc(O)c(O)cc1)c(O)cc(O)c2	1
CHEMBL502	O(C)c1cc2c(CC(CC3CC[NH+](CC3)Cc3ccccc3)C2=O)cc1OC	1
CHEMBL505597	s1nc(nc1-c1ccccc1)\C=[N+](/[O-])\C(C)(C)C	1
CHEMBL509467	O(C(=O)C=1C(C(C#N)=C(NC=1C)N)c1ccc(cc1)-c1ccccc1)CC	1
CHEMBL510656	O(C)c1ccc(cc1)C1C(C(OCC)=O)=C(NC(N)=C1C#N)C	1
CHEMBL512226	OC1=C2[C@](CCCC2(C)C)(c2c(cc(O)c(O)c2)C1=O)C	1
CHEMBL512565	O(C(=O)C=1C(C(C#N)=C(NC=1C)N)c1ccc(cc1)C)CC	1
CHEMBL513161	O=C1C2=C(Nc3[nH+]c4c(CCCC4)c(N)c3C2c2ccc(cc2)C)CC(C1)(C)C	1
CHEMBL538371	O1c2c(OC1)cc1c(-	1

	c3c(cc(OC)c(OC)c3OC)[C@H](C(=O)\C(=C\C)\C)[C@H](C)[C@@H](C)[C@H]1OC(=O)CC)c2OC	
CHEMBL553164	O(C)c1ccc(cc1)[C@H](O)[C@@H](O)C	1
CHEMBL559796	O1c2c(OC1)cc1c(-c3c(cc(OC)c(OC)c3OC)C[C@@H](C)[C@@H](C)[C@H]1OC(=O)C)c2OC	1
CHEMBL561908	O1[C@]2([C@@]3(CC1=O)[C@](O)(CC2)[C@@]1(COC(=O)[C@@]1(C)[C@H]3O)C)C	1
CHEMBL566961	O1[C@@H](COCCOc2cc(O)c3c(OC(=CC3=O)c3cc(O)c(O)cc3)c2)[C@H](O)[C@@H](O)[C@H](O)C1O	1
CHEMBL567663	Fc1ccc(cc1)[C@H]1OCC2([NH+]1[C@@H](OC2)c1ccc(F)cc1)CO	1
CHEMBL570886	O1c2cc(ccc2OC(CO)C1c1cc(OC)c(OCC=C)cc1)C=1Oc2c(C(=O)C=1O)c(O)cc(OCC=C)c2	1
CHEMBL571128	O1c2cc(ccc2OC(CO)C1c1cc(OC)c(OC\C=C(\C)/C)cc1)C=1Oc2c(C(=O)C=1O)c(O)cc(OC\C=C(\C)/C)c2	1
CHEMBL571588	Clc1cc(Cl)ccc1NC(=O)COc1ccc(cc1OC)C1Oc2cc(ccc2OC1CO)C=1Oc2c(C(=O)C=1O)c(O)cc(OCC(=O)Nc1ccc(Cl)cc1Cl)c2	1
CHEMBL571723	O1c2cc(ccc2OC(CO)C1c1cc(OC)c(OCC(=O)N2CCCC2)cc1)C=1Oc2c(C(=O)C=1O)c(O)cc(OCC(=O)N1CCCC1)c2	1
CHEMBL571752	O1c2cc(ccc2OC(CO)C1c1cc(OC)c(O)cc1)C=1Oc2c(C(=O)C=1O)c(O)cc(OCC(=O)N(CC)CC)c2	1
CHEMBL571753	O1c2cc(ccc2OC(CO)C1c1cc(OC)c(OCCC=C)cc1)C=1Oc2c(C(=O)C=1O)c(O)cc(OCCC=C)c2	1
CHEMBL571975	Clc1cc(ccc1)C(OCC1Oc2c(OC1c1cc(OC)c(O)cc1)cc(cc2)C=1Oc2c(C(=O)C=1O)c(O)cc(O)c2)=O	1
CHEMBL572707	O1[C@@H](COCCOc2cc(O)c3c(OC(=C(OC)C3=O)c3cc(O)c(O)cc3)c2)[C@H](O)[C@@H](O)[C@H](O)C1O	1
CHEMBL572941	O1[C@@H](COC(=O)COc2cc(O)c3c(OC(=C(OC)C3=O)c3cc(O)c(O)cc3)c2)[C@H](O)[C@@H](O)[C@H](O)C1O	1
CHEMBL574682	O1[C@@H](CO)[C@H](O)[C@@H](O)[C@H](O)C1Oc1cc(O)c2c(OC(=C(OC)C2=O)c2cc(O)c(O)cc2)c1	1
CHEMBL575787	O1[C@@H](COC(=O)COc2cc(O)c3c(OC(=CC3=O)c3cc(O)c(O)cc3)c2)[C@H](O)[C@@H](O)[C@H](O)C1O	1
CHEMBL600	SC[C@H](NC(=O)C)C(=O)[O-]	1

Decoy001	s1c(nnc1S[C@H](C(=O)Nc1ccc(F)c(F)c1F)C)N	0
Decoy002	O(Cc1ccccc1)C[C@](O)([C@H](OCc1ccccc1)[C@@H](OCc1ccccc1)[C@H](OCc1ccccc1)C=C)C=C	0
Decoy003	Br[C@H](Cl)[N+](=O)[O-]	0
Decoy004	O(C(=O)N1[C@@H]2CC=CC[C@]12C)C	0
Decoy005	S=C=NC(=O)[C@H]1CCOC1	0
Decoy006	Fc1c2C=C(C#N)C(Oc2ccc1)=O	0
Decoy007	P(OCCCC)(OCCCC)(=O)C(NCC[NH2+]C(P(OCCCC)(OCCCC)=O)(C)C)(C)C	0
Decoy008	[NH2+]1CCN(CC1)c1cc2c(cc1)ccnc2	0
Decoy009	n1c(CC#N)c(C)c(nc1C)CC	0
Decoy010	o1nc(cc1[C@@H](C#N)C)C1CC1	0
Decoy011	S1(=O)(=O)N(CC=C)C(C(=O)c2ccccc2)=C(OC(=O)c2ccc([N+](=O)[O-])cc2)c2c1cccc2	0
Decoy012	O(C)c1cc(O[C@H]([C@@H]([NH3+])C)c2cc(ccc2)C)ccc1	0
Decoy013	Clc1cc(ccc1)[C@H]1[C@@H]2C(=CC[C@@H](C2)C)C(C#N)=C([NH3+])C1(C#N)C#N	0
Decoy014	S([C@H](C(=O)NC(=O)NC12CC3CC(C1)CC(C2)C3)C)[C@@H]([C@H](O)C)C	0
Decoy015	S\1[C@](CS/C/1=N\C(C)C)(\C=N\O)C	0
Decoy016	O=C([O-])CCC=1C2=[NH+]C(=Cc3[nH]c(C=C4[NH+]=C(C=c5[nH]c(=C2)c(C)c5CCC(=O)[O-])C(C)=C4CCC(=O)[O-])c(C)c3CCC(=O)[O-])C=1C	0
Decoy017	Clc1c(cccc1Cl)-c1oc(cc1)C[NH2+]CCO	0
Decoy018	O1[C@H](CC[C@]12O[C@@H](OC)CC2)C	0
Decoy019	Br[C@H](\C(=N\OC(=O)c1ccccc1)\c1ccccc1)c1ccccc1	0
Decoy020	s1cc(nc1CCCC)CS(=O)[C@@H](C)c1onc(n1)CCCC	0
Decoy021	FC(F)(F)c1occ(c1)[C@H]1OC=CC1=N	0
Decoy022	O1[C@@H]([C@H](N=[N+]=[N-])COC(=O)C(C)(C)C)[C@@H](OC(=O)C(C)(C)C)[C@H](OC(=O)C(C)(C)C)[C@@H]1OC(=O)C(C)(C)C	0
Decoy023	Clc1cc(ccc1)[C@H](O)c1ncncc1	0
Decoy024	Brc1ccc(S(=O)(=O)N[C@@H]2CCCCC[C@H]2[NH3+])cc1	0

Decoy025	Fc1ccc(N(C)C)c(C#N)c1C=O	0
Decoy026	S=C(Nc1ccc(OCC)cc1)NCc1ccccc1C[NH+](C(C)C)C	0
Decoy027	ClCC1=C2C[C@H](CCC2=NNC1=O)C	0
Decoy028	Brc1cc(cc(Br)c1NC(=[NH2+])C1CCCC1)C	0
Decoy029	s1c(C)c(nc1[C@H]1c2c(OC1)c(oc2)C=O)C	0
Decoy030	O(C(=O)C1(CCCC1)CNC(=O)C1(CCC1)C#N)C	0
Decoy031	n1nn(c2c1cccc2)C=C=C	0
Decoy032	O=C(NC(C)C)c1ccccc1NC(=O)CNc1cc(ccc1)C#C	0
Decoy033	ClC(Cl)(Cl)/C(=[NH+]/P(=S)(Nc1ccccc1)Nc1ccccc1)/Nc1ccccc1	0
Decoy034	O(Cc1ccccc1)c1nc(cc(-c2ccccc2)c1C#N)-c1ccccc1	0
Decoy035	Ic1ccc(cc1)[C@H]([NH3+])c1cc(oc1C)C	0
Decoy036	s1c(ccc1Cn1ccnc1)C#CCO	0
Decoy037	OC1C[NH+](C[NH+](C1)C(C)(C)C)C(C)(C)C	0
Decoy038	O1[C@@H](\C=C\C(=C\[C@@H](C\C=C\C(=C\[C@@H](C(=O)[C@H]([C@H](O)[C@H](C\C(=C\C(=O)[O-])\C)C)C)C)\C)C)\CC)[C@H](C=CC1=O)C	0
Decoy039	Brc1ccc(Nc2ncnc(NC3CC([NH2+]C(C3)(C)C)(C)C)c2[N+](=O)[O-])cc1	0
Decoy040	Oc1cc(ccc1)C(=O)NNC(=O)[C@@H]1C[C@H]1c1ccccc1C	0
Decoy041	Clc1nnc(n1[C@@H](C)[C@@H]1OCCC1)C1CC1	0
Decoy042	Clc1cc(cc(Cl)c1OCCCCCC)C(=O)C=1C(C)=C(C#N)C(=O)N(CCCOC(C)C)C=1[O-]	0
Decoy043	s1cc(nc1-c1ncccc1)C#N	0
Decoy044	N(N1C=C(CC=C1C#N)CC)(C)C	0
Decoy045	s1cccc1[C@@H](N(C(=O)c1occc1)C)C#N	0
Decoy046	Clc1oc(cc1)C[C@@H]1CCS(=O)(=O)CC1=O	0
Decoy047	O(\N=C\1/C[C@@H]2CC[C@@]/1(C)C2(C)C)Cc1ccc(cc1)-c1ccccc1C#N	0
Decoy048	S1[C@@H](C)C(=CC1=N)c1n(C)c(nc1C)C	0
Decoy049	s1c(cnc1CCN/C(=[NH+]\[C@@H](C)c1sccc1)/NC(C)C)CC	0
Decoy050	S(=O)(=O)(CC[NH+](CC(OC)=O)C1CC1)c1ccc(cc1)C(C)(C)C	0
Decoy051	FC(F)(F)[C@@]1(O)N2NC(=CC2=[NH+][C@](O)(C1)C(F)(F)F)c1ccccc1	0
Decoy052	O=C(c1cc(n2c1-c1c(C=C2)cccc1)C(=O)c1ccccc1)c1ccccc1	0

Decoy053	ClC(Cl)(Cl)[C@@H](O)N1CCCC1=O	0
Decoy054	S1[C@H]2C(=NC(=NC2=O)C[NH+]2C[C@@H](C[C@H](C2)C)C)C=C1	0
Decoy055	Clc1cccc(Cl)c1[C@@H]([NH2+]CC(C)C)C(=O)[O-]	0
Decoy056	s1c(C)c(nc1[C@]1([NH2+]C)CCCOC1)C	0
Decoy057	O=C(N[C@H](CCC(C)C)C)c1cc([nH+]cc1)N(C)C	0
Decoy058	s1cccc1[C@@H]1CC(=O)c2c([nH]nc2)C1	0
Decoy059	o1c(ccc1C(c1oc(cc1)-c1cc([N+](=O)[O-])ccc1)c1oc(cc1)-c1cc([N+](=O)[O-])ccc1)-c1cc([N+](=O)[O-])ccc1	0
Decoy060	FC(F)Oc1ccc(cc1)CNC(=O)NC[C@@H]1C[C@H](O)CCC1	0
Decoy061	Ic1ccc(cc1)[C@H]([NH3+])c1cc2NC(=O)COc2cc1	0
Decoy062	ClCC#Cc1cc(OCc2cnoc2)cnc1	0
Decoy063	Clc1cc2nc(ccc2cc1)CCc1cc(ccc1)[C@H](SCC1(CC1)CC(=O)[O-])CCc1ccccc1C(O)(C)C	0
Decoy064	Brc1ccc(OC\C=N\NC(=[NH2+])c2ccccc2OCC)cc1	0
Decoy065	O(C)c1ccc(cc1)C[C@@H]([NH2+]Cc1cn(nc1)C)C	0
Decoy066	Brc1cc2c(nc(nc2-c2ccccc2)NCc2ccc[nH+]c2)cc1	0
Decoy067	Clc1cc(ccc1)CN/C(=[NH+]/CC=C)/NCC1(SC)CCOCC1	0
Decoy068	Oc1c2c(ccc1)C([C@@H]1C(=C([O-])[C@@]3(O)[C@H]([C@@H]([NH+](C)C)C(=O)/C(=C(/[O-])\N)/C3=O)[C@@H]1O)C2=O)=C	0
Decoy069	O1CCCC[C@H]1CO[C@H]1COCC[C@@H]1[NH2+]CCC	0
Decoy070	S(CCCOc1ccc(cc1)C#N)c1[nH+]cc[nH]1	0
Decoy071	S(=O)([C@H]1O[C@@H]2[C@H](O[C@H](OC2)c2ccccc2)[C@@H](OCc2ccc(OC)cc2)[C@H]1OCc1ccc(OC)cc1)c1ccc(cc1)C	0
Decoy072	o1cccc1C(Oc1ccc(cc1)C(=O)COC(=O)c1ccc(N2C(=O)[C@@H]3[C@H]([C@@H]4C=C[C@H]3C4)C2=O)cc1)=O	0
Decoy073	Cl[C@@H](C)c1oc(cc1)C(=O)N[C@H](C(OC)=O)C	0
Decoy074	o1c2CC[C@@H](Cc2nc1C=O)C	0
Decoy075	[NH+](C[C@]([NH3+])(C#N)c1ccccc1)(C)C1CCC(CC1)CC	0
Decoy076	S=C(N)[N-]\N=C/1\c2c(oc(C(=O)NNC(=O)c3ccc([N+](=O)[O-])cc3)c2C)CCC\1	0
Decoy077	O=C(C)c1cn(nc1C)C(C)(C)C	0
Decoy078	S(=O)(=O)(C)c1c2nc(n(c2ccc1)C(C)C)C	0

Decoy079	BrC(CNC(=O)Nc1cc(ccc1Cl)C(=O)NC)=C	0
Decoy080	FC(F)(F)COc1ccccc1OCC(OC[C@H]1OCCCC1)=O	0
Decoy081	S1(=O)(=O)NC[C@]23[C@H]1C[C@H](CC2)C3(C)C	0
Decoy082	Brc1cc([nH]c1)C(=O)NN\C=C(\C#N)/C#N	0
Decoy083	S(c1ccccc1C#N)c1ccccc1C(OCC(=O)N[C@@H](COC)C)=O	0
Decoy084	FC(F)(F)[C@H]1c2c(COC1)c[nH]c2C=O	0
Decoy085	o1c(ccc1CN(C(=O)C[NH2+]C(C)C)C)[C@@H]1C[C@H]1C	0
Decoy086	S=C(NC(C)(C)C)[N-]NC(=O)\C=C\c1nc2c(cc1)cccc2	0
Decoy087	Brc1cc2nc(sc2cc1)-c1nc([nH]c1)C1([NH3+])CCC1	0
Decoy088	S1C[C@@H](CC1)C(=O)Nc1ccc(cc1)C#N	0
Decoy089	[S-]C=1[NH+]=C(C[C@H]([NH+]=1)c1cc2OCOc2cc1)C12CC3CC(C1)CC(C2)C3	0
Decoy090	O(c1ccc(cc1)C(OC)=O)c1nc(Oc2ccc(cc2)C(OC)=O)nc(Oc2ccc(cc2)C(OC)=O)n1	0
Decoy091	o1nc(nc1[C@@H]([NH3+])C1CCCCC1)C1CCCC1	0
Decoy092	Oc1c2c([C@@H]3[C@H]([C@@H]4CC[C@H](O)[C@]4(CC3)C)CC2)c(-[n+]2c3nc[nH]c3c(nc2)N)cc1[O-]	0
Decoy093	s1cccc1/C(=N/N1C[NH+](P(N=C1N)Nc1[nH]ncn1)[C@@H](C(=O)[O-])C)/C	0
Decoy094	S(C)c1ccc(cc1)[C@@H](NC(=O)N[C@@H]1CCCCNC1=O)C	0
Decoy095	Clc1ccc(NC(=O)CCC(=O)CCC(=O)c2sccc2)cc1C(=O)N(C)C	0
Decoy096	S1/C(=C\C=C\c2occc2)/C(=O)[N-]C1=S	0
Decoy097	Clc1cc(Nc2[nH+]cnc(Nc3ccc(OC)cc3)c2N)c(cc1[C@@H](C#N)c1ccc(Cl)cc1)C	0
Decoy098	O(C(=O)C)C1[C@@H](OC(=O)C(C)(C)C)[C@H](OC(=O)C(C)(C)C)C(OC(=O)C)[C@H](OC(=O)C(C)(C)C)[C@H]1OC(=O)C(C)(C)C	0
Decoy099	S=C(N)c1cc2CCCc2nc1O[C@H](CC(C)C)C	0
Decoy100	s1c2c(ncnc2SCc2ccccc2)c2c3c(CCC3)c(nc12)C(C)C	0
Decoy101	Oc1ccccc1\C=N\[C@H]([C@@H](\[NH+]=C\c1ccccc1O)c1ccccc1O)c1ccccc1O	0
Decoy102	Fc1ccccc1[C@](Nc1ccc(OC)cc1)(CO)C	0
Decoy103	O=C1C=C(NC(=C1)C)[C@@H]1[NH+](CCC1)C(C)C	0

Decoy104	s1cc(nc1[C@@H](OCC)C)C[NH+]([C@H](C(OC)=O)c1ccccc1F)C	0
Decoy105	ClC(Cl)(Cl)[C@@H](P(OCC)(OCC)=O)NS(=O)(=O)N(C)C	0
Decoy106	s1ccc(C)c1C[C@@]1(NC(=NC1=O)N)c1ccc(OC)cc1	0
Decoy107	O1c2[nH]nc(c2[C@H](C(C#N)=C1[NH3+])c1ccc(N(CC)CC)cc1)-c1ccc(cc1)CC(C)C	0
Decoy108	O=C1N(CC=C)C(=O)NC(=O)C1(CCc1ncccc1)CCc1ncccc1	0
Decoy109	s1c(C[NH3+])c(nc1N(CC1CCCCC1)C)C1CC1	0
Decoy110	O(CCCC)c1ccc(cc1)/C(=N\O)/CCCCCCCC\C(=N\O)\c1ccc(OCCC)cc1	0
Decoy111	O1N=C([C@@H]2C[C@H]3[C@H]4[C@@H](CC[C@]3(C)[C@]12/C(=N/OC(=O)C)/C)[C@@]1(C(C[C@@H](OC(=O)C)CC1)=CC4)C)C(OC)=O	0
Decoy112	Clc1ccc(OP(Oc2ccc(Cl)cc2)(=O)N2CCN(CC2)c2ccc([N+](=O)[O-])cc2)cc1	0
Decoy113	Clc1cc(ccc1)[C@@H]1N[C@@H](CC=2[C@H]1[NH+]=C1C=2C=CC=C1)C(OC)=O	0
Decoy114	S(CC(=O)NCc1occc1)C=1NC(=O)C(NC(=O)c2occc2)=C(N=1)N	0
Decoy115	S(=O)(=O)(\N=C(\N)/N)c1ccc(NC(=S)NC(=O)c2ccncc2)cc1	0
Decoy116	S1c2n(C=C1C[NH3+])c(nc2)Cc1occc1	0
Decoy117	Ic1[nH+]cccc1C(=O)[O-]	0
Decoy118	O=C1N(c2c(cc(cc2)[C@@H](O)C(C)C)[C@H]1C)C	0
Decoy119	o1cccc1C[NH2+][C@@H](C#N)c1ccc(OCC)cc1	0
Decoy120	O(C(OC)[C@@H]([NH2+][C@H](C)c1c(cc(nc1C)C)C)C)C	0
Decoy121	S=C1N(C=N[N-]1)c1cc(OCC)c(OCC)cc1	0
Decoy122	o1nc(cc1C)C[NH+]1C[C@@](CC1)(CCC)C(=O)[O-]	0
Decoy123	Brc1ncc(OC)nc1	0
Decoy124	o1c(C)c(cc1C)[C@@H](N=C=O)C	0
Decoy125	Brc1cc(ccc1)[C@H]([NH2+][C@@H]1CCc2c1cccc2O)C	0
Decoy126	Brc1ccc(Br)cc1NC(=O)[C@@]1(CC[NH2+]C1)C	0
Decoy127	s1c2n(nc(c2cc1C(=O)N(C)C1CC1)C)C	0
Decoy128	S1c2n(N=C1C1CC1)c(nn2)-c1ccsc1	0
Decoy129	O1[C@H]2[C@H](OC[C@@H]2NC(=O)Nc2c3c(ccc2)cccc3)[C@@H](Nc2nc(ccn2)-c2ccc([NH+](C)C)cc2)C1	0
Decoy130	FC(F)(C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)[C@H](\C=N\Nc1cc	0

	c([N+](=O)[O-])cc1[N+](=O)[O-])CC	
Decoy131	Brc1ccc(cc1)[C@H]1[NH+]=C([O-])c2c3CC[C@H](Cc3sc2N1)C	0
Decoy132	Clc1snnc1C[NH+]1CCC[NH+]2[C@H](CCC2)C1	0
Decoy133	Fc1c(N[N-]C(=O)NCCC(F)(F)F)c(F)c(F)[nH+]c1F	0
Decoy134	Brc1sc(cc1)C[NH+]([C@H](C(=O)NC(=O)N)c1ccccc1)C	0
Decoy135	FC(F)(F)C[NH+]1C[C@@H](CC1)CN/C(=[NH+]\C1CC1)/NCC1CCCCC1	0
Decoy136	s1cccc1[C@H](NC(=O)Nc1ccc(cc1)C#N)CCO	0
Decoy137	O=C([O-])[C@@H](C[NH2+][C@H](C)C12CC3CC(C1)CC(C2)C3)C	0
Decoy138	S=C=NCc1nc(ncc1)C	0
Decoy139	Fc1ccccc1[C@H]1O[C@H]2N=CC=C2NC1	0
Decoy140	O(c1c(Oc2cc(C#N)c(cc2)C#N)cccc1Oc1cc(C#N)c(cc1)C#N)c1cc(C#N)c(cc1)C#N	0
Decoy141	Fc1ccc(cc1)-c1c(CO[C@H]2O[C@@H](C(=O)[O-])[C@@H](O)[C@@H](O)[C@@H]2O)c([nH+]c(C(C)C)c1\C=C\[C@@H](O)C[C@@H](O)CC(=O)[O-])C(C)C	0
Decoy142	O1[C@@H](C)[C@@H](O)[C@@H](O)[C@@H](O)[C@@H]1Nc1cc(N[C@H]2O[C@@H](C)[C@@H](O)[C@@H](O)[C@H]2O)ccc1C	0
Decoy143	Fc1cc2n(CCC#N)c(nc2cc1)C([NH3+])(C)C	0
Decoy144	Brc1cc(OCCO\N=C/2\c3c(-c4c\2cccc4)cccc3)ccc1	0
Decoy145	O=C(N[C@@H](C(=O)NC(C)(C)C)C)CCc1c2cc(ccc2[nH]c1)C	0
Decoy146	S(=O)(=O)(C(S(=O)(=O)CCCC)=C(Nc1ccc(OCCCC)cc1)Nc1ccc(OCCCC)cc1)CCCC	0
Decoy147	o1cccc1C[NH2+]Cc1ccc(nc1)-n1nccc1	0
Decoy148	O=C(N([C@H](C(=O)NCCCC)c1ccc(N(C)C)cc1)CCCCCC)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1	0
Decoy149	S=C(N)[N-]\N=C(\c1ccc(N(C)C)cc1)/c1ccc(N(C)C)cc1	0
Decoy150	s1cc(nc1NCC=C)[C@]1(OC(=O)[C@@]2(C1)C[C@H](OC2=O)COCC(C)C)C	0
Decoy151	S1c2n(nc(n2)C)C(O)=C1[C@@H]([NH+]1CCC2(OCCO2)CC1)c1ccc(cc1)C(C)C	0
Decoy152	Brc1c(n(nc1C(F)(F)F)[C@@H](C(=O)N[C@H](C(=O)N(CC=C)CC	0

	=C)C)C)C	
Decoy153	S(CC(C)=C)C1=NC(=O)[C@H]2C(=N1)c1c(C[C@]2(CC)C2CCCCC2)cccc1	0
Decoy154	O([C@H]([C@H](C\C=C\C=C)C)[C@H](N(C(=O)[C@@H](NC(=O)[C@@H]([NH2+]C)CC(C)C)C(C)C)C)C(=O)CCCCCCC)C(=O)C	0
Decoy155	s1cnnc1SCc1cc(ncc1)/C(=N\O)/N	0
Decoy156	Clc1sc(S(=O)(=O)N(CCCOCC)CC(F)(F)F)cn1	0
Decoy157	O(C)c1ccc(cc1)C(=O)[C@H](CCCC[C@@H](C(=O)c1ccc(OC)cc1)C[NH2+]C(C)(C)C)C[NH2+]C(C)(C)C	0
Decoy158	o1c2[C@@H]3[C@H](OCc2cc1C=O)CCC3	0
Decoy159	Oc1ccc(cc1)[C@@H]1Nc2c([C@@H]3[C@@H]1CC=C3)cc(cc2)C(=O)NCC[NH+](CC)CC	0
Decoy160	Clc1cc2c([nH+]cc(C(=O)NNC(=O)C3=CNc4c(cccc4C(F)(F)F)C3=O)c2N)cc1	0
Decoy161	Fc1ccc(N2CCN(CC2)C(=O)[C@@H]2OCCC2)cc1	0
Decoy162	[nH]1cc(nc1)-c1ccc(NCc2ccccc2CC)cc1	0
Decoy163	o1nc(C)c(C(=O)NC[C@H](OC)C(C)(C)C)c1C	0
Decoy164	F[C@@]12[C@H]([C@@H]3C[C@@H](C)[C@](OC(=O)CCCCC)(C(=O)COC(=O)CCCCC)[C@]3(C[C@@H]1OC(=O)CCCCC)C)CCC1=CC(=O)C=C[C@@]12C	0
Decoy165	s1cc(cc1)-c1nc(C)c(cc1)C(=O)NC	0
Decoy166	S(=O)(=O)(N(OC)C)c1cc(ccc1)C(=O)N[C@@H](CC)c1ccc(OC)cc1	0
Decoy167	O=C1[C@@H](C)[C@H]([NH2+][C@H]([C@H]1C)c1ccc(N(C)C)cc1)c1ccc(N(C)C)cc1	0
Decoy168	ClCc1nc([nH]c1)[C@H]1[C@H]2O[C@@H](C1)CC2	0
Decoy169	Brc1cc(N)c2onc(c2c1)CC(=O)NCC=C	0
Decoy170	O=C(Nc1ccc(cc1)[C@H](NC(=O)N[C@H](C(C)C)C)C)C1CC1	0
Decoy171	O(C)[C@@H]1[C@@]2(O)C[C@@H]3[C@@H]([C@@](O)([C@@H]4[C@H]5[NH+](C[C@]6([C@H]([C@@]35[C@@H](OC)C[C@H]6O)[C@H]4OC)COC)CC)[C@H]1O)[C@H]2O	0
Decoy172	S(CC(=O)N(CC)C1CCCC1)c1[nH]nc(n1)C	0
Decoy173	Clc1nc(c2C[C@H](Oc2n1)C)C	0
Decoy174	Clc1ccc(cc1[N+](=O)[O-])[C@H]1C2C(N=C(C)C1C(OCCOC)=O)=C[C@H](C)[C@H](C(O	0

	C)=O)C2=O	
Decoy175	ClC(Cl)(Cl)C(=O)Nc1ccc(nc1)NC(CO)(C)C	0
Decoy176	O(CCNC=1[N-]C2=NNC(=[NH2+])C2=C2C=1C[NH+](CC2)C1CCCCC1)CCO	0
Decoy177	O=C1N(N=C(C=C1)C(=O)N[C@@H](CC(OC)=O)c1ccc(cc1)C(C)C)CC	0
Decoy178	s1cccc1[C@@H]([NH2+]Cc1cn[nH]c1C)C1CCCC1	0
Decoy179	s1ccnc1Oc1ccc(OC(=O)CCOCC(F)(F)F)cc1	0
Decoy180	OC/1=Nc2c(cccc2)\C\1=N\NC(=O)COC[C@H](O)N\N=C/1\c2c(N=C\1O)cccc2	0
Decoy181	Oc1ccccc1[C@H](NC(=O)N[C@H](C(C)C)c1ncccc1)CC	0
Decoy182	o1c2C[C@H](CCc2c2c1CC[NH+](C2)C)CO	0
Decoy183	Brc1cccc(C[NH2+]CC)c1O[C@@H](C(=O)N[C@H](CC)C)C	0
Decoy184	O=C(\N=C(\Nc1ccc(cc1)C(C)C)/NCCC=1C[NH+]=C2C=1C=CC=C2)c1ccc(NC(=O)C)cc1	0
Decoy185	Clc1ccc([N+](=O)[O-])cc1[C@H](N(C(=O)c1c(O)cccc1O)Cc1occc1)C(=O)NC(C)(C)C	0
Decoy186	Clc1cccc(F)c1\C=N/n1c(nnc1C)C	0
Decoy187	O(CC)c1cc(ccc1OCC)-c1c-2n(CCc3cc(OCC)c(OCC)cc-23)c2c1cc(OCC#C)c1c2cccc1	0
Decoy188	S=C1N([C@H](CC(C)C)C[NH+](C)C)C(=N[N-]1)C(C)C	0
Decoy189	Brc1cc(oc1Br)[C@H](N1CCCCCCC1)C[NH3+]	0
Decoy190	S(=O)(=O)(N[C@]1(C2=C(NC1=O)N(C)C(=O)NC2=O)C(F)(F)F)c1ccc(N)cc1	0
Decoy191	O=C([O-])[C@@H](CN(CC)c1n[nH+]cc2c1cccc2)C	0
Decoy192	s1nc(C(=O)N)c(N)c1C(=O)N([C@@H](C(=O)NC[C@H]1OCCC1)C)c1cc(ccc1)C	0
Decoy193	Clc1cccc(F)c1[C@H]1O[C@H](CO1)CO	0
Decoy194	Clc1ccc(cc1)[C@@H](O)[C@H](NC(=O)N[C@H](C1CC1)c1sccn1)C	0
Decoy195	Clc1ccc(cc1)[C@H](N(C)c1cc([nH+]cc1)/C(=N/O)/N)C	0
Decoy196	S(CC[NH+](C)C)c1ccc(NC(=O)CNc2cc(F)ccc2)cc1	0
Decoy197	ClCc1nc(on1)[C@@H]1C[C@H]1C	0
Decoy198	Brc1ccc(Sc2c3c(ncc2C(=[NH2+])N)cccc3)nc1	0

Decoy199	s1cccc1C1=C2C(SC1)=NC(=NC2=O)[C@H](S[C@@H]1NN=C(N1[NH3+])C1CCCCC1)C	0
Decoy200	o1cccc1C(=O)Nc1cc(ccc1C)C(=O)Nc1ccc(NC(=O)N)cc1	0
Decoy201	S(C)[C@H]1NC(=[NH2+])C(=C1)Cc1oc(C)c(n1)C	0
Decoy202	o1cccc1[C@@H]([NH2+][C@H](C(C)C)CC)c1nccn1C	0
Decoy203	O1C[C@H]([NH+](C[C@@H]1C)Cc1cc(ncc1)C#N)CC	0
Decoy204	S1c2c(cccc2F)[C@@H](NC(=O)NC2CC([NH2+]C(C2)(C)C)(C)C)CC1	0
Decoy205	Brc1sc(cc1)[C@@H]([NH3+])c1cc2OCCOc2cc1Cl	0
Decoy206	S([C@@H]([C@@H]([NH3+])CC)c1cc(ccc1)C)c1nc(ccn1)C	0
Decoy207	Brc1c2c(c(N)ccc2OC)c(nc1)NC[C@@H]1OCCC1	0
Decoy208	FC(F)(F)Oc1ccc(OCC[NH+](C[C@H]2CCOC2)CCC#N)cc1	0
Decoy209	S(\C(=N\C#N)\N1CCCCC1)C	0
Decoy210	FC(F)(F)c1ccccc1NNC(=O)[C@@H](NC(=O)C(C)(C)C)C	0
Decoy211	[NH2+](Cc1nc(nc(c1)C)Cc1ccncc1)CC(C)C	0
Decoy212	O(C)c1ncnc(OC)c1C[NH2+]C1CCC(CC1)C	0
Decoy213	O=Cc1c2n(CCC2)c2c1cncc2	0
Decoy214	O[C@@H]1c2c(CCC[C@H]1n1nccc1)cccc2	0
Decoy215	[nH+]1ccc(cc1N)CN(C)c1ccc(cc1)C#N	0
Decoy216	S=C1NC(=O)C=CN1c1cccc(F)c1F	0
Decoy217	s1cccc1C\C(=C/c1n(Cc2ccc(cc2)C(O[C@@H]2O[C@@H](C(OC)=O)[C@@H](O)[C@@H](O)[C@H]2O)=O)c(nc1)CCCC)\C(=O)[O-]	0
Decoy218	S(C)c1cc(NC(=O)[C@@H](Nc2cc(ccc2)C(=O)NC)C)ccc1	0
Decoy219	S(C[C@@H](NC(=O)[N-]NC(=O)c1cc(ccc1)C)c1ccccc1)C	0
Decoy220	s1c2cc(\N=C\c3ccc(N(C)c4ccccc4)cc3)ccc2nc1SC	0
Decoy221	Clc1cc(ccc1Cl)-c1sc2cc(ccc2n1)C(OCC#C)=O	0
Decoy222	Fc1cc(ccc1C)CN\C(=[NH+]/CC(C)=C)\NCCc1cccnc1	0
Decoy223	S1(=O)(=O)C[C@@H](CC1)Cc1nc2c(n1C[C@@H](O)COCc1occc1)cccc2	0
Decoy224	Ic1nc(N)c2ncn(c2n1)[C@@H]1O[C@H](C(=O)NCC)[C@H](O)[C@H]1O	0
Decoy225	[NH+]=1[C@@H]2C(=C3C=1C=CC=C3)CCN(C\C(=C\C)\C)[C@H]2[C@@H]1Nc2c(N1C)cccc2	0
Decoy226	Clc1sc(cn1)C[NH+]1C[C@@H](O)CCC1	0

Decoy227	O([C@H](C)c1nc2c(n1Cc1cc3c(cc1)cccc3)cccc2)c1ccccc1	0
Decoy228	s1cc(nc1C)-c1cc([nH]c1)C(=O)NCc1[nH]ccn1	0
Decoy229	Brc1cc([nH]c1)C(Oc1cc(ccc1)C(=O)N)=O	0
Decoy230	Clc1ccccc1S(=O)Cc1oc(cc1)C(=O)NCCC[NH+]1CC[NH+](CC1)CC	0
Decoy231	Fc1cc(ccc1C(=O)N\\N=C\c1cc(n(c1C)-c1cc2OCOc2cc1)C)C#N	0
Decoy232	s1cc(nc1-c1scc(n1)-c1ccc(OC)cc1)-c1ccc(cc1C)C	0
Decoy233	Fc1cc(F)c(F)cc1NC(=O)NC[C@](O)(C)c1cc(oc1C)C	0
Decoy234	S\1C=C(N(\N=C\c2ccc(SC)cc2)/C/1=N/CC=C)c1ccccc1F	0
Decoy235	s1ccnc1C=1C(OCC=1C(C)(C)C)=N	0
Decoy236	S(Cc1[nH+]c2c([nH]1)cccc2)[C@H]1[NH+](Cc2occc2)[C@@H](NN1)c1cc(OC)ccc1	0
Decoy237	Fc1ccc(cc1C)-c1[nH+]c2n(C=C(C=C2)C)c1CC(=O)Nc1ccc(cc1)C(=O)N	0
Decoy238	O[C@@H]1CC[C@]2([C@H](C1)CC[C@H]1[C@H]3CC[C@@H]([NH2+]CC#N)[C@]3(CC[C@H]12)C)C	0
Decoy239	s1cccc1[C@@H]1N2NC=[NH+]C2=NC(=C1)c1ccc(cc1)-c1ccccc1	0
Decoy240	s1cc(nc1C)Cc1oc(SC[C@H](O)COCc2ccccc2F)nn1	0
Decoy241	S1(=O)(=O)c2c(cc(cc2C)C)[C@H]([NH2+]C)CCC1	0
Decoy242	s1c2O[C@@H](CNc2cc1)c1ncccc1	0
Decoy243	O(C(=O)C\N=C(/[O-])\[C@H]([NH+]1CC(C)(C)C1(C)C)C)C	0
Decoy244	Brc1cc(Cl)c(-n2c3c([nH+]c2N)cc(cc3)C)cc1	0
Decoy245	s1c(cnc1N=S(=O)([O-])N(C(C)C)C)C#CC[NH3+]	0
Decoy246	S(=O)(=O)(C(C)C)[C@@H]1[NH+](CCC(C)C)[C@H](C=N1)C[NH+]([C@@H](C)C=1[C@H](N=NC=1C)C)C	0
Decoy247	Brc1cc([C@H]([NH3+])c2sc(C)c(n2)CC)c(F)cc1	0
Decoy248	Brc1cc(Cl)c(cc1)[C@@H]([NH3+])c1c(F)cc(OC)cc1F	0
Decoy249	O=C(N1C[C@H](CCC1)c1n[nH]c(c1)C(=O)N)C1CCC1	0
Decoy250	O=C(Nc1ccc(cc1)C(=O)N)c1ccc(N(C(C)C)CC)cc1	0
Decoy251	S=C(N(CCOC)C1CCN(CC1)C(OCC)=O)Nc1cc(F)ccc1	0
Decoy252	FC(F)(F)C=1Oc2c(cc(C[NH+](C)C)c(O)c2C)C(=O)C=1c1ccccc1C	0
Decoy253	o1c(nnc1[C@H]([NH3+])c1ccc(cc1)C(C)(C)C)C	0
Decoy254	Clc1cc(\[NH+]=C\2/Oc3c(C=C/2C(=S)N)c(cnc3C)CO)ccc1	0
Decoy255	FC(F)(F)c1ccccc1[C@@H]([NH2+][C@@H](C(=O)Nc1ccc(OC)cc1	0

	OC)C)C	
Decoy256	O=Cc1[nH]cc2c1[C@@H](C[NH+](CC2)C)C(C)C	0
Decoy257	O1N2[C@](CCC2(C)C)(C)[C@H](C1)C#N	0
Decoy258	Fc1ccc(F)cc1[C@H](NC(=O)N1C[C@H]2[C@H](CCCC2)C1)c1cc[nH+]cc1	0
Decoy259	S([C@@H]1CCS(=O)(=O)C1)c1nncc2c1cccc2	0
Decoy260	O=C(Nc1ccc(NC[C@@H]2CCC=CC2)cc1)C1CC1	0
Decoy261	O=C1Nc2cc(ccc2C=C1CN(C(=O)c1cc([N+](=O)[O-])ccc1)c1ccccc1)C	0
Decoy262	s1c(ccc1CCCC)[C@H]1[C@H]2C(=CCCC2)[C@@H](C#N)C(=[NH2+])C1(C#N)C#N	0
Decoy263	FC(F)(F)c1nc(ncc1)[C@H]1[NH2+]CCC1	0
Decoy264	Oc1ccc(cc1)C(=O)N1CC[C@H](C[C@@H]1C)C	0
Decoy265	S=C1NC(=O)C(/C(=N\[N-]C(=S)[N-])N)/C(=O)Nc2cc(O)ccc2)C(=O)N1	0
Decoy266	s1cc(N)cc1S(=O)(=O)NC[C@H]1Oc2c(C1)cccc2	0
Decoy267	FC(F)(F)[C@@](O)(CCNC(=O)c1cc2[nH]cnc2cc1)c1ccccc1	0
Decoy268	[S-]\C(=[NH+]/Cc1ccncc1)\Nc1ccccc1C(C)C	0
Decoy269	O=C(NCCNC(=O)N[C@H](C)C12CC3CC(C1)CC(C2)C3)C1CC1	0
Decoy270	s1c(C(=O)N[C@H](CC(C)C)C[NH+](C)C)c(cc1NC(=O)C(C)(C)C)C	0
Decoy271	Sc1n(nc(c1)C)-c1ccncc1	0
Decoy272	s1cccc1C1=NN(C(=O)COC(=O)c2cc([N+](=O)[O-])ccc2N(C)C)[C@@H](C1)c1sccc1	0
Decoy273	Clc1cc(Nc2nc[nH+]c(Nc3ccc(S(=O)(=O)N(CC)CC)cc3)c2N)ccc1C	0
Decoy274	Brc1cc(ccc1OCCCCCC)C(=O)NC(=S)Nc1cc(OCCOCC)ccc1	0
Decoy275	Fc1ccc(cc1)C[C@@]1(CCCN(C1)c1nc(N)ccn1)CO	0
Decoy276	O=C(N[C@@H](CC)C)c1cc(NC(=O)CCCCCCCC(=O)Nc2cc(ccc2)C(=O)N[C@@H](CC)C)ccc1	0
Decoy277	Brc1cc(cc(Br)c1[O-])\C=N\[NH+]=C(/N)\c1nonc1N	0
Decoy278	Ic1c[nH+]n(c1N)C1CCC(CC1)C(C)C	0
Decoy279	O=C(Nc1cc(N(C)C)ccc1)[C@H]1c2c(cc(cc2)C(C)(C)C)C[NH+](C1)C	0
Decoy280	FC(F)(F)Oc1ccccc1C[NH2+]C[C@@H](O)CO[C@@H](C)c1ccccc	0

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Decoy281	S=C(N)c1c[nH+]c2c(cccc2)c1N(C[C@H](CC)C)C	0
Decoy282	S1C=C(N(CCCC(O[C@H](C(=O)c2[nH]c(C)c(C(=O)C)c2C)C)=O)C1=O)C	0
Decoy283	O(CC)c1ccc(N(C(=O)COC(=O)Cc2ccc(OC)cc2)CCC#N)cc1	0
Decoy284	s1c(ccc1CCNC(=O)C)C(=O)COC(=O)Cc1c2c(oc1)cc1CCCc1c2	0
Decoy285	O1CC[C@@H](Nc2ccc(cc2)CCO)C[C@H]1C(C)C	0
Decoy286	Clc1ccc(cc1)[C@@H]1[NH+](CC)[C@@](C[C@@H]1C[NH2+]Cc1ccc(OCC)cc1)(CO)C	0
Decoy287	O1[C@H]2[C@@H](OC1(C)C)O[C@H]([C@@H](O)CO[C@@H]1O[C@H](COC(=O)C)[C@@H](OC(=O)C)[C@H](OC(=O)C)[C@H]1NC(=O)C)[C@@H]2OCCCCC	0
Decoy288	Clc1cc(F)cc2c1[nH+]cc(C#N)c2NC	0
Decoy289	s1c(C)c(CC)c(C(=O)N)c1NC(=O)c1ccc(OCC)cc1	0
Decoy290	Clc1cc(ccc1)C(=O)N[N-]C(=S)Nc1ccc(OC)cc1	0
Decoy291	Clc1cc(ccc1Cl)C1=N[C@@H]2NC(=O)NC(=O)[C@H]2[C@@H]1[C@@H]1C(=NC(=O)NC1=O)N	0
Decoy292	O(C)c1c(OC)cc(cc1OC)C[C@]1(C[NH+]2C[C@H]3C=4N(C[C@H](C3)C2)C(=O)C=CC=4)C(=O)N(c2ccc(cc2)CC)C(=O)N=C1[O-]	0
Decoy293	s1cccc1[C@@](O)(CNC(=O)C(=O)Nc1ccc(cc1)C)C1CC1	0
Decoy294	O1CCC(Oc2c3c(ccc2)[C@H](O)CC3)CC1	0
Decoy295	S1C2(SC(C(OC)=O)=C1C(OC)=O)C1=C(SC(C(OC)=O)=C2C(OC)=O)C(N(c2cc(OC)ccc12)C(=O)c1ccc(F)cc1)(C)C	0
Decoy296	Brc1cc([C@@H]2N(CCC[C@H]2[NH3+])CC(C)C)c(F)cc1	0
Decoy297	Clc1cc([N+](=O)[O-])ccc1C(=O)Nc1cc(ccc1)-c1nc2SCCn2c1	0
Decoy298	o1nc(nc1CC)-c1ccc(-n2nc(C)c(c2)C(=O)Nc2cc(C)c(cc2)C)cc1	0
Decoy299	S(=O)([O-])(=Nc1nc(nc(OCCO)c1Oc1ccccc1OC)-c1cc(ncc1)-c1nnn[n-]1)c1[nH+]cc(cc1)C(C)C	0
Decoy300	Clc1ccc(cc1C)[C@@]1(NC(=O)N(C[C@@H]([NH3+])CC)C1=O)CC	0
Decoy301	s1c2cc(ccc2nc1Nc1nc[nH+]c(N(Cc2ccccc2)c2ncccc2)c1N)C	0
Decoy302	FC(F)(F)c1cc(N(C)C)ccc1NC(=O)NC1CCC(O)CC1	0
Decoy303	Brc1cc\2c(NC(=O)/C/2=N/c2ccc(cc2)Cc2cc[nH+]cc2)cc1	0
Decoy304	S(C(F)(F)F)c1ccc(cc1)C(=O)Nc1cc(NC(=O)NCc2cc[nH+]cc2)ccc1	0

Decoy305	s1c2c(CC[NH2+]C2)c(C#N)c1NC(=O)CC1CC1	0
Decoy306	Clc1c(cccc1Cl)-c1oc(cc1)[C@H]1[NH2+]CCc2[nH]cnc12	0
Decoy307	Clc1ccc(cc1)COc1cc(ccc1)C=1NN[C@@H](C=1)C(=O)N\N=C\C=1C[NH+]=C2C=1C=CC=C2	0
Decoy308	S1(=O)(=O)C[C@H](N(C)c2ccc(cc2F)C#N)CC1	0
Decoy309	Oc1ccc(cc1)[C@@H](Nc1ccccc1N(C)C)CC	0
Decoy310	n1n(CC)c(C)c(/C(=C/C#N)/C)c1C	0
Decoy311	o1c(C)c(cc1CO[C@@H]1C[C@H](OC)CCC1)C[NH2+]C	0
Decoy312	Clc1ncnc(N2CCC2)c1	0
Decoy313	s1cc2c(C[NH+](C[C@H]2c2ncoc2)C)c1C=O	0
Decoy314	O(CC)c1cc(ccc1OCC)[C@H](NC(=O)[C@@H]1C[C@@H]1c1cn(nc1)C)C(C)C	0
Decoy315	o1nc(/C(=[NH+]\N=C/c2cc([N+](=O)[O-])c(N3CC[NH+](CC3)C)cc2)/N)c(n1)N	0
Decoy316	O([C@H]1CCCC[C@H]1[NH+](CC)CC)c1ccccc1N	0
Decoy317	S(CC1=NC(=O)c2c(N1)cccc2)c1[nH+]c2c(cc(cc2C)C)c(c1)C	0
Decoy318	Fc1ccc(cc1C)[C@H](O)c1[nH+]c(c[nH]1)-c1c2c(ccc1)cccc2	0
Decoy319	S([C@@H]([C@@H]([NH3+])C)c1occc1)c1ncnc2[n-]cnc12	0
Decoy320	O=C1NC[C@@H]([NH2+][C@@H]1CCC)c1cc([nH+]cc1)C	0
Decoy321	S1Cc2c(CSCC[NH2+][C@H](CC([NH2+]CC1)(C)C)C)cccc2	0
Decoy322	FC(F)(F)c1ccc(cc1)[C@H](N(CCCCCC)C(=O)[C@@H](CCCC)CC)C(=O)NC(CC(C)(C)C)(C)C	0
Decoy323	S(=O)(=O)(CCN(C(=O)N[C@@H](C(C)C)C)C)C	0
Decoy324	Clc1cc(Cl)ccc1[C@@H](N(C(=O)c1[nH]c([nH+]c1)C(C)C)C)C	0
Decoy325	BrCCCCN1c2c(cccc2)\C(=N/[N-]C(=S)N)\C1=O	0
Decoy326	O(C[C@]([NH3+])(C#N)c1ccccc1)c1ccccc1C(C)C	0
Decoy327	s1ccc(C)c1\C=C\1/Oc2c(ccc(OCc3ccccc3C)c2C)C/1=O	0
Decoy328	S1C[C@@H](CC1)C(=O)N(C)c1ccc(O)cc1	0
Decoy329	O(C)c1cc2ncc3CC[NH2+]Cc3c2cc1	0
Decoy330	Brc1cnc(nc1)NCC(OC)OC	0
Decoy331	s1cccc1C\[NH+]=C(/NCC1(CC1)c1ccccc1OC)\NC(C)C	0
Decoy332	S(CC[C@H](NC(=O)[C@@H](N1C(=O)c2c(N=C1[O-])cccc2)Cc1ccccc1)C(=O)N[C@H](Cc1ccccc1)C(=O)[O-])C	0
Decoy333	s1cccc1[C@@H](NC(=O)N[C@H](C)c1cc2CC(=O)Nc2cc1)C	0

Decoy334	s1cccc1CNC(=O)COc1ccc2N=CN(CC=C)C(=O)c2c1CC=C	0
Decoy335	O(C)c1ccc(NC(=O)c2cc(cc(NC(=O)c3ccc([N+](=O)[O-])cc3)c2)C(=O)Nc2ccc(OC)cc2)cc1	0
Decoy336	O1c2cc(ccc2N(CC#C)C(=O)[C@@H]1C(C)C)C[NH3+]	0
Decoy337	Brc1ccc(cc1)C=1N=C2N(N=CN2)[C@H](C=1)c1cc([N+](=O)[O-])ccc1	0
Decoy338	S(=O)(=O)(C(F)(F)F)c1cc([N+](=O)[O-])c(NC[C@]2(CC(C[C@@H]([NH3+])C2)(C)C)C)cc1	0
Decoy339	s1ccnc1NC(=O)C[NH+]([C@@H](C)c1occc1)C	0
Decoy340	Clc1c(C)c([C@H](O)[C@@H]([NH2+]C(C)C)C)c(OC)cc1C	0
Decoy341	S1CCN(S(=O)(=O)N2C[C@@H](CCC2)C)CC1	0
Decoy342	Fc1cccc(F)c1C[C@@H](NC(=O)Nc1cc(NC(=O)C)ccc1F)C	0
Decoy343	O=C(NC(=O)NCC=C)[C@H]([NH2+][C@@H](C)c1c2c(ccc1)cccc2)C	0
Decoy344	s1cc(nc1)Cc1oc(cn1)[C@@H]1CCC[C@@H]1[NH3+]	0
Decoy345	O=C([O-])CC1(CCCC1)Cc1nc(nn1C)C(C)C	0
Decoy346	O1CC[C@@]([NH+](C)C)(C[C@@H]1CC)C#N	0
Decoy347	Clc1nc(nc(NCCc2scc(n2)C(F)(F)F)c1)N	0
Decoy348	s1c(ccc1C[NH2+]CCNC(=O)c1occc1)-c1ccc(F)cc1	0
Decoy349	FC(F)(F)CN1C[C@@H](CC1=O)C(O[C@@H](CC[NH+](C)C)c1ccccc1)=O	0
Decoy350	s1c(ccc1CC)-c1oc(nn1)C[NH2+]CCC	0
Decoy351	O=C1[NH+]=C(C)C(CC(=O)[O-])=C(N1CCC(C)C)C	0
Decoy352	Brc1oc(cc1)\C=N\Nc1nc2n(c3c(c2nn1)cccc3)CCC	0
Decoy353	Brc1cc(OCCC(=O)Nc2cc(C(=O)N)c(cc2)C)ccc1	0
Decoy354	s1c2nc(nc(NN)c2cc1)COc1cccc(F)c1F	0
Decoy355	O[C@H](c1ccc(cc1)C(C)C)c1nc(cc2ncccc12)-c1cc[nH+]cc1	0
Decoy356	O1CC[C@@H](\[NH+]=C(\NC2CC2)/NCCc2ccc(N(C)C)cc2)c2c1cccc2	0
Decoy357	O1CCC(CC1)(C[NH2+][C@@H](C(=O)NC[C@H](C)c1ccccc1)C)c1ccccc1	0
Decoy358	O1c2c(ccc(OC[C@@H](O)C[NH+](Cc3occc3)C[C@H](O)COc3ccc4c(OC(=O)C=C4c4ccccc4)c3C)c2C)C(=CC1=O)c1ccccc1	0
Decoy359	s1cc(nc1C)COc1ccc(cc1)C[NH2+][C@H](CO)C1CCCCC1	0

Decoy360	s1cc(nc1-c1ccccc1F)CS\C(=[NH+]/[C@H](COC)C)\N	0
Decoy361	s1cccc1[C@@H]1O[C@@H](C)C(=N1)CS[C@H]1[NH+]=C2C(=[NH+]1)C=[NH+]C=C2	0
Decoy362	S(=O)(=O)(Nc1cc(ccc1)[C@H]1[NH+]=C2C(=C1)C=CC=C2)c1ccccc1F	0
Decoy363	Oc1cc(O)cc(O)c1[C@H](N(C(=O)[C@H]1NC(=O)CC1)C)C(=O)NC(C)(C)C	0
Decoy364	Fc1cc(ccc1F)C=1NC=C(C#N)C(=O)C=1	0
Decoy365	O1[C@@H](C[NH+](C[C@H]1C)C[C@H](O)Cn1nc(C)c(N)c1C)C	0
Decoy366	S(=O)(=O)(NC=1C=CC(=O)N(C=1)CC)c1ccccc1C(=O)N(CCCC)C	0
Decoy367	S1C[C@H](CC1)c1[nH]c2c(n1)nccc2C	0
Decoy368	P(=O)([O-])([O-])N1N=C(NC1=O)C[NH+]1CCO[C@H](O[C@H](C)c2cc(cc(c2)C(F)(F)F)C(F)(F)F)[C@@H]1c1ccc(F)cc1	0
Decoy369	Fc1cc(OCc2cc(N)ccc2OCC)ccc1F	0
Decoy370	Clc1cc(Cl)cc2c1ncnc2OCc1ccc(cc1)C(C)(C)C	0
Decoy371	O1[C@@H](C[C@@H](OC(=O)c2ccccc2)COC(=O)c2ccccc2)[C@H](OC(=O)c2ccccc2)[C@H](OC(=O)c2ccccc2)[C@@H]1OC(=O)c1ccccc1	0
Decoy372	O1CC[NH+](CC1)[C@H]1CCCCCC[C@@H]1O	0
Decoy373	O1CCC(CC1)(C[NH+]1CC[C@H](CCC1)C(C)C)C[NH2+]C	0
Decoy374	O=C(NNc1ncnc(NC(c2ccccc2)c2ccccc2)c1N)c1ncccc1	0
Decoy375	O(C)c1cc(N2C[C@H]([NH3+])CCC2)cc(OC)c1	0
Decoy376	S1C=Cn2c1nc(N(CC)C[C@H](C#N)C)c2CO	0
Decoy377	Oc1ccccc1C[NH+]1C[C@@H](CCC1)C1=NN=C[C@@H]1c1c2c(ccc1)cccc2	0
Decoy378	s1cccc1[C@@H]([NH+](C)C)CNC(=O)Nc1cc(OCC(F)(F)F)ccc1	0
Decoy379	Brc1c(O)c(cc(Br)c1O)[C@@H](C=1[C@H](N=NC=1O)C)c1c([nH]nc1O)C	0
Decoy380	O=C(N[C@@H](Cc1[nH]nc(c1)C)C)[C@H]1[NH2+][C@@H]2C(C=C(C=C2)C)=C1C	0
Decoy381	S=C(N(Cc1cc(OC)ccc1OC)C[C@H]1OCCC1)NCc1occc1	0
Decoy382	s1c2c(CC[C@H](C2)C(C)(C)C)c(C(OCC)=O)c1NC(=O)c1nn2c(N[C@H](C[C@H]2C(F)(F)F)c2sccc2)c1	0

Decoy383	O1[C@@](CO)(C)[C@](O)(C)[C@](O)(C)[C@](O)(C)[C@]1(OC[C@@]1(O[C@@H](O)[C@@](O)(C)[C@@](O)(C)[C@@]1(O)C)C)C	0
Decoy384	O=C(N[C@H](CCC(C)C)C)c1nc2n(c1)C=CC=N2	0
Decoy385	o1c(cnc1C(C)C)-c1ccncc1	0
Decoy386	S=C1O\C(=C\c2ccc(N(C)C)cc2)\C(=O)N1C	0
Decoy387	Clc1cc(Cl)c2nsnc2c1NC(=O)C1CCC([NH3+])CC1	0
Decoy388	Clc1sc(cc1)CN(C(=O)c1ccc(OCCOC)nc1)CC=C	0
Decoy389	o1c2c(\C(=N\NC(=O)c3cc(OC)ccc3)\CCC2)c(C)c1C(Oc1ccc(cc1)-c1ccc(cc1)C#N)=O	0
Decoy390	Clc1ccccc1[C@H](CNC(=S)NC[C@@H]1OCCC1)C=1C[NH+]=C2C=1C=CC=C2	0
Decoy391	O=C1N[C@@H](Cc2ccccc2)C(=O)N[C@H](C[C@]2([NH3+])c3c(N[C@@H]2[NH3+])cccc3)C(=O)N[C@@H]1Cc1ccccc1	0
Decoy392	O(C)c1ccc(cc1)C(NOCc1nc-2n(n1)C=Nc1n(Cc3ccccc3)c(c(c1-2)-c1ccccc1)-c1ccccc1)=C	0
Decoy393	S(=O)(=O)(C)c1ccccc1NC1CC[NH+](CC1)c1cc(F)ccc1	0
Decoy394	S=C1NC([O-])=C(C[NH2+]\C=C/C=2CCCCC=2)C(=O)N1[C@@H](CC)C	0
Decoy395	Clc1ccc(cc1)[C@@H]([NH2+][C@H](C)C1=NC(=O)C=2C(S[C@H](C)C=2C)=N1)C	0
Decoy396	ClC=1C=CC2=[NH+][C@@H]3C(=C2C=1)CCN[C@@]13c2c(N(CC=C)C1=O)cccc2	0
Decoy397	s1c2cc(ccc2nc1-c1ccc(NC(=O)CSc2nc(cc(-c3cccc(OC)c3OC)c2C#N)-c2ccccc2)cc1)C	0
Decoy398	O(C(=O)c1cccnc1NC(C)C)CC(=O)N(Cc1ccc(N(C)C)cc1)C	0
Decoy399	Fc1cc(ccc1F)[C@@H](O)C\[NH+]=C\c1ccc(N(CC)CC)cc1O	0
Decoy400	O=C1N(C=CN=C1NCC([NH+](C)C)(C)C)C(C)(C)C	0
Decoy401	Clc1cc(NC(=O)N[C@@H]([C@H](CO)C)C)ccc1N(C)C	0
Decoy402	O=C1[C@@H]2[C@@](C[C@@H](O)[C@H](C(C(OC)=O)=C)[C@@H]2O)(C)[C@@H](O)CC1	0
Decoy403	[NH3+]Cc1cc(nc2c1cccc2)N(CC1CC1)C(C)C	0
Decoy404	Brc1cc(\C=N\Nc2[nH]nc(SCC(=O)Nc3ccc(cc3)[C@@H](CC)C)n2)c(O)cc1	0

Decoy405	S1(=O)(=O)C[C@](NC(=O)c2n(cc(N)c2)C2CC2)(CC1)C	0
Decoy406	O([C@H]([C@H]([NH3+])C)c1ncccc1)c1ccc(cc1)C(C)(C)C	0
Decoy407	Brc1ccc(cc1[N+](=O)[O-])C[NH2+][C@H]1CC[C@@H](C[C@H]1C)C	0
Decoy408	FC(F)Oc1ccc(cc1)[C@@H](O)CN1c2c(cccc2)[C@H](C[C@@H]1C)C(=O)N	0
Decoy409	[NH+]=1[C@@H](CCc2ccccc2)C(=N)N(CC#C)C=1C(C)C	0
Decoy410	O1[C@@H](COC1(C)C)[C@@H]1O[C@H]2OC(O[C@H]2[C@@H]1OC(=O)c1ccc(N=Nc2ccc(N(C)C)cc2)cc1)(C)C	0
Decoy411	S1CC[C@@H](C(=O)[O-])[C@]12C[C@H]([NH+](CC2)C)C	0
Decoy412	O=C1NC(=O)C[C@H]1[NH2+]Cc1ccc(cc1)-c1n[nH]cc1	0
Decoy413	Brc1ccc(cc1)/C(=N/NC(=O)CC=1C[NH+]=C2C=1C=CC=C2)/C	0
Decoy414	Clc1cc2[nH]c(nc2nc1)C[C@@H]1C[C@@H](C(C)C)[C@@H](C=C1C)CNC(=O)[C@@H](OC(=O)C)[C@H](OC(=O)C)C(=O)[O-]	0
Decoy415	FC(F)(F)c1nn(cc1)C[C@]([NH2+]CCC)(C#N)C	0
Decoy416	S(C/C(/[O-])=C\1/[C@H]([NH3+])N(C2CC2)C([O-])=NC/1=O)c1[nH+]c(c([nH]1)-c1ccccc1)-c1ccccc1	0
Decoy417	Brc1cc(ccc1N)C(=O)N[C@H]([C@@H](CC)C)C(OC)=O	0
Decoy418	FC(F)(F)Oc1ccc(NC(=O)c2c3c(c[nH+]c2)c(ccc3)C)cc1	0
Decoy419	s1c2c(nc1N[C@](P(OCCC(C)C)(OCCC(C)C)=O)(C(OC)=O)C(F)(F)F)cccc2	0
Decoy420	S(CCOc1ccc(F)cc1)C1=N\C(=C\c2ccc(OC(C)C)cc2)\C(=O)N1c1ccc(OCC)cc1	0
Decoy421	Oc1c2c(ccc1)[C@H](NC(=O)c1ccc(NC(=O)C3CC3)cc1)CC2	0
Decoy422	o1cccc1C[NH2+][C@H]([C@@H](O)c1cc2CCCCc2cc1)C	0
Decoy423	Clc1sc(Cl)cc1S(=O)(=O)N[C@@H]([C@@H](CC)C)C(=O)N	0
Decoy424	Clc1ccccc1CC(=O)NCCCCCc1nc2c(n1CCCCOc1cc(C)c(cc1)C)cccc2	0
Decoy425	OCC[C@H](CNC(=O)N([C@H](C(C)C)c1ccc[nH+]c1)CC)c1ccccc1	0
Decoy426	O=C(N1CCC[C@@H]1c1n[nH]cc1-c1nc(ncc1)N(C)C)[C@H](C)c1ccc(cc1)C	0
Decoy427	FC(F)(F)COCCC[NH+]1CC[NH+](CC1)[C@H](C)c1onc(n1)C(C)(C)C	0

Decoy428	Oc1ccc(cc1[N+](=O)[O-])C[C@H](NC(=O)CO\N=C/1\CC[C@@]2([C@H]3[C@H]([C@@H]4CC[C@H](O)[C@]4(CC3)C)CCC2=C\1)C)C(OC)=O	0
Decoy429	FC(F)(F)Oc1ccc(NC(=O)N[C@@H]2C=C(C[C@@H](O)[C@@H]2O)C(=O)N[C@@H](C(=O)N)C)cc1	0
Decoy430	S(CC(=O)Nc1cccnc1)C1=NC(=O)N(C2=C1CCC2)CC[NH+](CC)CC	0
Decoy431	S=C(NC1C[C@@H]2[NH+]([C@H](C1)CC2)Cc1occc1)Nc1ccc(cc1)CC	0
Decoy432	S1C=CN2C1=NC1=C(CCC1)C2=O	0
Decoy433	s1cccc1[C@H](O)CNC(=O)NC1=CC=CN(C)C1=O	0
Decoy434	FC(F)(F)c1cc(cnc1-c1noc(c1)C)C#N	0
Decoy435	s1c2c([nH+]c1-c1ccsc1)[C@@H](CC(=O)Nc1ccccc1)[C@@]1([C@H](C2)[C@@](CO)(C)[C@H](O)CC1)C	0
Decoy436	s1c2c(NC(=S)N(CCC)C2=O)cc1	0
Decoy437	S(CC(C)C)C1=N[N-]C(=O)N1C[C@H]1OCCC1	0
Decoy438	s1cccc1C(=O)NC(=S)Nc1cccc(NC(=O)C2CC2)c1C	0
Decoy439	Brc1cc2NC(=O)Nc2cc1[C@H]([NH2+]C)c1oc(Br)cc1	0
Decoy440	Ic1c(nc(SC)nc1O)N[C@@H]1OC[C@@H](O)[C@H](O)[C@H]1O	0
Decoy441	Fc1cc(C#N)c(N=C=O)cc1	0
Decoy442	Brc1oc(cc1)[C@@H]([NH3+])c1cc2c3c(oc2cc1)cccc3	0
Decoy443	Clc1sc(Cl)cc1C(=O)Nc1oc(nn1)-c1cc(OC)cc(OC)c1	0
Decoy444	Brc1cc(oc1Br)CNc1cc2OCOc2cc1[N+](=O)[O-]	0
Decoy445	S(CC#C)c1n2c(nn1)C=CC=C2	0
Decoy446	s1c(C)c(cc1C(=O)N1C[C@H](O)CC1)C	0
Decoy447	S1(=O)(=O)C[C@@H](NC(=O)COC(=O)c2ccc(OCC(C)C)cc2)CC1	0
Decoy448	FC(F)c1c2c(nc(c1)-c1ccc(cc1)CC)n(nc2C)Cc1ccccc1	0
Decoy449	[NH2+]1C[C@H](CCC1)[C@@H](Nc1nc(ccc1C#N)C)C	0
Decoy450	O1c2cc(ccc2OC1)[C@H](NCC)C[NH+](C(C)C)C	0
Decoy451	S(=O)(=O)(C(F)F)c1cc(NC(=O)CCCc2onc(n2)CCC)ccc1	0
Decoy452	[NH2+](Cc1nnnn1-c1ccccc1C(C)C)C1CC1	0
Decoy453	Ic1cc(ccc1[O-])\C=C(/C#N)\C1[NH+]=C2C(=[NH+]1)C=CC=C2	0
Decoy454	O=C(N(C)C1CC1)c1cc2nc(C)c(nc2cc1)C	0

Decoy455	Clc1ccccc1C1=NN(C[NH+](CCC)C)C(=S)N1CCCOC	0
Decoy456	s1c(ccc1CNC(=O)C)C(=O)COC(=O)Cn1nc(cc1)C(F)(F)F	0
Decoy457	Fc1ccc(cc1)[C@@H]1N(C)C(=O)CO[C@@H]1C(=O)N[C@H](C(=O)N(CC=C)CC=C)C	0
Decoy458	Brc1cc2OCCOc2cc1N[C@@H]1C[C@@H]([NH+](C[C@H]1C)C)C	0
Decoy459	s1cccc1C\[NH+]=C(/N[C@H]1C[C@H](SC)CC1)\NCCc1occc1	0
Decoy460	S1c2cc(OCC)ccc2-n2cc(nc12)[C@@H]([NH3+])C	0
Decoy461	Clc1ccccc1Cc1c(nc(SC)nc1N1CC[NH2+]CC1)C	0
Decoy462	Clc1n(nc(C)c1CN1C(C)=C(SC1=O)C)C	0
Decoy463	S(=O)(=O)(Nc1ccc(cc1)C(O[C@@H](C(=O)NC(=O)Nc1ccccc1)C)=O)c1cccc(F)c1C	0
Decoy464	S1CCn2cc([nH+]c12)-c1cc(NC(=O)c2ccc(cc2)C(C)(C)C)ccc1	0
Decoy465	s1cccc1[C@H]1CC(=O)C2C(=NC(=C)C(C(OCCSCC)=O)[C@@H]2c2cc(OC)c(OC)c(OC)c2)C1	0
Decoy466	Fc1ccccc1[C@@H](O)CNC(=O)C(=O)Nc1ccc(cc1)-c1ccccc1	0
Decoy467	O=C(N(CC1CCCC1)C)NCCn1ccnc1	0
Decoy468	s1cccc1[C@@H](NC(=O)N)CC(=O)N1CCC(=CC1)c1ccccc1	0
Decoy469	Clc1ccc(O[C@@H]([C@@H]([NH3+])CC)c2occc2)cc1C	0
Decoy470	Clc1cc(ccc1Cl)COc1ccc(cc1)-c1nc2c(nc1)cccc2	0
Decoy471	Clc1ccc(cc1)[C@@H]([C@@]1(OC(=O)c2c1cccc2)C)c1ccccc1N(C)C	0
Decoy472	S(Oc1ccccc1[C@H]1N(O[C@H]2[C@@H]1C(=O)N(c1ccc(OCCC)cc1)C2=O)c1ccccc1)(=O)(=O)c1ccccc1	0
Decoy473	O1CCC[C@@H]1Cn1cc[nH+]c1-c1ccc(N)cc1	0
Decoy474	O(CC#N)c1ccccc1C[NH2+][C@@H]1CCC[C@@H]1OC	0
Decoy475	O1CCC(CC1)[C@@H](O)CNC(=O)N[C@H]1C[C@H]1c1ccc(cc1)C(C)C	0
Decoy476	Clc1ccc(cc1)[C@H](NC(=O)C[NH2+][C@@](CC)(C)c1sccn1)CC	0
Decoy477	O=C1N(C[NH+]2C[C@@H](CCC2)C)C(=O)CC12CCCC2	0
Decoy478	S(=O)(=O)([C@H](C)c1ccccc1OC)CCCCCn1ncc(c1)C	0
Decoy479	O1CCCOc2c1cc(cc2)-c1nn(cc1C[NH2+]CCCOCCOC)C	0
Decoy480	s1c(SCCOc2ccc(F)cc2)c(nc1N)C	0
Decoy481	O(C)c1ccc(cc1)[C@@H](Nc1ccccc1[C@H](O)C)C	0

Decoy482	S1\C(=C/c2ccccc2F)\C(=O)N(CCNC(=O)CSCC(OCC)=O)C1=O	0
Decoy483	ClC=1C=CC2=[NH+]CC(=C2C=1)CC[N-]/C(=N\C(=O)CS[C@H]1S[C@H](NN1)C)/Nc1nc(cc(n1)C)C	0
Decoy484	[NH+]1(CCN(\N=C/C(=C/c2ccccc2)/C)CC1)C1c2c(-c3c1cccc3)cccc2	0
Decoy485	S\1c2n(nc(n2)\C=C\c2ccc(OCC=C)cc2)C(=O)/C/1=C/c1cn(nc1-c1occc1)-c1ccccc1	0
Decoy486	s1c(C)c(cc1C)-c1[nH]c2N(C)C(=O)NC(=O)c2c1C=1C(=O)NC(=O)N(C)C=1N	0
Decoy487	s1c2cc(ccc2nc1[C@H]1[NH2+]CCC1)C#N	0
Decoy488	[NH3+]C[C@@H]1CCCC[NH+](C(C)C)[C@H]1c1cn(nc1)C	0
Decoy489	O=C(N1C[C@]2(CCC=CC2)CCC1)[C@@H]1[NH2+]CCC1	0
Decoy490	s1ccnc1[C@](NC(=O)Cc1nocc1)(CC)C	0
Decoy491	S=C(N)c1ccc(cc1)C(=O)NCc1nncn1C	0
Decoy492	S(c1c(n(nc1C)C(=O)[C@@H]1N(S(=O)(=O)c2ccc(cc2)C)CCC1)C)c1ccccc1[N+](=O)[O-]	0
Decoy493	S(CC(=O)c1cc(OC)ccc1)[C@H]/1CC[NH+](C\C\1=C/C(OCC)=O)[C@H](C(=O)C1CC1)c1ccccc1F	0
Decoy494	O=C/1Nc2c(N=C(\C\1=C\[C@@H](O)[C@H](O)[C@H](O)[C@H](O)CO)c1ccccc1)cccc2	0
Decoy495	O=C1NC(=NC(=C1)CC)c1cc(NC(=O)C[C@H](NC(=O)N)c2ccccc2C)ccc1	0
Decoy496	O1C[C@@](O)(C)[C@@H](N(C(OC(C)(C)C)=O)C)[C@@H](O)[C@H]1O[C@H]1[C@@H](O)[C@H](O)[C@@H](NC(OC(C)(C)C)=O)C[C@H]1NC(OC(C)(C)C)=O	0
Decoy497	Brc1ccc(cc1)\C=N\NC(=O)[C@@H](NC(=O)c1ccccc1)C1=NNC(=O)c2c1cccc2	0
Decoy498	Clc1ccccc1-c1nnc(SCc2cc(ccc2)C)n1C(C)(C)C	0
Decoy499	O(C(=O)c1ccccc1-c1ccccc1C(OCC(=O)c1ccc([N+](=O)[O-])cc1)=O)CC(=O)c1ccc([N+](=O)[O-])cc1	0
Decoy500	OC1C2(C[NH+](CC1(C[NH+](C2)CC)C)CC)C	0
Decoy501	Clc1cc(NC(=O)N(Cc2cc(F)ccc2)C2CC2)ccc1C(=O)N	0
Decoy502	Fc1cccc(NC(=O)N([C@@H](c2ccc(cc2)C)c2[nH+]cccc2)C)c1C	0
Decoy503	Brc1cc2OCCOc2cc1CO	0

Decoy504	o1c2c(cc(cc2)C(=O)[C@@H]2CCC[NH2+]C2)cc1	0
Decoy505	Clc1ccc(cc1NC(=O)CS[C@H]1NN[C@@H](N1N)[C@@H]1N=NC(=C1)c1ccc(cc1)C)C(F)(F)F	0
Decoy506	O1CCOc2c1cc1C=C(C[NH+]([C@@H](C(C)C)c3nnnn3Cc3ccc(OC)cc3)Cc3ccc(OC)cc3)C(=O)Nc1c2	0
Decoy507	O(C)c1cc2c(cc(cc2)-c2n[nH]cc2C[NH2+][C@H](C(C)C)c2[nH]c3c(n2)cc(cc3)C)cc1	0
Decoy508	O=C(N(CC(C)C)C1CC1)C[NH+](CC1CCN(CC1)c1ncccc1)CC	0
Decoy509	S(C)c1ncc(cc1)C(=O)N[N-]C(=S)N[C@H]1CCCC[C@@H]1C	0
Decoy510	o1cccc1CN([C@H](C(=O)NC(CC(C)(C)C)(C)C)c1cc(OC)ccc1)C(=O)C[C@H](C)c1ccccc1	0
Decoy511	O(C[C@H](O)C[NH+](Cc1ccccc1)CCO)C12CC3CC(C1)CC(C2)C3	0
Decoy512	Ic1ccc(cc1)[C@H](Nc1c([nH][nH+]c1C)C)C	0
Decoy513	FC(F)(F)[C@@H]1CCCN(C1)C(=O)c1ncc(nc1)C	0
Decoy514	Fc1ccc(cc1)-c1n(CC[C@@H](O)C[C@@H](O)CC(=O)[O-])c(C(C)C)c(C(=O)Nc2ccccc2)c1-c1ccccc1	0
Decoy515	S1C=C(N2C1=NC(=CC2=O)CN1C(=O)[C@@](NC1=O)(C)c1ccc(cc1)C(C)(C)C)C	0
Decoy516	Clc1ccccc1[C@@H]1n2nc([nH+]c2N=C(C1)c1ccc(cc1)C)N=S(=O)([O-])C	0
Decoy517	S=C(Nc1cc(ccc1)C(=O)NC)NC(=O)C12CC3CC(C1)CC(C2)C3	0
Decoy518	O(C(=O)C1(CCC1)C(=O)NC)[C@H]1C[C@@H](OC)CCC1	0
Decoy519	S(C)c1ccc(cc1)[C@H](NC(=O)N1CCCCC[C@@H]1c1cc[nH+]cc1)C	0
Decoy520	S(C)[C@@H]1O[C@H]([C@H](NC(=O)[C@H]2[NH+](C[C@@H](C2)CCC)C)[C@H](O)C)[C@H](O)[C@@H](O)[C@@H]1O	0
Decoy521	Brc1sc(cc1)[C@@H]([NH+]1CCC2(CCCC2)CC1)[C@@H](N)C	0
Decoy522	S(CC[C@H](NC(=O)c1cc(ccc1)C)C(=O)N(Cc1cn(nc1)C)CC)C	0
Decoy523	O=C(Nc1ccc(NC(=O)[C@@H](n2ncnc2)C)cc1)c1ccc(NC(=O)N)cc1	0
Decoy524	Clc1nc2SC=Cn2c1\C=C\C(=O)[C@@H](C(=O)NCCCOC(C)C)C#N	0
Decoy525	S(CC(=O)Nc1ccc(cc1)C(OCC)=O)c1oc(nn1)CCCCCN1C(=O)c2c3c(cccc3ccc2)C1=O	0
Decoy526	Brc1cc(Cl)c(S(=O)(=O)N2[C@@H]3[C@@H](C[C@@H]2C)C[NH2+]C3)cc1	0

Decoy527	S(=O)(=O)(N1CCC(CC1)CO)c1ccc(nc1)N	0
Decoy528	Clc1cc2c([nH]c(C)c2CCN(Cc2cc[nH+]cc2)C(=S)NC(C)(C)C)cc1	0
Decoy529	Fc1cc2cc(n(c2cc1)C)[C@H]1OC=CC1=N	0
Decoy530	S(CC(=O)NC(c1ccccc1)c1ccccc1)c1nnc(n1-c1ccccc1)-n1nnc2c1cccc2	0
Decoy531	o1cccc1CNc1c2c3c(noc3-c3c(cccc3)C2=O)c(N2CCOCC2)c1	0
Decoy532	S(=O)(=O)(CNC(=O)[C@@H](N(Cc1oc(cc1)C)C(=O)[C@@H](CCCC)CC)\C=C\CCC)c1ccc(cc1)C	0
Decoy533	o1c2c(cccc2C)c(C)c1C(=O)N[C@@H](c1ccccc1)c1ccc[nH+]c1	0
Decoy534	S(=O)(=O)(\N=C\1/Nc2c(N=C/1Nc1ccccc1C(O[C@H]1C[C@H](CC[C@@H]1C(C)C)C)=O)cccc2)c1ccc(cc1)C	0
Decoy535	FC(F)(F)C1CCC(CC1)CNC(=O)NCC[NH+](CC(F)(F)F)C	0
Decoy536	Clc1cn(nc1C)[C@@H](C[NH3+])c1oc(cc1)C	0
Decoy537	O(C)[C@@H]1CCC[C@H]1n1c2c(cc1)[C@@H](O)CCC2	0
Decoy538	Clc1ccc(cc1[N+](=O)[O-])-c1nc([nH]c1)[C@@H]([NH3+])C	0
Decoy539	Brc1ccc(cc1)C(=O)C=1[C@@H](N(CCC[NH+](CCCC)CCCC)C(=O)C=1[O-])c1occc1	0
Decoy540	FC(F)(F)c1cc(N2C3=C([C@@H](C(C#N)=C2N)c2cc(COc4ccc(cc4[N+](=O)[O-])C)c(OC)cc2)C(=O)CCC3)ccc1	0
Decoy541	S(=O)(=O)(N)c1cc(C#N)c(N[C@@H](C)c2cccc(C)c2C)cc1	0
Decoy542	Clc1cccc(Cl)c1[C@@H](O)CNc1ncc(cc1)C(=O)NC1CC1	0
Decoy543	S(C)c1ccc(cc1)[C@H](NC(=O)N(Cc1cc(ccc1)C(=O)N)C)C	0
Decoy544	s1c(ccc1[C@H](N(C(=O)c1n[nH]c(C(C)C)c1N)C)C)C	0
Decoy545	S\1CC(=NN/C/1=[NH+]\C1CC1)c1cc(n(c1C)-c1cc(C)c(cc1)C)C	0
Decoy546	S(Cc1[nH+]c(Nc2ccc(OC)cc2)c(C)c(N)c1C)C=1n2nc(C)c(c2N=C(C=1)C)-c1ccccc1	0
Decoy547	S(=O)(=O)(c1cc2nc(oc2cc1)-c1cc(N)cc(N)c1)c1cc2nc(oc2cc1)-c1cc(N)cc(N)c1	0
Decoy548	s1c(C)c(nc1NC(=O)[C@@H]1[NH2+]CSC1)CC	0
Decoy549	O1CC[NH2+]CCOc2c(NCCCCCNc3c1cccc3)cccc2	0
Decoy550	Brc1ccc(cc1)[C@H](n1c2c([nH+]c1CO)cc(N)cc2)C	0
Decoy551	S(=O)(=O)(n1cc(c2c1cccc2)\C=C(/NC(=O)c1ccccc1F)\C(=O)NCCc1c2cc(OC)ccc2[nH]c1)N(C)C	0
Decoy552	Clc1cc(c2NC(=O)[C@@]3([NH2+][C@H](C[C@@H]3C(=O)Nc3c	0

	c(OC)ccc3OC)CCSC)c2c1)C	
Decoy553	S(C)c1ccc(cc1)C(=O)COC(=O)CNS(=O)(=O)c1ccc(cc1)C#N	0
Decoy554	Brc1cc2c([nH]cc2C(=O)NCC(=O)NCC)cc1	0
Decoy555	Clc1cc(cnc1Nc1[nH+]cnc(N(CC(C)C)CC(C)C)c1N)C(F)(F)F	0
Decoy556	S\1c2c(N(C)/C/1=C/C=C/C=N\c1cc(OC)ccc1)c1c(cc2)cccc1	0
Decoy557	Brc1cc(Cl)c(Cc2sc([nH+]c2)N)c(Cl)c1	0
Decoy558	Fc1ccccc1OCC[NH+](Cc1nnnn1-c1ccc(OC(F)F)cc1)C	0
Decoy559	S(=O)(=O)(CCC)c1c(n2c(c1S(=O)(=O)CCC)C(=CC(=C2)C)C)C(=O)c1ccc([N+](=O)[O-])cc1	0
Decoy560	Clc1cc(ccc1Cl)C1=Nc2n(nc(c2)C(=O)Nc2cc([N+](=O)[O-])cc(Oc3ccc(Cl)cc3C3CCCCC3)c2)C(=C1)C(F)(F)F	0

Table S4. Structures of the 200 Compounds (in SMILE format) from the Test set together with their activities (1 or 0) for H_2O_2-induced models.

Name	Structure	Activity
CHEMBL1080274	s1c2sccc2cc1C(=O)N[C@@H](CCC(=O)NCCC1CC[NH+](CC1)Cc	1

	1ccccc1)C(OCCCCCC)=O	
CHEMBL1082082	O(CCCCCC)C(=O)[C@@H](NC(OCc1ccccc1)=O)CCC(=O)NCCC1CC[NH+](CC1)Cc1ccccc1	1
CHEMBL1163575	Clc1ccc(cc1)-c1nc(SCCC)nnc1-c1ccc(Cl)cc1	1
CHEMBL1782114	O1c2c(OC1)cc1c(-c3c(cc(OC)c(OC)c3OC)[C@H](OC(=O)C)[C@@H](C)[C@@H](C)[C@H]1OC(=O)C)c2OC	1
CHEMBL1938457	Clc1cc2Sc3c(N(NC(=O)C[NH+]4CCCCC4)c2cc1)cccc3	1
CHEMBL1938460	Clc1cc2Sc3c(N(NC(=O)C[NH+]4CCCC4)c2cc1)cccc3	1
CHEMBL2012545	O1c2c(OC1)cc1c(-c3c(cc(OC)c(OC)c3OC)[C@H](OC(=O)C)[C@@H](C)[C@@H](C)[C@H]1OC(=O)\C(=C\C)\C)c2OC	1
CHEMBL2012547	O1c2c(OC1)cc1c(-c3c(cc(OC)c(OC)c3OC)[C@H](OC(=O)\C=C\c3ccccc3)[C@@H](C)[C@@H](C)[C@H]1OC(=O)\C(=C/C)\C)c2OC	1
CHEMBL2036260	S(C(=O)C)CCC(=O)NCCCCNc1c2CCCCc2[nH+]c2c1cccc2	1
CHEMBL2036261	SCCC(=O)NCCCCNc1c2CCCCc2[nH+]c2c1cccc2	1
CHEMBL2151788	Clc1cc2[nH+]c3c(CCCC3)c(NCCCNC(=O)\C=C\c3cc(O)c(O)cc3)c2cc1	1
CHEMBL2151789	Clc1cc2[nH+]c3c(CCCC3)c(NCCCCCCNC(=O)\C=C\c3cc(O)c(O)cc3)c2cc1	1
CHEMBL2312738	O1c2c(c(O)c(O)c(O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@@H]3O)c2)C(=O)C=C1c1ccc(O)cc1	1
CHEMBL2312739	O1c2c(c(O)c(O)c(O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)c2)C(=O)C=C1c1ccc(O)cc1	1
CHEMBL2337717	o1cc(cc1)[C@@H]1CC(=O)[C@]2(O)CCCC[C@]12C	1
CHEMBL2337719	o1cc(cc1)C1=CC(=O)[C@]2(O)CCCC[C@]12C	1
CHEMBL2391350	O=C(NC1CCCCC1)CC[NH+]1[C@H]2C[C@H]([NH2+]C2)C1	1
CHEMBL2391360	O=C(N1CC[NH+](CC1)CC(=O)NCC(CC)C)CC	1
CHEMBL2391362	O=C(N(CCCC)CCC)C[NH+]1C[C@@H]([NH2+]C[C@H]1C)C	1
CHEMBL2397176	Oc1cc(ccc1O)\C=C\C(=O)CCCc1ccccc1	1
CHEMBL2397180	O(C(=O)C)c1cc(ccc1OC(=O)C)\C=C\C(=O)CCc1cc(OC)c(OC)cc1	1
CHEMBL2397183	O(C(=O)C)c1cc(ccc1OC(=O)C)\C=C\C(=O)CCCc1ccccc1	1
CHEMBL2414565	S(=O)(=O)(NCCCc1ccccc1)\C=C\c1cc(O)c(O)cc1	1

CHEMBL2414567	Clc1ccc(cc1)CNS(=O)(=O)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2414568	S(=O)(=O)(NCc1ccc(cc1)C(F)(F)F)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2414570	S(=O)(=O)(NCc1ccc(cc1)C)\C=C\c1cc(O)c(O)cc1	1
CHEMBL2414574	S(=O)(=O)(NCc1ccccc1)\C=C\c1cc(OC(=O)C)c(OC(=O)C)cc1	1
CHEMBL2414576	S(=O)(=O)(NCCCc1ccccc1)\C=C\c1cc(OC(=O)C)c(OC(=O)C)cc1	1
CHEMBL2414580	S(=O)(=O)(NCc1ccc(F)cc1)\C=C\c1cc(OC(=O)C)c(OC(=O)C)cc1	1
CHEMBL2414581	S(=O)(=O)(NCc1ccc(cc1)C)\C=C\c1cc(OC(=O)C)c(OC(=O)C)cc1	1
CHEMBL290916	O=C1N(N=C(C1)C)c1ccccc1	1
CHEMBL468002	O=C1C2=C(Nc3[nH+]c4c(CCCC4)c(N)c3C2c2ccncc2)CC(C1)(C)C	1
CHEMBL493074	s1nc(nc1\C=[N+](/[O-])\C(C)(C)C)-c1ccccc1	1
CHEMBL506792	O1c2c(OC1)cc1c(-c3c(cc(OC)c(OC)c3OC)C[C@@H](C)[C@@H](C)[C@H]1O)c2OC	1
CHEMBL508313	O(C(=O)C=1C(C(C#N)=C(NC=1C)N)c1cccnc1)CC	1
CHEMBL512096	O=C1C2=C(Nc3[nH+]c4c(CCCC4)c(N)c3C2c2ccccc2)CC(C1)(C)C	1
CHEMBL571751	O1c2cc(ccc2OC(CO)C1c1cc(OC)c(OCC(=O)N(CC)CC)cc1)C=1Oc2c(C(=O)C=1O)c(O)cc(OCC(=O)N(CC)CC)c2	1
CHEMBL571754	O1c2cc(ccc2OC(CO)C1c1cc(OC)c(OCCC=C)cc1)C=1Oc2c(C(=O)C=1OCCC=C)c(O)cc(OCCC=C)c2	1
CHEMBL574683	O1[C@@H](CO)[C@H](O)[C@@H](O)[C@H](O)C1Oc1cc(O)c2c(OC(=CC2=O)c2cc(O)c(O)cc2)c1	1
CHEMBL585388	O1c2cc(ccc2OC(CO)C1c1cc(OC)c(O)cc1)C=1Oc2c(C(=O)C=1O)c(O)cc(OC\C=C(\C)/C)c2	1
Decoy561	S(=O)(=O)(N[C@H]1C[C@@H]1[NH3+])c1cc2C=CC(Oc2cc1)=O	0
Decoy562	S(=O)(=O)(N(C)c1nc(-c2ccc(F)cc2)c(\C=C\[C@@H](O)C[C@@H](O)CC(O[C@@H]2O[C@H](C(=O)[O-])[C@@H](O)[C@H](O)[C@H]2O)=O)c(n1)C(C)C)C	0
Decoy563	O=C(N)c1cc(C)c(NCC(=O)N2C[C@H](C[C@H](C2)C)C)cc1	0
Decoy564	[NH+]1(CCCCCC1)[C@H](C)c1nc2c(n1Cc1cc(ccc1C)C)cccc2	0
Decoy565	Brc1oc(cc1)C(=O)Nc1ccc(cc1)[C@H]1[NH+]=C2C(=C1)C=CC=C2	0
Decoy566	O(C)c1cc(cc(OC)c1)C#N	0
Decoy567	O1CCC[C@H]1CN\1C=2N=C3N(C=CC=C3C)C(=O)C=2C=C(C(OCC)=O)/C/1=N/C(=O)c1cc(cc(c1)C)C	0
Decoy568	O1[C@@H]2O[C@H](C1)[C@@H](NC(=O)Nc1ccc(OC)cc1)[C@	0

	H](O)[C@H]2[NH+]1CCC(CC1)C(=O)N	
Decoy569	Fc1cc(cc(NC(=O)[C@@H]2[NH2+]CCC2)c1C)C(=O)N[C@@H](C)c1ccccc1	0
Decoy570	O(CCC)c1ccc(OCC[NH+]2CC[NH+](CC2)CC[NH+]2CCCC2)cc1	0
Decoy571	Clc1ccc(cc1N(C(=O)c1ccccc1[N+](=O)[O-])C(=O)c1ccccc1[N+](=O)[O-])C(F)(F)F	0
Decoy572	O=C([C@@H]([NH2+]CCN(C)C)c1ccccc1)c1c2c([nH]c1)c(ccc2)CC	0
Decoy573	O1[C@@H]2[C@@H]([NH+](CC1)CC[C@@H]([NH2+]CCC)C#N)CCCC2	0
Decoy574	o1cccc1CC[C@H](NC(=O)c1ncc(nc1)C)C	0
Decoy575	S1C(=S)N(N=C1S[C@@H](C(=O)C)C(OCC)=O)CCOc1ccc(cc1)C	0
Decoy576	S(C[C@H](O)COc1ccc(cc1)C#N)c1nnc(n1C1CC1)-c1ccncc1	0
Decoy577	S=C1NC(=O)C([C@](O)(C(OC)=O)C(F)(F)F)=C(N)N1CCc1c2c([nH]c1)cccc2	0
Decoy578	O(Cc1cc(ncc1)C[NH3+])c1cc(C)c(cc1)C(C)C	0
Decoy579	O(CC(OCC(=O)c1cc(n([C@@H](COC)C)c1C)C)=O)c1ccc(OC)cc1	0
Decoy580	S=C(NC1CC([NH2+]C(C1)(C)C)(C)C)N(Cc1ccc(OC)cc1)C[C@@H]1OCCC1	0
Decoy581	O=C(NCC(C)C)C1=C[NH+](CC(C(=O)NCC2[NH+]=C3C(=[NH+]2)C=CC=C3)=C1[O-])C(C)C	0
Decoy582	Brc1cc(N)ccc1COc1c2[nH+]c(ccc2ccc1)C	0
Decoy583	Fc1ccc(cc1)C=1NN2[C@@H](C=1)c1c(OC23CC[NH+](CC3)CCC)cccc1	0
Decoy584	Brc1ccc(nc1)CNc1ccc(cc1)-c1[nH]nc(O)c1	0
Decoy585	FC(F)(F)C[NH+]1CCN(CC1)c1ccc(cc1[NH3+])C(=O)[O-]	0
Decoy586	Brc1cc(C(=O)[O-])c(NC(=O)CC[NH2+]C(C)(C)C)cc1	0
Decoy587	S1CCC(NC(=O)Nc2cc(C(=O)NC(C)C)c(cc2)C)CC1	0
Decoy588	O1[C@@H](COC(=O)C)[C@@H](OC(=O)C)[C@H](OC(=O)C)[C@H](OC(=O)C)[C@@H]1O[C@H]1OC=C[C@@H]2[C@H]1C(=C[C@H]2OC(=O)C)COC(=O)C	0
Decoy589	Brc1cc(ccc1C(C)(C)C)C(=O)NC(=S)[N-]NC(=O)c1cc([N+](=O)[O-])c(Cl)cc1	0
Decoy590	S(C)c1cc2nc(-	0

	c3cc(ccc3)C)c(cc2cc1)CN(C(=O)c1cccc(OC)c1OC)CCCOC	
Decoy591	S=C1NC(=N[N-]1)NC(=O)\C(=N/NC(C)(C)C)\[C@H]1S(=O)c2c(NC1=O)cccc2	0
Decoy592	S(CCCNc1[nH+]cc(cc1)C=1NC(=CC(=O)N=1)CC)c1ccc(F)cc1	0
Decoy593	s1c2C[C@H](CCc2c2c1N=C(NCC[NH3+])N(C)C2=O)C(C)(C)C	0
Decoy594	FC(F)(F)C1=NN(C(=O)c2ccc([N+](=O)[O-])cc2)[C@](O)(C1)c1ccc(cc1)CC	0
Decoy595	O=C1CCCc2c1cc(NC(=O)N[C@H](CO)c1ccccc1)cc2	0
Decoy596	O[C@@H]1[C@H]2[C@H](C)[C@@H](NC(=O)C3CC3)CC[C@@]2(CC[C@@H]1[C@@H](C(=O)NC(C)C)C)C	0
Decoy597	Fc1ccc(NC(=O)[C@@H](NC(=O)c2[nH]c3c(occ3-c3ccc[nH+]c3)c2)CC(C)C)cc1	0
Decoy598	O=C(Nc1cccc(C)c1C)[C@H]([NH2+][C@H](C(C)C)C)C	0
Decoy599	S1C[C@H](N(CC1)c1nc(ccc1)CO)C	0
Decoy600	Brc1cnc(Sc2nccn2C)nc1	0
Decoy601	Clc1cc([C@@H]2N=C(O)c3c4CC[NH+](Cc4sc3N2)C(C)C)c(O)c(OC)c1	0
Decoy602	S(c1oc(cc1)C[NH+](Cc1ncccc1)C[C@@H]1[NH+](CCC1)CC)c1nccn1	0
Decoy603	s1cccc1CN(C(=O)C[NH+](Cc1cn(nc1)-c1ccccc1)C)CC=C	0
Decoy604	o1c(C)c(cc1C)-c1[nH]c(nc1)CC1CC[NH2+]CC1	0
Decoy605	o1c(C[NH3+])c(cc1C[NH+]1C[C@@H](OCCC1)C)C	0
Decoy606	Brc1cc(NC(=O)[C@@H]2C[C@H]([NH3+])CCC2)c(N(C)C)cc1	0
Decoy607	s1cccc1[C@H]1N(S(=O)(=O)c2ccc(cc2)C(C)(C)C)CCCCC1	0
Decoy608	O1C2=C([C@H](C[C@H](CCCC(C)C)C)C(C#N)=C1[NH3+])C(=O)N(C)C(=C2)CCC	0
Decoy609	FC(F)(C(F)(F)C(F)(F)F)C(=O)N\N=C/1\c2c(oc(C(=O)N[NH2+]C(C)(C)C)c2C)CCC\1	0
Decoy610	FC(F)(F)c1n(nc(C)c1C#N)C	0
Decoy611	[nH+]1c-2n(c3c1cccc3)[C@@H](Nc1c-2cccc1)c1cc(n(c1C)C1CC1)C	0
Decoy612	[NH+]12[C@H](CCCC1)[C@H](NCc1c(n[nH]c1C)C)CC2	0
Decoy613	Brc1cc2nc(n(c2cc1)C1CC1)[C@]1([NH3+])C[C@@H](CCC1)C	0
Decoy614	S1CC(=NN=C1Nc1c(cccc1C)C)c1sc(cc1)CC(=O)N	0

Decoy615	S(c1ncccc1NC(=O)NC[C@H](O)C1CC1)c1ccccc1	0
Decoy616	s1nnc(c1)[C@@H](N(Cc1ccccc1F)C(=O)CN1C(=O)c2c(cccc2)C1=O)C(=O)Nc1ccc(OC)cc1OC	0
Decoy617	O=C1c2c(N(CC[NH+](C)C)C1=O)cc(cc2C)C	0
Decoy618	O1CCCC[C@H]1C[NH+]1CCC[C@H]1c1cn(nc1)C	0
Decoy619	Clc1ccccc1NC(=O)[C@@H](S(=O)Cc1nnnn1CCCC)C	0
Decoy620	s1c(nnc1CSc1[nH+]c2sc3C[C@@H](CCc3c2c(n1)N)C)C(=O)Nc1ccc(OC)cc1	0
Decoy621	S(=O)(=O)(N(C)C)c1cc(ccc1)CS(=O)(=O)C(CCC)CCC	0
Decoy622	Clc1ccc(\N=C\2/SC=C(N/2C[C@@H]2OCCC2)c2ccccc2)cc1	0
Decoy623	FC(F)(F)c1ccccc1NC(=O)Nc1cc(ccc1)C(=O)NCC(OCC)(OCC)c1[nH+]cccc1	0
Decoy624	O=C1C=2CC[NH2+]CC=2N(c2c1cc(cc2)CC)C	0
Decoy625	S(=O)(=O)(N([C@H](Cc1ccc(OS(=O)(=O)c2c3c(ccc2)cncc3)cc1)C(=O)N1CCN(CC1)c1ccccc1)C)c1c2c(ccc1)cncc2	0
Decoy626	S\1C[C@H](N/C/1=N/c1cc(S(=O)(=O)N)ccc1)CC(C)C	0
Decoy627	Clc1cc(cnc1NCCN1C[C@H](C(=[NH2+])N)C([O-])=NC1=O)C(F)(F)F	0
Decoy628	S(=O)(=O)(N)c1ccc(-n2cccc2\C=N\N=C(/N)\c2nonc2N)cc1	0
Decoy629	Fc1ccc(cc1)[C@H](O)c1nc(C)c(n1C)C	0
Decoy630	Clc1nc(nc(Cl)c1)C[NH+]1CCOCC1	0
Decoy631	S(=O)(=O)(Cc1nc(oc1)-c1ccc(OC)cc1)CCCOCC(F)(F)F	0
Decoy632	Brc1cc(\C=N\Nc2nc(nc(n2)N2CCCCC2)N2CCCCC2)c(OCc2ccc(Cl)cc2)cc1	0
Decoy633	Fc1cc2c(cc1C)CC[NH2+][C@H]2c1ncccn1	0
Decoy634	Brc1cc2c(cc(Oc3ncc(nc3)C(=[NH2+])N)cc2)cc1	0
Decoy635	S(=O)(=O)(N(CC)CC)c1cc(ccc1F)C(OCC(=O)NC1CC1)=O	0
Decoy636	Clc1cccc(Cl)c1[C@@H]1N2NC=NC2=[NH+][C@H](C1)c1ccc(Cl)cc1	0
Decoy637	FC(F)(F)Oc1ccc(NC(=O)[C@H]2[NH+]=C3C(=C2)C(=CC(=C3)C)C)cc1	0
Decoy638	O=C([O-])[C@@H](n1c2c(nc1C[NH+](C)C)cccc2)CC	0
Decoy639	Clc1sc(S(=O)(=O)c2c[nH+]c(SCC(=O)Nc3ccccc3)nc2N)cc1	0
Decoy640	O=C(N1CCC(CC1)c1nn2c(N=C3C(C[NH+](CC3)C3CCCC3)=C2[	0

	O-])c1)C(C)(C)C	
Decoy641	O=C(NC[C@@H](O)c1cc2c(cc1)cccc2)N[C@@H](C(C)C)c1ccncc1	0
Decoy642	Brc1ccc(cc1)[C@@H](NC(=O)NCc1n[nH]cc1)C	0
Decoy643	S1(=O)(=O)c2cc(F)c(F)cc2[C@H]([NH2+]C)[C@H]1C	0
Decoy644	o1c(C)c(cc1C[NH+](C[C@@H]1OCCCC1)C)C(=O)[O-]	0
Decoy645	S=C1Nc2c([nH]c3c2cc(OC)cc3)C(=O)N1Cc1ccc(cc1)C(=O)NCc1ccc(OC)cc1	0
Decoy646	s1c2N=C(NC(=O)c2c(C)c1C)[C@@H](Nc1cc(ccc1)CO)C	0
Decoy647	S=C(Nc1cccc(C)c1C)[N-]NC(=O)[C@@H]1CCOc2c1cccc2	0
Decoy648	s1c(CCC)c(cc1C(=O)N(CCC#N)CC[NH+]1CCOCC1)CC	0
Decoy649	FC(F)(F)c1ccccc1\N=C(/[O-])\C[NH+](C(C)C)CC(=O)N(CCC#N)C	0
Decoy650	S\1c2c(N(CC=C)/C/1=N/C(=O)c1cc(ccc1)C(F)(F)F)c(F)ccc2	0
Decoy651	O1CCC([NH+]2CCC(CC2)C(=O)Nc2ccc(cc2)-c2cc(ccc2)C)CC1	0
Decoy652	O1CCC([NH+](CCC(OC)=O)CC(=O)N(C2CCC(CC2)C)C2CC2)CC1	0
Decoy653	O([C@@H](CC[NH+](C)C)c1ccccc1)C(=O)[C@@H](Cc1c(n(nc1C)C)C)C	0
Decoy654	FC(F)Oc1cc(ccc1)CN/C(=[NH+]\C1CCOCC1)/NC1CCCC1	0
Decoy655	Brc1ccc(cc1)-c1oc(cc1)C[NH+](CC(=O)Nc1ccc(cc1)C(=O)N)C	0
Decoy656	o1cccc1C(=O)Nc1ccc(cc1)/C(=N/NC(=O)c1cc(O)c(O)c(O)c1)/C	0
Decoy657	S1[C@@H](CN(C[C@@H]1C)c1n(nc(C)c1C=O)C)C	0
Decoy658	S(CC(=O)Nc1ccc(S(=O)(=O)N)cc1)C1=NN[C@@H](N1N)[C@H]1N=NC2=C1CCC2	0
Decoy659	O(C)c1cccc([C@H]2Nc3c([C@@H]4[C@H]2CC=C4)cccc3C(=O)NCCC)c1O	0
Decoy660	Clc1cc(Cl)ccc1OCCCC(=O)Nc1sc(C(OCCOC)=O)c(C)c1C(OCC)=O	0
Decoy661	FC(F)(F)c1cc(OC/C(=[NH+]/NC(=O)c2cccnc2Oc2ccccc2)/N)ccc1	0
Decoy662	S([C@H](C#N)C)c1ncc(cn1)C	0
Decoy663	n1c(c2CCCCc2nc1C)CC#N	0
Decoy664	Clc1ccc(cc1)C(=O)N(CCC(OCC)=O)CCCOC(C)C	0
Decoy665	O=C1[C@H](CN(C[C@@H]1\C=N\OCc1ccc(cc1)C)c1ccc([N+](=O)[O-])cc1)\C=N/OCc1ccc(cc1)C	0

Decoy666	Oc1c(cccc1\C=[NH+]\NC(=O)c1[nH]nc(c1)C12CC3CC(C1)CC(C2)C3)CC=C	0
Decoy667	Clc1nc(OC)ncc1C	0
Decoy668	S(CC(=O)N(Cc1ccc(OC)cc1)C1CC1)c1nc(C)c(n1C[C@H]1OCCC1)C	0
Decoy669	S\1C=2N([C@H](C(C(OC)=O)=C(N=2)C)c2ccc(OC(=O)c3occc3)cc2)C(=O)/C/1=C/c1ccc(OCC=C)cc1	0
Decoy670	Fc1ccc(cc1)[C@@H]1N(CCC=2[C@H]1[NH+]=C1C=2C=CC=C1)Cc1oc(cc1)CO	0
Decoy671	s1c2nc(cc(c2c(N)c1C(OCC(=O)Nc1sc2c(CCC2)c1C(=O)N)=O)C)C	0
Decoy672	S(Cc1ccccc1)C=1N=C2N(C=CC=C2C)C(=O)C=1\C=N\NC(=O)c1cc2nc(n(c2cc1)CC)C	0
Decoy673	Brc1cc(OC(C)C)c(OCC)cc1\C=C(\C(=O)Nc1cc([N+](=O)[O-])ccc1Cl)/C#N	0
Decoy674	s1cc(nc1[C@H]([NH3+])c1ccccc1C)-c1c2c(ccc1)cccc2	0
Decoy675	s1c(nnc1S(=O)(=O)[C@H](C(=O)N(CC)CC)C)NCC(F)(F)F	0
Decoy676	S(=O)(=O)(N(Cc1oc(cc1)C)CC[NH+](C)C)c1cc(OC(F)(F)F)ccc1	0
Decoy677	O1[C@@H](C(OC)=O)[C@H](OC(=O)C)[C@@H](OC(=O)C)[C@@H](OC(=O)C)[C@H]1Oc1c2O[C@@H]3[C@]45CC[NH+]([C@H](Cc(c24)cc1)[C@]5(O)CCC3=O)CC1CC1	0
Decoy678	Brc1cc(C(=O)N)c(NC(=O)c2oc(cc2)CC)cc1	0
Decoy679	Br[C@@H](CC1=NC=Cn2c1nnc2C)C	0
Decoy680	Brc1cc(F)cc(F)c1NC(=O)c1cc(N)c[nH+]c1C	0
Decoy681	Fc1cc(ccc1)[C@H]1[NH2+]Cc2c(-n3c1ccc3)n(nc2C)-c1ccccc1	0
Decoy682	s1c(C(=O)Nc2ccc(cc2)-c2[nH+]c3c([nH]2)cccc3)c(cc1NC(=O)c1occc1)C	0
Decoy683	Clc1oc(cc1)C[NH2+]C[C@@H](N(C)C)c1occc1	0
Decoy684	FCCN1C[C@](N(c2c1cc(N)cc2)CCC)(CC)C	0
Decoy685	[NH3+][C@@H]1CCN(C1)c1nc(nc(c1)C(C)C)CC	0
Decoy686	s1c(C)c(nc1NC(=O)Nc1cc(ccc1)[C@H](O)C)CC	0
Decoy687	Brc1cc(OC)c(OC)cc1CNCC([NH2+][C@H](C)c1ccccc1)(C)C	0
Decoy688	FC(F)(F)C(OC[C@@H](O)C[NH+]1CC[NH+](CC1)Cc1cc2OCOc2cc1)C(F)(F)F	0
Decoy689	s1c(ccc1C)C[NH+](C(C)C)CC(=O)N(Cc1oc(C)c(c1)C(OC)=O)C	0

Decoy690	Fc1ccccc1C[C@@H](CNc1nc([nH+]c(c1)CC)-c1ccncc1)CO	0
Decoy691	Clc1nc(N)cc(c1)C(=O)NC[C@@H]1OCCOC1	0
Decoy692	o1c2c([C@@H]([NH+]3CCOCC3)CC2)c(C)c1C(=O)C	0
Decoy693	Fc1cc(N2CCCC2)cc(NC(=O)NCC(C[C@H](O)C)(C)C)c1	0
Decoy694	O(CC)c1ccc(cc1)C(=O)CCC(=O)N[C@@H](C)c1ccc(-n2ccnc2)cc1	0
Decoy695	O(CC)c1ccccc1C[NH+](CC(=O)Nc1cccc(C)c1C)C[C@@H](O)C	0
Decoy696	Brc1sc(cc1)[C@@H](SC1=N[N-]C(=O)N1CC)[C@@H]([NH3+])CC	0
Decoy697	s1cc(nc1NC(=O)C1=CC=CNC1=O)CCC(=O)Nc1ccc(cc1)C(=O)N	0
Decoy698	O1[C@@H]2O[C@@]3(OO[C@]24[C@@H](CC[C@H]([C@@H]4CC3)C)[C@@H](C)[C@@H]1OC(=O)CCC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H]([C@H](CC)C)C(=O)[O-])C	0
Decoy699	S=C(Nc1ccc(F)cc1F)NC[C@@H]([NH+]1CCCC1)c1ccccc1OC	0
Decoy700	O(CC(C)C)c1ccc(cc1)C(=O)N1CCNC(=O)[C@@H]1CC(OCCC)=O	0
Decoy701	O1c2c(cc3c(oc(C)c3-c3ccccc3)c2C)C(C)=C(CCC(=O)N[C@@H](Cc2ccccc2)C(=O)NCC(C)C)C1=O	0
Decoy702	Clc1cc(N2C(C)=C(C(OC)=O)\C(=C/c3oc(cc3)CNC(=O)C(=O)Nc3ccc(cc3)C(OCC)=O)\C2=O)ccc1C	0
Decoy703	O=C1[C@H](C(OC)=O)C(CC(N2CCN(CC2)C=2CC(C)(C)C(C(OC)=O)=C([O-])C=2C(=O)CCC)=C1C(=O)CCC)(C)C	0
Decoy704	O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@](OC(=O)C)(C(=O)COC(=O)CCC(=O)N5CCC[C@H]5C(=O)[O-])[C@]4(CC3)C)CCC2=C1)C	0
Decoy705	S([C@H](C(=O)c1cc2NC(=O)COc2cc1)C)c1n-2c(nn1)C=C(c1c-2cccc1)C	0
Decoy706	S=C(Nc1cc2nn(nc2cc1C)-c1ccc([NH+](CC)CC)cc1)NC(=O)c1ccccc1[N+](=O)[O-]	0
Decoy707	S(Cc1onc(n1)-c1cc(F)ccc1)C1=Nc2c(cc3OCOc3c2)C(=O)N1C[C@H]1OCCC1	0
Decoy708	Brc1cc(C)c(NCC(=O)NC(=O)NC(C)C)cc1	0
Decoy709	Fc1cccc(F)c1[C@@H](O)CNC(=O)NC[C@H]1Cc2c(OC1)cccc2	0
Decoy710	Oc1ccc(cc1)C=1CCN(CC=1)C(=O)N[C@@H](CCCO)c1ccccc1	0

Decoy711	Clc1c(n(nc1C)-c1ccc(cc1)C(=O)NCCSCCC(OC)=O)C	0
Decoy712	O(CCOC)c1ccc(cc1)C[NH+]1CCC[C@@H]1C=1NC(=O)C=C(N=1)c1ncccc1	0
Decoy713	Clc1cc(N([C@@H](C(=O)NC(CC(C)(C)C)(C)C)c2cc(OC)ccc2)C(=O)[C@H](CCCC)CC)ccc1	0
Decoy714	Fc1cc(ccc1)-c1[nH]c([nH+]c1)[C@@H]1N(CCCC1)C(=O)C[C@H]1C[C@H](CCC1)C	0
Decoy715	O1c2c(C=C(C(OCC(=O)N3N=C/4[C@@H](CCC\C\4=C/c4occc4)[C@@H]3c3occc3)=O)C1=O)cccc2	0
Decoy716	O(CC)c1ccc(NC2=Nc3c(N4C2=Nc2n(nc(c2[C@H]4c2ccc(cc2)C(OC)=O)C)-c2ccccc2)cccc3)cc1	0
Decoy717	O=C(Nc1ccccc1)C=1[C@H](N2NC=C(C2=[NH+]C=1C)C(=O)Nc1ccccc1)CC(C)C	0
Decoy718	O(c1ccc(cc1OC)[C@H]([NH2+]Cc1cc(O)ccc1)C)C1CCCC1	0
Decoy719	O=C1Nc2cc(ccc2N1)[C@@H](NC(=O)c1ccccc1NC(=O)NC(C)C)C	0
Decoy720	O(C)c1ccc(cc1)[C@@H]1[NH+](CCC[NH2+]C1)C	0

Table S5. The detailed performance of 24 single classification models for the training set and test set using different combinational of molecular properties.

NO	Model	Descriptors	Training set (5-fold cross validation)				Test set			
			TP	FN	FP	TN	TP	FN	FP	TN
1	NN-a1	12	139	61	27	773	41	11	8	200
2	NN-b1	23	151	49	36	764	46	6	3	205
3	NN-c1*	26	155	45	36	764	48	4	4	204
4	kNN-a1	12	161	39	71	729	51	1	11	197

5	kNN-b1	23	170	30	66	734	52	0	21	187
6	kNN-c1*	26	174	26	65	735	52	0	14	194
7	CT-a1	12	132	68	83	717	43	9	14	194
8	CT-b1	23	140	60	78	722	48	4	15	193
9	CT-c1*	26	147	53	82	718	47	5	14	194
10	RF-a1	12	83	117	23	777	28	24	3	205
11	RF-b1	23	123	77	22	778	47	5	5	203
12	RF-c1*	26	138	62	41	759	47	5	5	203
13	NN-a2	12	73	67	23	537	29	11	5	155
14	NN-b2*	26	108	32	14	546	35	5	4	156
15	NN-c2	24	100	40	19	541	37	3	2	158
16	kNN-a2	12	100	40	48	512	38	2	9	151
17	kNN-b2*	26	120	20	38	522	40	0	10	150
18	kNN-c2	24	116	24	43	517	40	0	4	156
19	CT-a2	12	85	55	63	497	36	4	18	142
20	CT-b2*	26	101	39	38	522	36	4	14	146
21	CT-c2	24	109	31	55	505	38	2	18	142
22	RF-a2	12	52	88	20	540	21	19	3	157
23	RF-b2*	26	108	32	30	530	36	4	8	152
24	RF-c2	24	99	41	26	534	34	6	7	153

1-12: neuroprotective models against glutamate induced neurotoxicity (NGN models); 13-24：neuroprotective models against H2O2 induced neurotoxicity (NHN models); a: models built by DS_2D descriptors; b: models built by MOE_2D descriptors; c: models built by DS_MOE 2D descriptors

Table S6. The detailed performance of the 26 Bayesian classification models for the training set and test set using different combinational of output probabilities and fingerprints.

NO	Model	Training set(5-fold cross validation)				Test set			
		TP	FN	FP	TN	TP	FN	FP	TN
1	NB	175	25	36	764	40	0	0	160
2	NB+ECFP4	188	12	11	789	40	0	6	154
3	NB+ECFP6	190	10	2	798	40	0	6	154
4	NB+EPFP4	185	15	48	752	37	3	15	145

5	NB+EPFP6	193	7	54	746	39	1	14	146
6	NB+FCFP4	179	21	9	791	40	0	5	155
7	NB+FCFP6	194	6	21	779	40	0	2	158
8	NB+FPFP4	188	12	40	760	39	1	16	144
9	NB+FPFP6	194	6	30	770	39	1	13	147
10	NB+LCFP4	192	8	18	782	40	0	4	156
11	NB+LCFP6	193	7	15	785	40	0	4	156
12	NB+LPFP4	197	3	6	794	40	0	10	150
13	NB+LPFP6	196	4	4	796	40	0	7	153
14	NB	118	22	14	546	40	0	0	160
15	NB+ECFP4	131	9	2	558	40	0	6	154
16	NB+ECFP6	130	10	0	560	40	0	6	154
17	NB+EPFP4	130	10	41	519	37	3	15	145
18	NB+EPFP6	135	5	39	521	39	1	14	146
19	NB+FCFP4	139	1	42	518	40	0	5	155
20	NB+FCFP6	132	8	5	555	40	0	2	158
21	NB+FPFP4	136	4	65	495	39	1	16	144
22	NB+FPFP6	128	12	17	543	39	1	13	147
23	NB+LCFP4	138	2	11	549	40	0	4	156
24	NB+LCFP6	138	2	8	552	40	0	4	156
25	NB+LPFP4	138	2	20	540	40	0	10	150
26	NB+LPFP6	136	4	8	552	40	0	7	153

1-13: combined naïve Bayesian models for neuroprotection against glutamate-induced neurotoxicity; 14-26: combined NB models for neuroprotection against H_2O_2-induced neurotoxicity

Table S7. Structures of the 70 virtual hits (in SMILE format) for neuroprotective assay.

Number	Cluster	Structure
J10216*	9	O1CC2C(COC2c2cc3OCOc3cc2)C1c1cc2OCOc2cc1
J10233*	14	O1C(C)C(O)C(OC)C(O)C1OC1CC2CCC3C(CCC4(C)C(CCC34O)C3=CC(OC3)=O)C2(CC1)C
J10244	13	O(C(=O)C)C1CCC2(C(CCC34C2C(OC(=O)C)CC(C3)C(C4)=C)C1(C)C)C
J11759	14	OC1C2=CC(O)CCC2(C2C(C3CCC(C(CCC(C(C)C)CC)C)C3(CC2)C)C1)C
J11762*	2	O1c2c(C(=O)C(=C1c1ccc(O)cc1)c1c3OC(CC(=O)c3c(O)cc1O)c1ccc(O)cc1)c(O)cc(O)c2
J11788	12	O1C2C(OC(=O)c3cc(O)c(O)c4oc5c(c(cc(O)c5O)C(OC2)=O)c34)C(O)C(O)C1Oc

		1ccccc1CO
J12115	12	O1C(C(=O)[O-])C(O)C(O)C(O)C1Oc1cc2OC(=CC(=O)c2c(O)c1O)c1ccc(O)cc1
J12129	11	O1C(CO)C(O)C(O)C(O)C1Oc1c2OC(=O)C=Cc2ccc1O
J12144	2	O1c2c(C(=O)C(OC3OCC(O)C(O)C3O)=C1c1cc(O)c(O)cc1)c(O)cc(O)c2
J12146*	2	O1C(CO)C(O)C(O)C1OC1=C(Oc2c(C1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
J14153	2	O1C(COc2cc(cc(O)c2O)C=2Oc3c(C(=O)C=2O)c(O)cc(O)c3)C(O)C(O)C1O
J14156*	2	O1c2c(C(=O)C(OC[C@H]3O[C@@H](O)[C@H](O)[C@@H](O)[C@@H]3O)=C1c1cc(O)c(O)cc1)c(O)cc(O)c2
J14157	11	O1C(COc2c3OC(=O)C=Cc3cc(OC)c2O)C(O)C(O)C(O)C1O
J14171	12	O1C(CO)C(O)C(O)C(O)C1Oc1cc(O)cc(O)c1C(=O)CCc1ccc(O)cc1
J14572*	17	O1c2c(OC1)c(OC)cc(C(=O)N1CC[NH+](CC1)Cc1c3c(cccc3)c(OC)cc1)c2-c1c2OCOc2c(OC)cc1C(OC)=O
J14576	17	O1c2c(OC1)c(OC)cc(C(=O)N1CC[NH+](CC1)Cc1cc(OC)c(OC)c(OC)c1)c2-c1c2OCOc2c(OC)cc1C(OC)=O
J14581*	17	O1c2c(OC1)c(OC)cc(C(=O)N1CC[NH+](CC1)Cc1cc(OC)c(OC)cc1)c2-c1c2OCOc2c(OC)cc1C(OCC)=O
J14590*	17	O1c2c(OC1)c(OC)cc(C(=O)N1CC[NH+](CC1)Cc1cc(Oc3ccccc3)ccc1)c2-c1c2OCOc2c(OC)cc1C(OCC)=O
J14591*	17	O1c2c(OC1)c(OC)cc(C(=O)N1CC[NH+](CC1)C\C=C\c1ccccc1)c2-c1c2OCOc2c(OC)cc1C(OCC)=O
J14593*	17	O1c2c(OC1)c(OC)cc(C(=O)N1CC[NH+](CC1)Cc1cc(OC)c(OC)cc1)c2-c1c2OCOc2c(OC)cc1C(OCCC)=O
J14599	17	O1c2c(OC1)c(OC)cc(C(=O)N1CC[NH+](CC1)Cc1ccc(OC)cc1)c2-c1c2OCOc2c(OC)cc1C(OCCC)=O
J14600	17	O1c2c(OC1)c(OC)cc(C(=O)N1CC[NH+](CC1)Cc1cc(OC)c(OC)c(OC)c1)c2-c1c2OCOc2c(OC)cc1C(OCCC)=O
J14656	12	O1c2c(c(O)c(OC)c(O)c2OC)C(=O)C=C1c1ccc(OC)cc1
J14658	12	O1C(C(O)C(OC(=O)C)C(O)C1CO)c1c2OC(=CC(=O)c2c(O)cc1O)c1ccc(O)cc1
J14664	2	O1C(C)C(O)C(O)C(O)C1OC1=C(Oc2c(C1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
J14691*	13	O(C(=O)\C=C\c1cc(O)c(O)cc1)C1CCC2(C(CCC3(C2CCC2(C4CC(CCC4(CC=C23)C(=O)[O-])C)C)C)C1(C)C)C
J14699	11	O1C(CO)C(O)C(O)C(O)C1Oc1cc2c-3c(OC(=O)c4cc(O)c(OC)c(OC2=O)c-34)c1O
J16037	14	O1C(C)C(O)C(OC)C(O)C1OC1CC2=CCC3C(CCC=4C5C(OC3=O)COC5(OC=4

		)C)C2(CC1)C
J16040	12	O1CC(O)C(O)C(O)C1Oc1cc(cc(O)c1)\C=C\c1ccc(O)cc1
J16048	2	O1c2c(CC(OC(=O)c3cc(O)c(O)c(O)c3)C1c1cc(O)c(O)cc1)c(O)cc(O)c2
J18461	6	O=C(CC[NH+](C)C)c1ccc(cc1)-c1ccc(cc1)C(=O)CC[NH+](C)C
J18803	13	FC(F)(F)c1cc(NC=2n3ncc(c3N=C(C=2)COCC[NH+]2CCNCC2)C#N)ccc1
J18811*	15	Fc1ccc(NC=2n3ncc(c3N=C(C=2)COCC[NH+]2CCNCC2)C#N)cc1C(F)(F)F
J18836*	7	O(CC1=Nc2n(ncc2C#N)C(Nc2cc(ccc2)C)=C1)CC[NH+]1CCNCC1
J18842*	7	Fc1ccc(NC=2n3ncc(c3N=C(C=2)COCC[NH+]2CCNCC2)C#N)cc1
J18848	7	Fc1ccccc1NC=1n2ncc(c2N=C(C=1)COCC[NH+]1CCNCC1)C#N
J18854	11	Clc1cc(NC=2n3ncc(c3N=C(C=2)COCC[NH+]2CCNCC2)C#N)ccc1
J18879*	6	O1CC[NH+](CC1)CC1=Nc2n(ncc2C#N)C(Nc2cc3OCOc3cc2)=C1
J18911	6	O(C)c1ccc(cc1)CNC=1n2ncc(c2N=C(C=1)C[NH+]1CCCC1)C#N
J27111	4	O1c2c(c(O)c(O)c(O)c2CN2CC[NH+](CC2)CCO)C(=O)C=C1c1ccccc1
J27114*	4	O1c2c(c(O)c(O)c(O)c2C[NH+]2CCCC2)C(=O)C=C1c1ccccc1
J27115*	4	O1c2c(c(O)c(O)c(O)c2C[NH+]2CC(CCC2)C)C(=O)C=C1c1ccccc1
J27118*	4	O1c2c(c(O)c(O)c(O)c2CN2CC[NH+](CC2)Cc2ccccc2)C(=O)C=C1c1ccccc1
J27139	8	O1C=C(C(=O)c2c1cc(OCC[NH+]1CCCCC1)cc2)c1ccc(OC)cc1
J27140	8	O1CC[NH+](CC1)CCOc1cc(O)c2c(OC=C(C2=O)c2ccc(OC)cc2)c1
J27143	8	O1C=C(C(=O)c2c1cc(OCC[NH+]1CCC(O)CC1)cc2)c1ccc(OC)cc1
J27151*	4	O1c2c(C(=O)C=C1c1cc(O)c(O)cc1)c(O)cc(O)c2C[NH+]1CCC(CC1)CO
J27152*	4	O1c2c(C(=O)C=C1c1cc(O)c(O)cc1)c(O)cc(O)c2C[NH+]1CCOCC1
J27153*	4	O1c2c(C(=O)C=C1c1cc(O)c(O)cc1)c(O)cc(O)c2CN1CC[NH+](CC1)C
J27155	4	O1c2c(C(=O)C=C1c1cc(O)c(O)cc1)c(O)cc(O)c2C[NH+]1CCCCC1C
J27162	4	O1c2c(C(=O)C=C1c1ccc(O)cc1)c(O)cc(O)c2CN1CC[NH+](CC1)Cc1ccccc1
J27166	8	O1C=C(C(=O)c2c1c(CN1CC[NH+](CC1)Cc1ccccc1)c(O)cc2O)c1ccc(O)cc1
J27167*	8	O1C=C(C(=O)c2c1c(CN1CC[NH+](CC1)CCO)c(O)cc2O)c1ccc(O)cc1
J27197	8	O1CC([NH+](Cc2c3OC=C(C(=O)c3ccc2O)c2ccc(OC)cc2)C(C1)C)C
J27198*	8	O1C=C(C(=O)c2c1c(C[NH+]1CCC(CC1)CO)c(O)cc2)c1ccc(OC)cc1
J27200	8	O1C=C(C(=O)c2c1c(C[NH+]1CCC(CC1)Cc1ccccc1)c(O)cc2)c1ccc(OC)cc1
J27201	8	O1C=C(C(=O)c2c1c(C[NH+]1CCCCC1C)c(O)cc2)c1ccc(OC)cc1
J27203	8	O1C=C(C(=O)c2c1c(CN1CC[NH+](CC1)Cc1ccccc1)c(O)cc2)c1ccc(OC)cc1
J27706*	9	O1c2c(OC1)cc1CC[N+]3(C(Cc4c(C3)c(OC)c(OC)cc4)c1c2)CC(OCC)=O
J27709*	9	O1c2c(OC1)cc1CC[N+]3(C(Cc4c(C3)c(OC)c(OC)cc4)c1c2)Cc1ccc(cc1)C(OC)=O

J27724	9	O(C)c1c2c(CC3[N+](C2)(CCc2cc(OC)c(OC)cc23)Cc2ccc(cc2)C(OC)=O)ccc1OC
J27727	9	O(C)c1c2c(CC3[N+](C2)(CCc2cc(OC)c(OC)cc23)CCCC(OCC)=O)ccc1OC
J32886	15	O1c2c(OC1)c(OC(=O)\C=C\c1ccccc1)cc(C(OC)=O)c2-c1c2OCOc2c(OC)cc1C(OC)=O
J32899*	17	O1c2c(OC1)c(OC)cc(\C=C\C(=O)CCCCC[NH3+])c2-c1c2OCOc2c(OC)cc1\C=C\C(=O)CCCCC[NH3+]
J32900	17	O1c2c(OC1)c(OC)cc(C(=O)CCCCC[NH3+])c2-c1c2OCOc2c(OC)cc1C(=O)CCCCC[NH3+]
J39065	16	O1c2c(OC1)cc-1c(CC[n+]3c-1cc1c(c3)c(OC(=O)\C=C\c3ccccc3)c(OC)cc1)c2
J39067	16	O1c2c(OC1)cc-1c(CC[n+]3c-1cc1c(c3)c(OC(=O)c3ccccc3OC(=O)C)c(OC)cc1)c2
J39068	16	O1c2c(OC1)cc-1c(CC[n+]3c-1cc1c(c3)c(OC(=O)\C=C\c3cc(OC)c(OC(=O)C)cc3)c(OC)cc1)c2
J39069	16	O1c2c(OC1)cc-1c(CC[n+]3c-1cc1c(c3)c(OCc3nc(C)c(nc3C)C)c(OC)cc1)c2
J100313*	19	O(CC(C)C)c1cc(O)c2c(c1)C(=O)c1c(C2=O)c(O)cc(c1)C

*represented that the compound showed neuroprotective activity against glutamate-induced and H_2O_2-induced neurotoxicity simultaneously in the preliminary assay.

Table S8. The preliminary assay result for 70 virtual hits on monosodium glutamate or H_2O_2-induced neurotoxicity on PC12 Cell.

Number	H_2O_2 (300 μM)	Monosodium glutamate (40mM)
J10216*	101.97	116.13
J10233*	61.26	83.58
J10244	3.18	<0
J11759	5.84	<0
J11762*	122.07	114.13
J11788	24.83	30.19
J12115	33.61	39.77

J12129	16.13	13.69
J12144	13.64	<0
J12146*	95.11	84.65
J14153	31.76	13.13
J14156*	66.14	50.05
J14157	<0	7.30
J14171	<0	22.95
J14572*	127.88	91.33
J14576	12.84	<0
J14581*	52.76	67.77
J14590*	57.66	87.02
J14591*	96.39	97.59
J14593*	85.26	63.80
J14599	25.21	<0
J14600	23.77	<0
J14691*	112.56	50.61
J14699	2.08	<0
J16037	5.20	<0
J16040	1.28	<0
J16048	15.20	1.82
J18461	6.76	<0
J18803	32.06	44.48
J18811*	73.73	95.00
J18854	32.82	26.70
J18836*	88.01	80.57
J18842*	105.99	69.10
J18848	28.41	<0
J18879*	69.09	91.35
J18911	38.92	26.16
J27111	34.03	26.77
J27114*	92.64	108.19
J27115*	81.28	98.16
J27118*	82.46	87.76
J27139	21.66	<0

J27140	15.97	2.18
J27143	13.18	<0
J27151*	124.71	96.18
J27152*	93.63	64.09
J27153*	115.35	89.62
J27155*	129.36	92.22
J27162	10.69	<0
J27166	<0	14.24
J27167*	59.14	69.31
J27197	31.23	40.15
J27198*	94.49	54.33
J27200	8.24	<0
J27201	35.59	4.56
J27203	20.06	19.58
J27706*	80.02	59.98
J27709*	67.51	86.47
J27724	15.46	<0
J27727	48.00	6.31
J32886	6.82	41.24
J32899*	110.32	58.82
J32900	30.43	19.38
J39065	5.88	45.56
J39067	0.25	14.87
J39068	36.77	28.78
J39069	<0	42.34
J100313*	67.72	89.49

*represented that the compound showed neuroprotective activity against glutamate-induced and H_2O2-induced neurotoxicity simultaneously in the preliminary assay.

The data (cell damage inhibition rate, measured by MTT assay) were expressed as the following formula.

$$\text{cell damage inhibition rate}=\frac{(\text{treatment group OD570 - model group OD570})}{(\text{control group OD570 - model group OD570})}\times 100\%$$