Supplementary file 1

Platinum(IV) compounds as potential drugs: a quantitative structure-activity relationship study

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Table S1. List of molecules constituting SARS-COV training set.

ChEMBL ID	Smiles	Relation	IC_{50}	Units	pIC_{50}
CHEMBL222234	O=C(Oc1cncc(Br)c1)c1ccco1	'='	50	nM	7.301
CHEMBL222840	O=C(Oc1cncc(Cl)c1)c1ccco1	'='	60	nM	7.222
CHEMBL222769	O=C(Oc1cncc(Cl)c1)c1ccc(-c2ccc(Cl)cc2)o1	'='	63	nM	7.201
CHEMBL225515	O=C(Oc1cncc(Cl)c1)c1cc2ccccc2[nH]1	'='	65	nM	7.187
CHEMBL222893	O=C(Oc1cncc(Cl)c1)c1cc2ccccc2s1	'='	95	nM	7.022
CHEMBL426898	O=C(Oc1cncc(Cl)c1)c1cc2ccccc2o1	'='	170	nM	6.770
CHEMBL2441741	CC(C)C[C@H](NC(=O)[C@H](Cc1cccc2ccccc12)NC(=O)OCc1ccccc1)C(=O)N[C@H](C=O)C[C@@H]1CCNC1=O	'='	230	nM	6.638
CHEMBL222628	O=C(Oc1cncc(Cl)c1)c1cscn1	'='	270	nM	6.569
CHEMBL212218	Cc1cc(S(=O)(=O)c2c([N+](=O)[O-])cc(C(F)(F)F)cc2[N+](=O)[O-])c(Cl)cc1Cl	'='	300	nM	6.523
CHEMBL222735	COc1cccc(C(=O)Oc2cncc(Cl)c2)c1	'='	340	nM	6.469
CHEMBL221366	O=C(Oc1cccnc1)c1cccs1	'='	500	nM	6.301
CHEMBL2441745	CC(C)C[C@H](NC(=O)[C@H](Cc1cccc2ccccc12)NC(=O)OCc1ccccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	'='	610	nM	6.215
CHEMBL212454	O=C(Oc1ccc(S(=O)(=O)c2ccc(OC(=O)C(Cl)=C(Cl)Cl)cc2)cc1)C(Cl)=C(Cl)Cl	'='	900	nM	6.046
CHEMBL190743	O=C1C(=O)N(Cc2cc3ccccc3s2)c2ccc(I)cc21	'='	950	nM	6.022
CHEMBL365134	O=C1C(=O)N(Cc2cc3ccccc3s2)c2c(Br)cccc21	'='	980	nM	6.009
CHEMBL3099526	CC1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3C)CC1	'='	1040	nM	5.983
CHEMBL3099541	CC1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3)CC1	'='	1180	nM	5.928
CHEMBL3105073	S=C(NCc1cccnc1)SCc1cc(Cl)sc1Cl	'='	160	nM	5.916
CHEMBL3099527	CC1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccccc2)CC1	'='	1690	nM	5.772
CHEMBL187717	O=C1C(=O)N(Cc2cc3ccccc3s2)c2c1cccc2[N+](=O)[O-]	'='	2000	nM	5.699

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CHEMBL4788119	CCN1/C(=C\C=C\C2=C/C(=C/c3sc4ccccc4[n+]3CC)CC(C)C2)Sc2ccccc21	'='	2000	nM	5.699
CHEMBL4214066	CC(C)C[C@H](NC(=O)OC1CCN(C(=O)OC(C)(C)C)CC1)C(=O)N[C@H](C=O)C[C@@H]1CCNC1=O	'='	2100	nM	5.678
CHEMBL3099542	CC1CCCCN1S(=O)(=O)c1ccc2c(c1)C(=O)C(=O)N2	'='	2250	nM	5.648
CHEMBL541163	CCN1/C(=C\C=C\c2sc3ccc(-c4nc5ccccc5s4)cc3[n+]2CC)Sc2ccc(-c3nc4ccccc4s3)cc21.[Cl-]	'='	2500	nM	5.602
CHEMBL1092796	CC1=CC[C@]2(C)CC[C@]3(C)C4=CC=C5C(=CC(=O)C(O)=C5C)[C@]4(C)CC[C@@]3(C)[C@@H]2C1	'='	2600	nM	5.585
CHEMBL3099529	CC1CC(C)CN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3C)C1	'='	2820	nM	5.550
CHEMBL208732	O=C(CSc1nccc(-c2csc(-c3ccccc3)n2)n1)Nc1cc(Cl)cc(Cl)c1	'='	3000	nM	5.523
CHEMBL379642	O=C(Sc1nnc(C(F)(F)F)[nH]1)c1ccc(C#Cc2ccccc2)o1	'='	3000	nM	5.523
CHEMBL4217568	CCOC(=O)N1CCC(OC(=O)N[C@@H](CC(C)C)C(=O)N[C@H](C=O)C[C@@H]2CCNC2=O)CC1	'='	3200	nM	5.495
CHEMBL540403	CCN1C(c2ccccc2)=C(c2ccccc2)S/C1=C/C=C/c1sc2c3ccccc3ccc2[n+]1CC.[Cl-]	'='	3800	nM	5.420
CHEMBL4214471	CC(C)C[C@H](NC(=O)OC1(Cc2ccccc2)CCN(S(C)(=O)=O)CC1)C(=O)N[C@H](C=O)C[C@@H]1CCNC1=O	'='	3900	nM	5.409
CHEMBL4216101	CCC1(OC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(O)S(=O)(=O)[O-])CCN(C(=O)OC(C)(C)C)CC1.[Na+]	'='	4100	nM	5.387
CHEMBL3099543	CC1CC(C)CN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3)C1	'='	4300	nM	5.367
CHEMBL4208764	CC(C)C[C@H](NC(=O)OC1(Cc2ccccc2)CCN(S(C)(=O)=O)CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(=O)(=O)[O-].[Na+]	'='	4300	nM	5.367
CHEMBL61320	O=C1Nc2ccc(S(=O)(=O)N3CCCCC3)cc2C1=O	'='	4450	nM	5.352
CHEMBL2316337	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OCc1ccccc1)C(C)C)C(=O)N[C@H](C#N)CCC(N)=O	'='	4600	nM	5.337
CHEMBL3099530	CC1CC(C)CN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccccc2)C1	'='	4700	nM	5.328
CHEMBL187598	O=C1C(=O)N(Cc2cc3ccccc3s2)c2ccc(F)cc21	'='	4820	nM	5.317
CHEMBL427404	Cc1noc(NC(=O)c2ccc(-c3cc(C(F)(F)F)nn3C)s2)c1[N+](=O)[O-]	'='	5000	nM	5.301
CHEMBL4208240	CC(C)C[C@H](NC(=O)OC1CCN(C(=O)OC(C)(C)C)CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(=O)(=O)[O-].[Na+]	'='	5100	nM	5.292
CHEMBL4202812	CC(C)C[C@H](NC(=O)OC1(Cc2ccccc2)CCN(C(=O)OC(C)(C)C)CC1)C(=O)N[C@H](C=O)C[C@@H]1CCNC1=O	'='	5200	nM	5.284
CHEMBL479172	CCC(=C\c1sc2c3ccccc3ccc2[n+]1CC)/C=C1/Sc2cc(C)c(C)cc2N1CC	'='	5400	nM	5.268
CHEMBL54804	COC(=O)[C@]1(C)CC[C@]2(C)CC[C@]3(C)C4=CC=C5C(=CC(=O)C(O)=C5C)[C@]4(C)CC[C@@]3(C)[C@@H]2C1	'='	5500	nM	5.260
CHEMBL1277046	N#Cc1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(C(=O)O)cc3)C2=O)cc1	'='	5500	nM	5.260

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CHEMBL4212620	CCC1(OC(=O)N[C@@H](CC(C)C)C(=O)N[C@H](C=O)C[C@@H]2CCNC2=O)CCN(C(=O)OC(C)(C)C)CC1	'='	5500	nM	5.260
CHEMBL3099521	CN1C(=O)C(=O)c2cc(S(=O)(=O)N3CCN(c4ccccn4)CC3)ccc21	'='	5520	nM	5.258
CHEMBL3808427	CC(C)(C)c1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4cc(Cl)ccc4C(=O)O)o3)C2=O)cc1	'='	5800	nM	5.237
CHEMBL213581	Nc1ncc(S(=O)(=O)c2ccc(Cl)cc2)c(N)n1	'='	6000	nM	5.222
CHEMBL3809329	CC(C)c1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4cc(Cl)ccc4C(=O)O)o3)C2=O)cc1	'='	6000	nM	5.222
CHEMBL4203883	CC(C)C[C@H](NC(=O)OC1(Cc2ccccc2)CCN(C(=O)OC(C)(C)C)CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(=O)(=O)[O-].[Na+]	'='	6300	nM	5.201
CHEMBL3809861	O=C(O)c1cccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4ccccc4)o3)C2=O)c1	'='	6400	nM	5.194
CHEMBL558828	CCC(=C\c1sc2cc(C)c(C)cc2[n+]1CC)/C=C1/Sc2cc(/C=C/c3ccccc3)ccc2N1CC.[Cl-]	'='	6600	nM	5.180
CHEMBL3809053	O=C(O)c1cccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4ccccc4)cc3)C2=O)c1	'='	6700	nM	5.174
CHEMBL1277227	O=C(O)c1ccc(/C=C2\C(=O)N(c3ccc(F)cc3)N=C2c2ccccc2)cc1	'='	6800	nM	5.167
CHEMBL187579	Cc1noc(C)c1CN1C(=O)C(=O)c2cc(C#N)ccc21	'='	7200	nM	5.143
CHEMBL515787	CCN1/C(=C\C(=C/c2sc3ccccc3[n+]2CCCS(=O)(=O)[O-])OC)Sc2ccc(OC)cc21	'='	7300	nM	5.137
CHEMBL3818000	CC(=O)N[C@@H](CC(N)=O)C(=O)N[C@@H](CO)C(=O)N[C@H](C(=O)N[C@@H](CO)C(=O)N[C@@H](CCC(N)=O)C(=O)O)[C@@H](C)O	'='	7500	nM	5.125
CHEMBL3818593	CC(=O)N[C@@H](CCC(=O)O)C(=O)N[C@@H](CO)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(N)=O)C(=O)O)[C@@H](C)O	'='	7500	nM	5.125
CHEMBL1651956	C/C=C/C[C@@H](C)[C@@H](O)[C@H]1C(=O)N[C@@H](CC)C(=O)N(C)[C@H](C)C(=O)N(CC)[C@@H](C(C)C)C(=O)N[C@@H](C(C)C)C(=O)N(C)[C@@H](CC(C)C)C(=O)N[C@@H](C)C(=O)N[C@H](C)C(=O)N(C)[C@@H](CC(C)C)C(=O)N(C)[C@@H](CC(C)C)C(=O)N(C)[C@@H](C(C)C)C(=O)N1C	'='	7700	nM	5.114
CHEMBL551131	N#Cc1cccc(COc2cc(O)c3c(=O)c(O)c(-c4ccc(O)c(O)c4)oc3c2)c1	'='	25400	nM	5.082
CHEMBL160	C/C=C/C[C@@H](C)[C@@H](O)[C@H]1C(=O)N[C@@H](CC)C(=O)N(C)CC(=O)N(C)[C@@H](CC(C)C)C(=O)N[C@@H](C(C)C)C(=O)N(C)[C@@H](CC(C)C)C(=O)N[C@@H](C)C(=O)N[C@H](C)C(=O)N(C)[C@@H](CC(C)C)C(=O)N(C)[C@@H](CC(C)C)C(=O)N(C)[C@@H](C(C)C)C(=O)N1C	'>'	8300	nM	5.081
CHEMBL63354	O=c1cc(-c2ccc(O)c(-c3c(O)cc(O)c4c(=O)cc(-c5ccc(O)cc5)oc34)c2)oc2cc(O)cc(O)c12	'='	8300	nM	5.081
CHEMBL1277228	O=C(O)c1ccc(/C=C2\C(=O)N(c3cccc([N+](=O)[O-])c3)N=C2c2ccccc2)cc1	'='	8400	nM	5.076
CHEMBL3105076	Nc1ncnc2[nH]c(C(F)(F)F)nc12	'='	2200	nM	5.068
CHEMBL3809579	CC(C)(C)c1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4ccccc4C(=O)O)o3)C2=O)cc1	'='	8600	nM	5.066

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CHEMBL471187	Oc1cc(O)cc(Oc2c(O)cc(O)c3c2Oc2c(O)cc(O)cc2O3)c1	'='	8800	nM	5.056
CHEMBL4204431	CCOC(=O)N1CCC(OC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(O)S(=O)(=O)[O-])CC1.[Na+]	'='	8800	nM	5.056
CHEMBL550256	O=c1c(O)c(-c2ccc(O)c(O)c2)oc2cc(OCc3ccc(Cl)cc3)cc(O)c12	'='	4100	nM	5.034
CHEMBL188487	O=C1C(=O)N(Cc2ccc(F)cc2Cl)c2ccc(I)cc21	'='	9400	nM	5.027
CHEMBL432519	CC1=C(O)C(=O)C=C2C1=CC=C1[C@@]3(C)CC[C@@]4(C)CC(=O)[C@H](C)C[C@H]4[C@]3(C)CC[C@@]21C	'='	9900	nM	5.004
CHEMBL3099523	CN1C(=O)C(=O)c2cc(S(=O)(=O)N3CCOCC3)ccc21	'='	9910	nM	5.004
CHEMBL212190	Cc1oc(C(C)(C)C)cc1-c1cc(NS(=O)(=O)c2cccs2)[nH]n1	'='	10000	nM	5.000
CHEMBL377150	Cn1nc(-c2ccc(-c3ccnc(SCC(=O)Nc4ccc(Cl)cc4)n3)s2)cc1C(F)(F)F	'='	10000	nM	5.000
CHEMBL478987	CCN1/C(=C\C=c2/s/c(=C\c3sc4ccccc4[n+]3CC)n(CC)c2=O)Sc2ccccc21	'='	10000	nM	5.000
CHEMBL3818400	CC(=O)N[C@@H](CC(=O)O)C(=O)N[C@@H](CO)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(N)=O)C(=O)O)[C@@H](C)O	'='	10000	nM	5.000
CHEMBL3099539	O=C1Nc2ccc(S(=O)(=O)N3CCN(C(=O)c4ccco4)CC3)cc2C1=O	'='	10070	nM	4.997
CHEMBL301982	CC1=C(O)C(=O)C=C2C1=CC=C1[C@@]3(C)CC[C@@]4(C)CC[C@@](C)(C(=O)O)C[C@H]4[C@]3(C)CC[C@@]21C	'='	10300	nM	4.987
CHEMBL518593	C(\C1=C2Sc3ccccc3N2CC1)=C1/CC[n+]2c1sc1ccccc12	'='	10500	nM	4.979
CHEMBL1277135	O=C(O)c1ccc(/C=C2\C(=O)N(c3cccc(Cl)c3)N=C2c2ccccc2)cc1	'='	10800	nM	4.967
CHEMBL210092	CSc1sc(-c2nc(C)cs2)c(C)c1-c1ccnc(SCC(=O)Nc2ccc(Cl)cc2)n1	'='	11000	nM	4.959
CHEMBL365469	O=C1C(=O)N(Cc2cc3ccccc3s2)c2cccc(Cl)c21	'='	11200	nM	4.951
CHEMBL3809506	CC(C)c1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4ccccc4C(=O)O)o3)C2=O)cc1	'='	11700	nM	4.932
CHEMBL3099544	CN1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3C)CC1	'='	11830	nM	4.927
CHEMBL378674	CSc1sc(-c2nc(C)cs2)c(C)c1-c1ccnc(SCC(=O)Nc2ccccc2Cl)n1	'='	12000	nM	4.921
CHEMBL380403	O=[N+]([O-])c1cc(C(F)(F)F)ccc1S(=O)(=O)c1ccc(Cl)cc1	'='	12000	nM	4.921
CHEMBL1276871	COc1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(C(=O)O)cc3)C2=O)cc1	'='	12000	nM	4.921
CHEMBL191575	O=C(Nc1ccc(Cl)cc1)c1ccc(CN2C(=O)C(=O)c3cc(I)ccc32)s1	'='	12570	nM	4.901
CHEMBL484273	O=C1Nc2ccc(S(=O)(=O)N3CCOCC3)cc2C1=O	'='	12660	nM	4.898
CHEMBL211969	Cc1ccc(S(=O)(=O)c2nc(C)c([N+](=O)[O-])c(C)c2C#N)cc1	'='	13000	nM	4.886
CHEMBL212504	Cc1nc(S(=O)(=O)c2ccccc2)c(C#N)c(C)c1[N+](=O)[O-]	'='	13000	nM	4.886

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CHEMBL426082	O=C1C(=O)N(Cc2cc3ccccc3s2)c2ccccc21	'='	13110	nM	4.882
CHEMBL185698	O=C1C(=O)N(CC2COc3ccccc3O2)c2ccc(I)cc21	'='	13500	nM	4.870
CHEMBL508791	Oc1cc(O)cc(Oc2c(O)cc(O)c3c2Oc2c(O)cc(Oc4c(O)cc(Oc5c(O)cc(O)c6c5Oc5c(O)cc(O)cc5O6)cc4O)cc2O3)c1	'='	68100	nM	4.868
CHEMBL1876821	CN(CC(=O)NC1CCCC1)S(=O)(=O)c1cccc(Cl)c1	'>'	200000	nM	4.863
CHEMBL3099524	O=C1C(=O)N(Cc2ccccc2)c2ccc(S(=O)(=O)N3CCOCC3)cc21	'='	13860	nM	4.858
CHEMBL3099547	CN1C(=O)C(=O)c2cc(S(=O)(=O)N3CCN(CCc4ccccc4)CC3)ccc21	'='	13860	nM	4.858
CHEMBL50	O=c1c(O)c(-c2ccc(O)c(O)c2)oc2cc(O)cc(O)c12	'='	23800	nM	4.857
CHEMBL1278125	O=C(O)c1ccc(/C=C2\C(=O)N(c3ccc(Cl)cc3)N=C2c2ccccc2)cc1	'='	13900	nM	4.857
CHEMBL209227	Cc1nc(-c2nc(-c3ccnc(SCC(=O)Nc4ccc(Cl)cc4)n3)cs2)cs1	'='	14000	nM	4.854
CHEMBL3099522	O=C1C(=O)N(Cc2ccccc2)c2ccc(S(=O)(=O)N3CCCCC3)cc21	'='	14000	nM	4.854
CHEMBL208763	O=C(CSc1nccc(-c2cc(-c3ccccc3)no2)n1)Nc1ccc(Cl)cc1	'='	15000	nM	4.824
CHEMBL209667	O=C(CSc1nccc(-c2cc(-c3ccccc3Cl)no2)n1)Nc1ccc(Cl)cc1	'='	15000	nM	4.824
CHEMBL210097	O=C(CSc1nccc(-c2cc(-c3ccc(Cl)cc3Cl)no2)n1)Nc1ccc(C(F)(F)F)cc1	'='	15000	nM	4.824
CHEMBL378700	CSc1[nH]nc(NC(=O)c2cccs2)c1S(=O)(=O)c1ccccc1	'='	15000	nM	4.824
CHEMBL384739	O=[N+]([O-])c1ccc(S(=O)(=O)c2ccc(Cl)cc2)[n+]([O-])c1	'='	15000	nM	4.824
CHEMBL3809926	O=C(O)c1cccc(N2N=C(c3ccccc3)/C(=C/c3ccc(OCc4ccccc4)cc3)C2=O)c1	'='	15700	nM	4.804
CHEMBL212019	CC1(C)CC(=O)c2c(NCc3ccco3)sc(C#N)c2C1	'='	16000	nM	4.796
CHEMBL212240	O=C(O)c1ccc(S(=O)(=O)c2cc(Br)c(O)c(Br)c2)cc1	'='	16000	nM	4.796
CHEMBL215732	CCOC(=O)/C(C#N)=C/Nc1ccc(S(=O)(=O)c2ccc(/N=C/C(C#N)=C(\O)OCC)cc2)cc1	'='	16000	nM	4.796
CHEMBL377253	CC(=O)c1ccccc1S(=O)(=O)c1ccccc1C(=O)O	'='	16000	nM	4.796
CHEMBL551130	O=c1c(O)c(-c2ccc(O)c(O)c2)oc2cc(OCc3cccc(Cl)c3)cc(O)c12	'>'	50000	nM	4.793
CHEMBL3105074	O=C(c1cncc(Br)c1)N1CCN(Cc2ccsc2)CC1	'='	24500	nM	4.789
CHEMBL3810328	O=C(O)c1ccc(Cl)cc1-c1ccc(/C=C2\C(=O)N(c3ccccc3)N=C2c2ccccc2)o1	'='	16400	nM	4.785
CHEMBL370923	O=C1C(=O)N(Cc2ccc(C(=O)N3CCCCC3)s2)c2ccc(I)cc21	'='	17500	nM	4.757
CHEMBL3099528	CC1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccc3ccccc3c2)CC1	'='	17820	nM	4.749
CHEMBL212399	CSc1nn(-c2c([N+](=O)[O-])c(C)nn2C)c(-c2cccs2)c1C#N	'='	18000	nM	4.745
CHEMBL215733	O=S(=O)(Cc1[nH]c(-c2ccc(Cl)s2)c[s+]1)c1cccs1.[Br-]	'='	18000	nM	4.745

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ChEMBL ID	Smiles	Relation	IC_{50}	Units	pIC_{50}
CHEMBL1277944	O=C(O)c1ccc(/C=C2\C(=O)N(c3ccccc3)N=C2c2ccccc2)cc1	'='	18000	nM	4.745
CHEMBL551529	N#Cc1cccc(COc2cc(O)c3c(=O)c(O)c(-c4ccc5c(c4)OCO5)oc3c2)c1	'='	8100	nM	4.730
CHEMBL3809498	N#Cc1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4ccccc4C(=O)O)o3)C2=O)cc1	'='	18700	nM	4.728
CHEMBL151	O=c1cc(-c2ccc(O)c(O)c2)oc2cc(O)cc(O)c12	'='	20000	nM	4.699
CHEMBL375130	Cc1nn(C)c(NCc2ccc(-c3cccs3)s2)c1[N+](=O)[O-]	'='	20000	nM	4.699
CHEMBL3818028	CC(=O)N[C@@H](CC(N)=O)C(=O)N[C@@H](CO)C(=O)N[C@H](C(=O)N[C@@H](CC(=O)O)C(=O)N[C@@H](CCC(N)=O)C(=O)O)[C@@H](C)O	'='	20000	nM	4.699
CHEMBL3808658	O=C(O)c1ccc(Cl)cc1-c1ccc(/C=C2\C(=O)N(c3ccc(F)cc3)N=C2c2ccccc2)o1	'='	20200	nM	4.695
CHEMBL551334	O=c1c(O)c(-c2ccc3c(c2)OCO3)oc2cc(OCc3ccc(Cl)cc3)cc(O)c12	'>'	50000	nM	4.666
CHEMBL1092797	Cc1c(O)c(O)cc2c1CC=C1[C@@]3(C)CC[C@@]4(C)CC[C@@](C)(C(=O)O)C[C@H]4[C@]3(C)CC[C@]12C	'='	21700	nM	4.664
CHEMBL399121	COc1ccc([C@@H]2CC(=O)c3c(O)cc(O)cc3O2)cc1O	'='	60000	nM	4.651
CHEMBL116438	COc1cc(/C=C/C(=O)/C=C(O)/C=C/c2ccc(O)c(OC)c2)ccc1O	'='	23500	nM	4.629
CHEMBL188983	O=C1C(=O)N(C/C=C/c2cc3ccccc3s2)c2ccc(I)cc21	'='	23500	nM	4.629
CHEMBL554041	CCCCC(CC)CNC(=N)NC(=N)NCCCCCCNC(=N)NC(=N)NCC(CC)CCCC.Cl.Cl	'='	17800	nM	4.629
CHEMBL1277136	O=C(O)c1ccc(/C=C2\C(=O)N(c3ccc(Cl)c(Cl)c3)N=C2c2ccccc2)cc1	'='	24300	nM	4.614
CHEMBL1487869	Cn1cnc2cc(NC(=O)c3ccc(Cl)cc3)ccc21	'='	18200	nM	4.603
CHEMBL215397	O=[N+]([O-])c1ccc(S(=O)(=O)c2ccc([N+](=O)[O-])cc2)cc1	'='	25000	nM	4.602
CHEMBL560933	O=c1c(O)c(-c2ccc3c(c2)OCO3)oc2cc(OCc3cccc(Cl)c3)cc(O)c12	'='	15400	nM	4.557
CHEMBL4209146	CC(C)C[C@H](NC(=O)OC1CCN(S(C)(=O)=O)CC1)C(=O)N[C@H](C=O)C[C@@H]1CCNC1=O	'='	28800	nM	4.541
CHEMBL3105075	C(=C/c1ccccc1)\C[N+]1(C/C=C/c2ccccc2)CCN(C(c2ccccc2)c2ccccc2)CC1	'='	28300	nM	4.537
CHEMBL208584	CCCc1cc(O)nc(SCC(=O)Nc2ccc(Cl)cc2)n1	'='	30000	nM	4.523
CHEMBL3809059	COc1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4ccccc4C(=O)O)o3)C2=O)cc1	'='	30700	nM	4.513
CHEMBL1478361	COc1ccc(N(CC(=O)NCc2ccco2)S(C)(=O)=O)cc1	'='	61900	nM	4.501
CHEMBL3099536	O=C1Nc2ccc(S(=O)(=O)N3CCN(Cc4cccc(Cl)c4)CC3)cc2C1=O	'='	31710	nM	4.499
CHEMBL377324	COc1cc(O)c2c(=O)cc(-c3ccc(OC)c(-c4c(O)cc(O)c5c(=O)cc(-c6ccc(O)cc6)oc45)c3)oc2c1	'='	32000	nM	4.495
CHEMBL378342	CCOC(=O)C(=CNc1ccc(S(=O)(=O)c2ccc(/N=C/C(C(=O)OCC)=C(\O)OCC)cc2)cc1)C(=O)OCC	'='	32000	nM	4.495
CHEMBL3099537	COc1cc(CN2CCN(S(=O)(=O)c3ccc4c(c3)C(=O)C(=O)N4)CC2)cc(OC)c1OC	'='	32080	nM	4.494
CHEMBL1906723	COc1ccc(C(=O)Cn2c(NCCO)nc3ccccc32)cc1	'='	40900	nM	4.464

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ChEMBL ID	Smiles	Relation	IC_{50}	Units	pIC_{50}
CHEMBL3099538	O=C1Nc2ccc(S(=O)(=O)N3CCN(CCc4ccccc4)CC3)cc2C1=O	'='	34910	nM	4.457
CHEMBL3810325	O=C(O)c1ccccc1-c1ccc(/C=C2\C(=O)N(c3ccc(F)cc3)N=C2c2ccccc2)o1	'='	37500	nM	4.426
CHEMBL208908	COc1ccc(-c2cc(=O)c3c(O)cc(O)c(-c4cc(-c5cc(=O)c6c(O)cc(OC)cc6o5)ccc4OC)c3o2)cc1	'='	38400	nM	4.416
CHEMBL1350514	Cc1ccc(C(=O)N/C(=C\c2ccc(-c3cccc([N+](=O)[O-])c3)o2)C(=O)NCCCN(C)C)cc1	'='	38570	nM	4.414
CHEMBL2391423	Oc1cc(O)cc(Oc2c(Oc3c(O)cc(O)cc3O)cc(O)c3c2Oc2c(O)cc(O)cc2O3)c1	'='	13300	nM	4.413
CHEMBL2316336	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)[C@H](CO)NC(=O)[C@@H](NC(=O)OCc1ccccc1)[C@@H](C)O)C(C)C)C(=O)N[C@H](C#N)CCC(N)=O	'='	39000	nM	4.409
CHEMBL3099525	O=C1C(=O)N(Cc2ccc3ccccc3c2)c2ccc(S(=O)(=O)N3CCOCC3)cc21	'='	39870	nM	4.399
CHEMBL210497	COc1cccc(-c2nc(SCC(=O)Nc3ccc(S(N)(=O)=O)cc3)nc(O)c2C#N)c1	'='	40000	nM	4.398
CHEMBL210612	CC(C)c1ccc(NC(=O)CSc2nccc(-c3cccs3)n2)cc1	'='	40000	nM	4.398
CHEMBL214372	O=C(Cc1nccs1)c1nccs1	'='	40000	nM	4.398
CHEMBL3810361	O=C(O)c1ccccc1-c1ccc(/C=C2\C(=O)N(c3ccccc3)N=C2c2ccccc2)o1	'='	41200	nM	4.385
CHEMBL1315054	Cc1ccc(C(=O)N/C(=C\c2ccc(-c3ccccc3[N+](=O)[O-])o2)C(=O)NCCCN(C)C)cc1	'='	41390	nM	4.383
CHEMBL1277047	O=C(O)c1ccc(/C=C2\C(=O)N(c3ccc(OC(F)(F)F)cc3)N=C2c2ccccc2)cc1	'='	42000	nM	4.377
CHEMBL4213159	CC(C)C[C@H](NC(=O)OC1CCN(S(C)(=O)=O)CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(=O)(=O)[O-].[Na+]	'='	42100	nM	4.376
CHEMBL3808795	O=C(O)c1cccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4cc(Cl)ccc4C(=O)O)o3)C2=O)c1	'='	44700	nM	4.350
CHEMBL194398	CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@@H](CC(=O)[C@@H](NC(=O)c1cc(C)on1)C(C)C)Cc1ccccc1	'='	45000	nM	4.347
CHEMBL380470	COc1ccc(NC(=O)CSc2nc(O)cc(-c3ccccc3)n2)cc1OC	'='	45000	nM	4.347
CHEMBL2316338	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OC(C)(C)C)C(C)C)C(=O)N[C@H](C#N)CCC(N)=O	'='	49000	nM	4.310
CHEMBL2316339	Cc1cc(C(=O)N[C@@H](C)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@H](C#N)CCC(N)=O)C(C)C)no1	'='	49000	nM	4.310
CHEMBL197308	CC(C)c1cc2c(cc1O)[C@@]1(C)CCCC(C)(C)[C@@H]1CC2	'='	49600	nM	4.305
CHEMBL549646	O=c1cc(CNCc2ccc(Cl)cc2)oc2ccc(O)c(O)c12	'>'	50000	nM	4.301
CHEMBL556501	O=c1c(O)c(-c2ccc3c(c2)OCO3)oc2cc(O)cc(O)c12	'>'	50000	nM	4.301
CHEMBL560136	O=c1cc(CNCc2cccc(Cl)c2)oc2ccc(O)c(O)c12	'>'	50000	nM	4.301
CHEMBL560392	N#Cc1cccc(CNCc2cc(=O)c3c(O)c(O)ccc3o2)c1	'>'	50000	nM	4.301
CHEMBL3808558	O=C(O)c1cccc(N2N=C(C(F)(F)F)/C(=C\c3ccc(-c4ccccc4C(=O)O)o3)C2=O)c1	'>'	50000	nM	4.301

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ChEMBL ID	Smiles	Relation	IC_{50}	Units	pIC_{50}
CHEMBL3809159	CC1=NN(c2cccc(C(=O)O)c2)C(=O)/C1=C\c1ccc(-c2ccccc2)o1	'>'	50000	nM	4.301
CHEMBL3809833	O=C(O)c1cccc(N2N=C(c3ccccc3)/C(=C/c3ccco3)C2=O)c1	'>'	50000	nM	4.301
CHEMBL3810010	CC1=NN(c2ccccc2)C(=O)/C1=C\c1ccc(-c2cc(Cl)ccc2C(=O)O)o1	'>'	50000	nM	4.301
CHEMBL3810058	O=C1/C(=C\c2ccc(-c3ccccc3)o2)C(c2ccccc2)=NN1c1ccccc1	'>'	50000	nM	4.301
CHEMBL3810109	O=C(O)c1cccc(N2N=C(C(F)(F)F)/C(=C/c3ccc(-c4cc(Cl)ccc4C(=O)O)o3)C2=O)c1	'>'	50000	nM	4.301
CHEMBL3810366	CC1=NN(c2cccc(C(=O)O)c2)C(=O)/C1=C\c1ccc(-c2cc(Cl)ccc2C(=O)O)o1	'>'	50000	nM	4.301
CHEMBL3818761	CC(=O)N[C@@H](Cc1cnc[nH]1)C(=O)N[C@@H](CO)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(N)=O)C(=O)O)[C@@H](C)O	'>'	50000	nM	4.301
CHEMBL3099540	O=C1Nc2ccc(S(=O)(=O)N3CCN(c4ccccn4)CC3)cc2C1=O	'='	51330	nM	4.290
CHEMBL510508	Oc1cc(O)cc(Oc2c(O)cc(O)c3c2Oc2c(O)cc4oc5c(Oc6cc(O)cc(O)c6)c(O)cc(O)c5c4c2O3)c1	'='	16700	nM	4.268
CHEMBL1774322	Nc1nc(CSc2nnc(-c3cccc4ccccc34)n2-c2ccccc2)cs1	'='	58350	nM	4.234
CHEMBL210487	CCC(Sc1nc(O)c(C#N)c(-c2cccc(OC)c2)n1)C(=O)Nc1ccc(C(C)=O)cc1	'='	60000	nM	4.222
CHEMBL210632	COc1cccc(-c2nc(SCC(=O)Nc3ccc(C(C)=O)cc3)nc(O)c2C#N)c1	'='	60000	nM	4.222
CHEMBL1774323	COc1cc(C2C(C(=O)c3ccc(OCC(C)C)cc3C)=C(O)C(=O)N2CCN(C)C)ccc1O	'='	62790	nM	4.202
CHEMBL459393	Oc1cc(O)c(Oc2cc(O)cc(O)c2Oc2cc(O)cc(O)c2-c2c(O)cc(O)cc2O)c(O)c1	'='	22500	nM	4.200
CHEMBL3099545	CN1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccccc2)CC1	'='	67200	nM	4.173
CHEMBL456228	Oc1cc(O)cc(Oc2c(O)cc(O)c3c2Oc2c(O)cc(Oc4c(O)cc(O)cc4O)cc2O3)c1	'='	112000	nM	4.163
CHEMBL1488602	COCCOCCn1c(CCCO)nc2ccccc21	'='	186000	nM	4.161
CHEMBL196635	CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC=C(C)C)CC(=O)[C@@H](NC(=O)c1cc(C)on1)C(C)C	'='	70000	nM	4.155
CHEMBL378188	COc1ccc(-c2cc(=O)c3c(O)cc(O)cc3o2)cc1-c1c(O)cc(O)c2c(=O)cc(-c3ccc(O)cc3)oc12	'='	72300	nM	4.141
CHEMBL238217	CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC=C(C)C)CC(=O)[C@@H](NC(=O)[C@H](CO)NC(=O)OC(C)(C)C)C(C)C	'='	75000	nM	4.125
CHEMBL3099533	CN1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3)CC1	'='	76740	nM	4.115
CHEMBL1774325	COc1cc(/C=N/NC(=O)/C(=C\c2ccccc2)NC(=O)c2ccccc2)cc(OC)c1O	'='	77090	nM	4.113
CHEMBL3105072	Nc1ccc(F)c(S(=O)(=O)Nc2cccc(C(F)(F)F)c2)c1	'='	29800	nM	4.112
CHEMBL3105071	COc1ccccc1CNC(=O)[C@H](C)NS(=O)(=O)c1ccccc1	'='	29900	nM	4.112
CHEMBL3099546	CN1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccc3ccccc3c2)CC1	'='	82910	nM	4.081

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ChEMBL ID	Smiles	Relation	IC_{50}	Units	pIC_{50}
CHEMBL1774326	O=C(CSc1ncnc2c1sc1nc(N3CCOCC3)c3c(c12)CCCC3)NCc1ccco1	'='	90720	nM	4.042
CHEMBL203308	NC(=O)c1cn([C@@H]2C=C(CO)[C@@H](O)[C@H]2O)nn1	'>'	100000	nM	4.000
CHEMBL204499	NC(=O)c1ncn([C@@H]2C=C(CO)[C@@H](O)[C@H]2O)n1	'>'	100000	nM	4.000
CHEMBL207207	Cc1cc(O)nc(SCC(=O)Nc2cc(Cl)ccc2Oc2ccccc2)n1	'='	1.00E+13	nM	4.000
CHEMBL224363	O=c1[nH]cc([C@@H]2C=C(CO)[C@@H](O)[C@H]2O)c(=O)[nH]1	'>'	100000	nM	4.000
CHEMBL225045	Nc1nc(O)c2[nH]cc([C@@H]3C=C(CO)[C@@H](O)[C@H]3O)c2n1	'>'	100000	nM	4.000
CHEMBL225046	Nc1nc(=O)c([C@@H]2C=C(CO)[C@@H](O)[C@H]2O)c[nH]1	'>'	100000	nM	4.000
CHEMBL235873	CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)[C@H](CO)NC(=O)OC(C)(C)C)C(C)C	'='	100000	nM	4.000
CHEMBL381539	NC(=O)c1cn([C@@H]2C=C(CO)[C@@H](O)[C@H]2O)cn1	'>'	100000	nM	4.000
CHEMBL397154	CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)[C@H](CO)NC(=O)OC(C)(C)C)C(C)C	'='	100000	nM	4.000
CHEMBL3099534	O=C1Nc2ccc(S(=O)(=O)N3CCN(c4ccc(F)cc4)CC3)cc2C1=O	'>'	100000	nM	4.000
CHEMBL3099535	O=C1Nc2ccc(S(=O)(=O)N3CCN(c4cccc(C(F)(F)F)c4)CC3)cc2C1=O	'>'	100000	nM	4.000
CHEMBL1774324	Cc1nc(C)c(C(=O)C2=C(O)C(=O)N(CCCN3CCOCC3)C2c2cccc([N+](=O)[O-])c2)s1	'='	101380	nM	3.994
CHEMBL8145	O=c1c(-c2ccc(O)cc2)coc2cc(O)ccc12	'='	105000	nM	3.979
CHEMBL1732790	OCCCc1nc2ccccc2n1CCOc1ccccc1	'>'	200000	nM	3.913
CHEMBL1392147	CCOc1ccc(S(=O)(=O)NCc2ccc3c(c2)OCO3)cc1C	'='	76700	nM	3.907
CHEMBL1277754	CC(=O)Oc1cc2c(cc1C(C)C)CC[C@@H]1[C@]2(C)CCC[C@@]1(C)CO	'='	128900	nM	3.890
CHEMBL40275	O=C1c2cccc(O)c2C(=O)c2c(O)cc(CO)cc21	'='	132000	nM	3.879
CHEMBL1277840	C=C1CC[C@H]2[C@](C)(CO)CCC[C@]2(C)[C@H]1CC/C(C)=C\CO	'='	137700	nM	3.861
CHEMBL559870	Oc1cc(O)c2oc3cc(O)c4oc5cc(O)cc(O)c5oc4c3oc2c1	'='	158300	nM	3.817
CHEMBL1277662	CC(C)c1cc2c(cc1O)[C@@]1(C)CCC[C@@](C)(C=O)[C@@H]1CC2	'='	163200	nM	3.787
CHEMBL2391422	Oc1cc(O)cc(Oc2c(O)cc(Oc3c(O)cc(O)cc3O)cc2O)c1	'='	164700	nM	3.783
CHEMBL71893	CC(C)C1=CC2=CC[C@H]3[C@](C)(C(=O)O)CCC[C@]3(C)[C@H]2CC1	'='	189100	nM	3.723
CHEMBL207381	CC(C)c1ccc(NC(=O)CSc2nccc(-c3csc(COc4ccccc4Cl)n3)n2)cc1	'='	200000	nM	3.699
CHEMBL207484	COC(OC)c1cc(O)nc(SCC(=O)Nc2ccc(C(F)(F)F)cc2)n1	'='	200000	nM	3.699
CHEMBL210511	Cc1cc(O)nc(SCC(=O)Nc2ccc(Oc3ccc(Cl)cc3)cc2)n1	'='	200000	nM	3.699

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ChEMBL ID	Smiles	Relation	IC_{50}	Units	pIC_{50}
CHEMBL210823	CCCCc1ccc(NC(=O)CSc2nc(O)c(C#N)c(C3CCCCC3)n2)c(C)c1	'='	200000	nM	3.699
CHEMBL377225	N#Cc1c(O)nc(SCC(=O)Nc2cccc(C(F)(F)F)c2)nc1-c1ccccc1	'='	200000	nM	3.699
CHEMBL473159	Oc1cc(O)cc(O)c1	'>'	200000	nM	3.699
CHEMBL12798	COC(=O)[C@]1(C)CCC[C@]2(C)c3ccc(C(C)C)cc3CC[C@H]21	'='	207000	nM	3.684
CHEMBL197310	CC(C)c1cc2c(cc1O)[C@@]1(C)CCC[C@@](C)(CO)[C@@H]1CC2	'='	220800	nM	3.656
CHEMBL1277661	CC(C)c1cc2c(cc1O)[C@@]1(C)CC[C@H](O)C(C)(C)[C@@H]1CC2	'='	233400	nM	3.632
CHEMBL207458	CCOC(=O)c1cnc(SCC(=O)Nc2ccc([N+](=O)[O-])cc2)nc1N	'='	250000	nM	3.602
CHEMBL28	O=c1cc(-c2ccc(O)cc2)oc2cc(O)cc(O)c12	'='	280800	nM	3.552
CHEMBL512164	C=C[C@@]1(C)CC[C@H]2C(=CC[C@H]3[C@](C)(C(=O)O)CCC[C@]23C)C1	'='	283500	nM	3.547
CHEMBL210145	CCOc1ccc(N2C(=O)CC(Sc3nc(C)cc(C)n3)C2=O)cc1	'='	300000	nM	3.523
CHEMBL210146	COc1cccc(-c2nc(SCC(=O)Nc3ccc([N+](=O)[O-])cc3)nc(O)c2C#N)c1	'='	300000	nM	3.523
CHEMBL210972	CC(Sc1nc(O)c(C#N)c(-c2ccccc2)n1)C(=O)Nc1ccc(Cl)cc1	'='	300000	nM	3.523
CHEMBL378677	CC(C)(C)c1ccc(NC(=O)CSc2nc(O)c(C#N)c(C3CCCCC3)n2)cc1	'='	350000	nM	3.456
CHEMBL210437	COc1ccc(-c2ccnc(SCC(=O)Nc3ccc(C(C)C)cc3)n2)cc1	'='	400000	nM	3.398
CHEMBL210195	Cc1cc(C(F)(F)F)nc(SCC(=O)Nc2ccc(Cl)cc2F)n1	'='	500000	nM	3.301
CHEMBL210216	Cc1nc(SCC(=O)Nc2ccc([N+](=O)[O-])cc2)nc(O)c1C	'>'	1000000	nM	3.000

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Table S1. List of molecules constituting SARS-CoV RNA dependent RNA polymerase training set.

ChEMBL ID	Smiles	Relation	IC_{50}	Units	pIC_{50}
CHEMBL2441741	CC(C)C[C@H](NC(=O)[C@H](Cc1cccc2ccccc12)NC(=O)OCc1ccccc1)C(=O)N[C@H](C=O)C[C@@H]1CCNC1=O	'='	230	nM	6.638
CHEMBL221366	O=C(Oc1cccnc1)c1cccs1	'='	500	nM	6.301
CHEMBL2441745	CC(C)C[C@H](NC(=O)[C@H](Cc1cccc2ccccc12)NC(=O)OCc1ccccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	'='	610	nM	6.215
CHEMBL3099526	CC1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3C)CC1	'='	1040	nM	5.983
CHEMBL3099541	CC1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3)CC1	'='	1180	nM	5.928
CHEMBL3105073	S=C(NCc1cccnc1)SCc1cc(Cl)sc1Cl	'='	160	nM	5.916
CHEMBL3099527	CC1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccccc2)CC1	'='	1690	nM	5.772
CHEMBL478119	CCN1/C(=C\C=C\C2=C/C(=C/c3sc4ccccc4[n+]3CC)CC(C)C2)Sc2ccccc21	'='	2000	nM	5.699
CHEMBL4214066	CC(C)C[C@H](NC(=O)OC1CCN(C(=O)OC(C)(C)C)CC1)C(=O)N[C@H](C=O)C[C@@H]1CCNC1=O	'='	2100	nM	5.678
CHEMBL3099542	CC1CCCCN1S(=O)(=O)c1ccc2c(c1)C(=O)C(=O)N2	'='	2250	nM	5.648
CHEMBL541163	CCN1/C(=C\C=C\c2sc3ccc(-c4nc5ccccc5s4)cc3[n+]2CC)Sc2ccc(-c3nc4ccccc4s3)cc21.[Cl-]	'='	2500	nM	5.602
CHEMBL1092796	CC1=CC[C@]2(C)CC[C@]3(C)C4=CC=C5C(=CC(=O)C(O)=C5C)[C@]4(C)CC[C@@]3(C)[C@@H]2C1	'='	2600	nM	5.585
CHEMBL3099529	CC1CC(C)CN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3C)C1	'='	2820	nM	5.550
CHEMBL4217568	CCOC(=O)N1CCC(OC(=O)N[C@@H](CC(C)C)C(=O)N[C@H](C=O)C[C@@H]2CCNC2=O)CC1	'='	3200	nM	5.495
CHEMBL540403	CCN1C(c2ccccc2)=C(c2ccccc2)S/C1=C/C=C/c1sc2c3ccccc3ccc2[n+]1CC.[Cl-]	'='	3800	nM	5.420
CHEMBL4214471	CC(C)C[C@H](NC(=O)OC1(Cc2ccccc2)CCN(S(C)(=O)=O)CC1)C(=O)N[C@H](C=O)C[C@@H]1CCNC1=O	'='	3900	nM	5.409
CHEMBL4216101	CCC1(OC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(O)S(=O)(=O)[O-])CCN(C(=O)OC(C)(C)C)CC1.[Na+]	'='	4100	nM	5.387
CHEMBL3099543	CC1CC(C)CN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3)C1	'='	4300	nM	5.367
CHEMBL4208764	CC(C)C[C@H](NC(=O)OC1(Cc2ccccc2)CCN(S(C)(=O)=O)CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(=O)(=O)[O-].[Na+]	'='	4300	nM	5.367
CHEMBL61320	O=C1Nc2ccc(S(=O)(=O)N3CCCCC3)cc2C1=O	'='	4450	nM	5.352
CHEMBL2316337	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OCc1ccccc1)C(C)C)C(=O)N[C@H](C#N)CCC(N)=O	'='	4600	nM	5.337
CHEMBL3099530	CC1CC(C)CN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccccc2)C1	'='	4700	nM	5.328

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CHEMBL4208240	CC(C)C[C@H](NC(=O)OC1CCN(C(=O)OC(C)(C)C)CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(=O)(=O)[O-].[Na+]	'='	5100	nM	5.292
CHEMBL4202812	CC(C)C[C@H](NC(=O)OC1(Cc2ccccc2)CCN(C(=O)OC(C)(C)C)CC1)C(=O)N[C@H](C=O)C[C@@H]1CCNC1=O	'='	5200	nM	5.284
CHEMBL479172	CCC(=C\c1sc2c3ccccc3ccc2[n+]1CC)/C=C1/Sc2cc(C)c(C)cc2N1CC	'='	5400	nM	5.268
CHEMBL54804	COC(=O)[C@]1(C)CC[C@]2(C)CC[C@]3(C)C4=CC=C5C(=CC(=O)C(O)=C5C)[C@]4(C)CC[C@@]3(C)[C@@H]2C1	'='	5500	nM	5.260
CHEMBL1277046	N#Cc1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(C(=O)O)cc3)C2=O)cc1	'='	5500	nM	5.260
CHEMBL4212620	CCC1(OC(=O)N[C@@H](CC(C)C)C(=O)N[C@H](C=O)C[C@@H]2CCNC2=O)CCN(C(=O)OC(C)(C)C)CC1	'='	5500	nM	5.260
CHEMBL3099521	CN1C(=O)C(=O)c2cc(S(=O)(=O)N3CCN(c4ccccn4)CC3)ccc21	'='	5520	nM	5.258
CHEMBL3808427	CC(C)(C)c1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4cc(Cl)ccc4C(=O)O)o3)C2=O)cc1	'='	5800	nM	5.237
CHEMBL3809329	CC(C)c1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4cc(Cl)ccc4C(=O)O)o3)C2=O)cc1	'='	6000	nM	5.222
CHEMBL4203883	CC(C)C[C@H](NC(=O)OC1(Cc2ccccc2)CCN(C(=O)OC(C)(C)C)CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(=O)(=O)[O-].[Na+]	'='	6300	nM	5.201
CHEMBL3809861	O=C(O)c1cccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4ccccc4)o3)C2=O)c1	'='	6400	nM	5.194
CHEMBL558828	CCC(=C\c1sc2cc(C)c(C)cc2[n+]1CC)/C=C1/Sc2cc(/C=C/c3ccccc3)ccc2N1CC.[Cl-]	'='	6600	nM	5.180
CHEMBL3809053	O=C(O)c1cccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4ccccc4)cc3)C2=O)c1	'='	6700	nM	5.174
CHEMBL1277227	O=C(O)c1ccc(/C=C2\C(=O)N(c3ccc(F)cc3)N=C2c2ccccc2)cc1	'='	6800	nM	5.167
CHEMBL515787	CCN1/C(=C\C(=C/c2sc3ccccc3[n+]2CCCS(=O)(=O)[O-])OC)Sc2ccc(OC)cc21	'='	7300	nM	5.137
CHEMBL3818000	CC(=O)N[C@@H](CC(N)=O)C(=O)N[C@@H](CO)C(=O)N[C@H](C(=O)N[C@@H](CO)C(=O)N[C@@H](CCC(N)=O)C(=O)O)[C@@H](C)O	'='	7500	nM	5.125
CHEMBL3818593	CC(=O)N[C@@H](CCC(=O)O)C(=O)N[C@@H](CO)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(N)=O)C(=O)O)[C@@H](C)O	'='	7500	nM	5.125
CHEMBL551131	N#Cc1cccc(COc2cc(O)c3c(=O)c(O)c(-c4ccc(O)c(O)c4)oc3c2)c1	'='	25400	nM	5.082
CHEMBL63354	O=c1cc(-c2ccc(O)c(-c3c(O)cc(O)c4c(=O)cc(-c5ccc(O)cc5)oc34)c2)oc2cc(O)cc(O)c12	'='	8300	nM	5.081
CHEMBL1277228	O=C(O)c1ccc(/C=C2\C(=O)N(c3cccc([N+](=O)[O-])c3)N=C2c2ccccc2)cc1	'='	8400	nM	5.076
CHEMBL3105076	Nc1ncnc2[nH]c(C(F)(F)F)nc12	'='	2200	nM	5.068
CHEMBL3809579	CC(C)(C)c1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4ccccc4C(=O)O)o3)C2=O)cc1	'='	8600	nM	5.066
CHEMBL471187	Oc1cc(O)cc(Oc2c(O)cc(O)c3c2Oc2c(O)cc(O)cc2O3)c1	'='	8800	nM	5.056

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CHEMBL4204431	CCOC(=O)N1CCC(OC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(O)S(=O)(=O)[O-])CC1.[Na+]	'='	8800	nM	5.056
CHEMBL550256	O=c1c(O)c(-c2ccc(O)c(O)c2)oc2cc(OCc3ccc(Cl)cc3)cc(O)c12	'='	4100	nM	5.034
CHEMBL432519	CC1=C(O)C(=O)C=C2C1=CC=C1[C@@]3(C)CC[C@@]4(C)CC(=O)[C@H](C)C[C@H]4[C@]3(C)CC[C@@]21C	'='	9900	nM	5.004
CHEMBL3099523	CN1C(=O)C(=O)c2cc(S(=O)(=O)N3CCOCC3)ccc21	'='	9910	nM	5.004
CHEMBL478987	CCN1/C(=C\C=c2/s/c(=C\c3sc4ccccc4[n+]3C)n(CC)c2=O)Sc2ccccc21	'='	10000	nM	5.000
CHEMBL3818400	CC(=O)N[C@@H](CC(=O)O)C(=O)N[C@@H](CO)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(N)=O)C(=O)O)[C@@H](C)O	'='	10000	nM	5.000
CHEMBL3099539	O=C1Nc2ccc(S(=O)(=O)N3CCN(C(=O)c4ccco4)CC3)cc2C1=O	'='	10070	nM	4.997
CHEMBL301982	CC1=C(O)C(=O)C=C2C1=CC=C1[C@@]3(C)CC[C@@]4(C)CC[C@@](C)(C(=O)O)C[C@H]4[C@]3(C)CC[C@@]21C	'='	10300	nM	4.987
CHEMBL518593	C(\C1=C2Sc3ccccc3N2CC1)=C1/CC[n+]2c1sc1ccccc12	'='	10500	nM	4.979
CHEMBL1277135	O=C(O)c1ccc(/C=C2\C(=O)N(c3cccc(Cl)c3)N=C2c2ccccc2)cc1	'='	10800	nM	4.967
CHEMBL3809506	CC(C)c1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4ccccc4C(=O)O)o3)C2=O)cc1	'='	11700	nM	4.932
CHEMBL3099544	CN1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3C)CC1	'='	11830	nM	4.927
CHEMBL1276871	COc1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(C(=O)O)cc3)C2=O)cc1	'='	12000	nM	4.921
CHEMBL484273	O=C1Nc2ccc(S(=O)(=O)N3CCOCC3)cc2C1=O	'='	12660	nM	4.898
CHEMBL508791	Oc1cc(O)cc(Oc2c(O)cc(O)c3c2Oc2c(O)cc(Oc4c(O)cc(Oc5c(O)cc(O)c6c5Oc5c(O)cc(O)cc5O6)cc4O)cc2O3)c1	'='	68100	nM	4.868
CHEMBL1876821	CN(CC(=O)NC1CCCC1)S(=O)(=O)c1cccc(Cl)c1	'>'	200000	nM	4.863
CHEMBL3099524	O=C1C(=O)N(Cc2ccccc2)c2ccc(S(=O)(=O)N3CCOCC3)cc21	'='	13860	nM	4.858
CHEMBL3099547	CN1C(=O)C(=O)c2cc(S(=O)(=O)N3CCN(CCc4ccccc4)CC3)ccc21	'='	13860	nM	4.858
CHEMBL50	O=c1c(O)c(-c2ccc(O)c(O)c2)oc2cc(O)cc(O)c12	'='	23800	nM	4.857
CHEMBL1278125	O=C(O)c1ccc(/C=C2\C(=O)N(c3ccc(Cl)cc3)N=C2c2ccccc2)cc1	'='	13900	nM	4.857
CHEMBL3099522	O=C1C(=O)N(Cc2ccccc2)c2ccc(S(=O)(=O)N3CCCCC3)cc21	'='	14000	nM	4.854
CHEMBL3809926	O=C(O)c1cccc(N2N=C(c3ccccc3)/C(=C/c3ccc(OCc4ccccc4)cc3)C2=O)c1	'='	15700	nM	4.804
CHEMBL551130	O=c1c(O)c(-c2ccc(O)c(O)c2)oc2cc(OCc3cccc(Cl)c3)cc(O)c12	'>'	50000	nM	4.793
CHEMBL3105074	O=C(c1cncc(Br)c1)N1CCN(Cc2ccsc2)CC1	'='	24500	nM	4.789

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CHEMBL3810328	O=C(O)c1ccc(Cl)cc1-c1ccc(/C=C2\C(=O)N(c3ccccc3)N=C2c2ccccc2)o1	'='	16400	nM	4.785
CHEMBL3099528	CC1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccc3ccccc3c2)CC1	'='	17820	nM	4.749
CHEMBL1277944	O=C(O)c1ccc(/C=C2\C(=O)N(c3ccccc3)N=C2c2ccccc2)cc1	'='	18000	nM	4.745
CHEMBL551529	N#Cc1cccc(COc2cc(O)c3c(=O)c(O)c(-c4ccc5c(c4)OCO5)oc3c2)c1	'='	8100	nM	4.730
CHEMBL3809498	N#Cc1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4ccccc4C(=O)O)o3)C2=O)cc1	'='	18700	nM	4.728
CHEMBL151	O=c1cc(-c2ccc(O)c(O)c2)oc2cc(O)cc(O)c12	'='	20000	nM	4.699
CHEMBL3818028	CC(=O)N[C@@H](CC(N)=O)C(=O)N[C@@H](CO)C(=O)N[C@H](C(=O)N[C@@H](CC(=O)O)C(=O)N[C@@H](CCC(N)=O)C(=O)O)[C@@H](C)O	'='	20000	nM	4.699
CHEMBL3808658	O=C(O)c1ccc(Cl)cc1-c1ccc(/C=C2\C(=O)N(c3ccc(F)cc3)N=C2c2ccccc2)o1	'='	20200	nM	4.695
CHEMBL551334	O=c1c(O)c(-c2ccc3c(c2)OCO3)oc2cc(OCc3ccc(Cl)cc3)cc(O)c12	'>'	50000	nM	4.666
CHEMBL1092797	Cc1c(O)c(O)cc2c1CC=C1[C@@]3(C)CC[C@@]4(C)CC[C@@](C)(C(=O)O)C[C@H]4[C@]3(C)CC[C@]12C	'='	21700	nM	4.664
CHEMBL399121	COc1ccc([C@@H]2CC(=O)c3c(O)cc(O)cc3O2)cc1O	'='	60000	nM	4.651
CHEMBL116438	COc1cc(/C=C/C(=O)/C=C(O)/C=C/c2ccc(O)c(OC)c2)ccc1O	'='	23500	nM	4.629
CHEMBL554041	CCCCC(CC)CNC(=N)NC(=N)NCCCCCCNC(=N)NC(=N)NCC(CC)CCCC.Cl.Cl	'='	17800	nM	4.629
CHEMBL1277136	O=C(O)c1ccc(/C=C2\C(=O)N(c3ccc(Cl)c(Cl)c3)N=C2c2ccccc2)cc1	'='	24300	nM	4.614
CHEMBL1487869	Cn1cnc2cc(NC(=O)c3ccc(Cl)cc3)ccc21	'='	18200	nM	4.603
CHEMBL560933	O=c1c(O)c(-c2ccc3c(c2)OCO3)oc2cc(OCc3cccc(Cl)c3)cc(O)c12	'='	15400	nM	4.557
CHEMBL4209146	CC(C)C[C@H](NC(=O)OC1CCN(S(C)(=O)=O)CC1)C(=O)N[C@H](C=O)C[C@@H]1CCNC1=O	'='	28800	nM	4.541
CHEMBL3105075	C(=C/c1ccccc1)\C[N+]1(C/C=C/c2ccccc2)CCN(C(c2ccccc2)c2ccccc2)CC1	'='	28300	nM	4.537
CHEMBL3809059	COc1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4ccccc4C(=O)O)o3)C2=O)cc1	'='	30700	nM	4.513
CHEMBL1478361	COc1ccc(N(CC(=O)NCc2ccco2)S(C)(=O)=O)cc1	'='	61900	nM	4.501
CHEMBL3099536	O=C1Nc2ccc(S(=O)(=O)N3CCN(Cc4cccc(Cl)c4)CC3)cc2C1=O	'='	31710	nM	4.499
CHEMBL377324	COc1cc(O)c2c(=O)cc(-c3ccc(OC)c(-c4c(O)cc(O)c5c(=O)cc(-c6ccc(O)cc6)oc45)c3)oc2c1	'='	32000	nM	4.495
CHEMBL3099537	COc1cc(CN2CCN(S(=O)(=O)c3ccc4c(c3)C(=O)C(=O)N4)CC2)cc(OC)c1OC	'='	32080	nM	4.494
CHEMBL1906723	COc1ccc(C(=O)Cn2c(NCCO)nc3ccccc32)cc1	'='	40900	nM	4.464
CHEMBL3099538	O=C1Nc2ccc(S(=O)(=O)N3CCN(CCc4ccccc4)CC3)cc2C1=O	'='	34910	nM	4.457

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CHEMBL3810325	O=C(O)c1ccccc1-c1ccc(/C=C2\C(=O)N(c3ccc(F)cc3)N=C2c2ccccc2)o1	'='	37500	nM	4.426
CHEMBL208908	COc1ccc(-c2cc(=O)c3c(O)cc(O)c(-c4cc(-c5cc(=O)c6c(O)cc(OC)cc6o5)ccc4OC)c3o2)cc1	'='	38400	nM	4.416
CHEMBL1350514	Cc1ccc(C(=O)N/C(=C\c2ccc(-c3cccc([N+](=O)[O-])c3)o2)C(=O)NCCCN(C)C)cc1	'='	38570	nM	4.414
CHEMBL2391423	Oc1cc(O)cc(Oc2c(Oc3c(O)cc(O)cc3O)cc(O)c3c2Oc2c(O)cc(O)cc2O3)c1	'='	13300	nM	4.413
CHEMBL2316336	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)[C@H](CO)NC(=O)[C@@H](NC(=O)OCc1ccccc1)[C@@H](C)O)C(C)C)C(=O)N[C@H](C#N)CCC(N)=O	'='	39000	nM	4.409
CHEMBL3099525	O=C1C(=O)N(Cc2ccc3ccccc3c2)c2ccc(S(=O)(=O)N3CCOCC3)cc21	'='	39870	nM	4.399
CHEMBL3810361	O=C(O)c1ccccc1-c1ccc(/C=C2\C(=O)N(c3ccccc3)N=C2c2ccccc2)o1	'='	41200	nM	4.385
CHEMBL1315054	Cc1ccc(C(=O)N/C(=C\c2ccc(-c3ccccc3[N+](=O)[O-])o2)C(=O)NCCCN(C)C)cc1	'='	41390	nM	4.383
CHEMBL1277047	O=C(O)c1ccc(/C=C2\C(=O)N(c3ccc(OC(F)(F)F)cc3)N=C2c2ccccc2)cc1	'='	42000	nM	4.377
CHEMBL4213159	CC(C)C[C@H](NC(=O)OC1CCN(S(C)(=O)=O)CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(=O)(=O)[O-].[Na+]	'='	42100	nM	4.376
CHEMBL3808795	O=C(O)c1cccc(N2N=C(c3ccccc3)/C(=C/c3ccc(-c4cc(Cl)ccc4C(=O)O)o3)C2=O)c1	'='	44700	nM	4.350
CHEMBL2316338	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OC(C)(C)C)C(C)C)C(=O)N[C@H](C#N)CCC(N)=O	'='	49000	nM	4.310
CHEMBL2316339	Cc1cc(C(=O)N[C@@H](C)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@H](C#N)CCC(N)=O)C(C)C)no1	'='	49000	nM	4.310
CHEMBL197308	CC(C)c1cc2c(cc1O)[C@@]1(C)CCCC(C)(C)[C@@H]1CC2	'='	49600	nM	4.305
CHEMBL549646	O=c1cc(CNCc2ccc(Cl)cc2)oc2ccc(O)c(O)c12	'>'	50000	nM	4.301
CHEMBL556501	O=c1c(O)c(-c2ccc3c(c2)OCO3)oc2cc(O)cc(O)c12	'>'	50000	nM	4.301
CHEMBL560136	O=c1cc(CNCc2cccc(Cl)c2)oc2ccc(O)c(O)c12	'>'	50000	nM	4.301
CHEMBL560392	N#Cc1cccc(CNCc2cc(=O)c3c(O)c(O)ccc3o2)c1	'>'	50000	nM	4.301
CHEMBL3808558	O=C(O)c1cccc(N2N=C(C(F)(F)F)/C(=C\c3ccc(-c4ccccc4C(=O)O)o3)C2=O)c1	'>'	50000	nM	4.301
CHEMBL3809159	CC1=NN(c2cccc(C(=O)O)c2)C(=O)/C1=C\c1ccc(-c2ccccc2)o1	'>'	50000	nM	4.301
CHEMBL3809833	O=C(O)c1cccc(N2N=C(c3ccccc3)/C(=C/c3ccco3)C2=O)c1	'>'	50000	nM	4.301
CHEMBL3810010	CC1=NN(c2ccccc2)C(=O)/C1=C\c1ccc(-c2cc(Cl)ccc2C(=O)O)o1	'>'	50000	nM	4.301
CHEMBL3810058	O=C1/C(=C\c2ccc(-c3ccccc3)o2)C(c2ccccc2)=NN1c1ccccc1	'>'	50000	nM	4.301

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CHEMBL3810109	O=C(O)c1cccc(N2N=C(C(F)(F)F)/C(=C/c3ccc(-c4cc(Cl)ccc4C(=O)O)o3)C2=O)c1	'>'	50000	nM	4.301
CHEMBL3810366	CC1=NN(c2cccc(C(=O)O)c2)C(=O)/C1=C\c1ccc(-c2cc(Cl)ccc2C(=O)O)o1	'>'	50000	nM	4.301
CHEMBL3818761	CC(=O)N[C@@H](Cc1cnc[nH]1)C(=O)N[C@@H](CO)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(N)=O)C(=O)O)[C@@H](C)O	'>'	50000	nM	4.301
CHEMBL3099540	O=C1Nc2ccc(S(=O)(=O)N3CCN(c4ccccn4)CC3)cc2C1=O	'='	51330	nM	4.290
CHEMBL510508	Oc1cc(O)cc(Oc2c(O)cc(O)c3c2Oc2c(O)cc4oc5c(Oc6cc(O)cc(O)c6)c(O)cc(O)c5c4c2O3)c1	'='	16700	nM	4.268
CHEMBL1774322	Nc1nc(CSc2nnc(-c3cccc4ccccc34)n2-c2ccccc2)cs1	'='	58350	nM	4.234
CHEMBL1774323	COc1cc(C2C(C(=O)c3ccc(OCC(C)C)cc3C)=C(O)C(=O)N2CCN(C)C)ccc1O	'='	62790	nM	4.202
CHEMBL459393	Oc1cc(O)c(Oc2cc(O)cc(O)c2Oc2cc(O)cc(O)c2-c2c(O)cc(O)cc2O)c(O)c1	'='	22500	nM	4.200
CHEMBL3099545	CN1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccccc2)CC1	'='	67200	nM	4.173
CHEMBL456228	Oc1cc(O)cc(Oc2c(O)cc(O)c3c2Oc2c(O)cc(Oc4c(O)cc(O)cc4O)cc2O3)c1	'='	112000	nM	4.163
CHEMBL1488602	COCCOCCn1c(CCCO)nc2ccccc21	'='	186000	nM	4.161
CHEMBL378188	COc1ccc(-c2cc(=O)c3c(O)cc(O)cc3o2)cc1-c1c(O)cc(O)c2c(=O)cc(-c3ccc(O)cc3)oc12	'='	72300	nM	4.141
CHEMBL3099533	CN1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3)CC1	'='	76740	nM	4.115
CHEMBL1774325	COc1cc(/C=N/NC(=O)/C(=C\c2ccccc2)NC(=O)c2ccccc2)cc(OC)c1O	'='	77090	nM	4.113
CHEMBL3105072	Nc1ccc(F)c(S(=O)(=O)Nc2cccc(C(F)(F)F)c2)c1	'='	29800	nM	4.112
CHEMBL3105071	COc1ccccc1CNC(=O)[C@H](C)NS(=O)(=O)c1ccccc1	'='	29900	nM	4.112
CHEMBL3099546	CN1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccc3ccccc3c2)CC1	'='	82910	nM	4.081
CHEMBL1774326	O=C(CSc1ncnc2c1sc1nc(N3CCOCC3)c3c(c12)CCCC3)NCc1ccco1	'='	90720	nM	4.042
CHEMBL3099534	O=C1Nc2ccc(S(=O)(=O)N3CCN(c4ccc(F)cc4)CC3)cc2C1=O	'>'	100000	nM	4.000
CHEMBL3099535	O=C1Nc2ccc(S(=O)(=O)N3CCN(c4cccc(C(F)(F)F)c4)CC3)cc2C1=O	'>'	100000	nM	4.000
CHEMBL1774324	Cc1nc(C)c(C(=O)C2=C(O)C(=O)N(CCCN3CCOCC3)C2c2cccc([N+](=O)[O-])c2)s1	'='	101380	nM	3.994
CHEMBL8145	O=c1c(-c2ccc(O)cc2)coc2cc(O)ccc12	'='	105000	nM	3.979
CHEMBL1732790	OCCCc1nc2ccccc2n1CCOc1ccccc1	'>'	200000	nM	3.913
CHEMBL1392147	CCOc1ccc(S(=O)(=O)NCc2ccc3c(c2)OCO3)cc1C	'='	76700	nM	3.907
CHEMBL1277754	CC(=O)Oc1cc2c(cc1C(C)C)CC[C@@H]1[C@]2(C)CCC[C@@]1(C)CO	'='	128900	nM	3.890
CHEMBL40275	O=C1c2cccc(O)c2C(=O)c2c(O)cc(CO)cc21	'='	132000	nM	3.879
CHEMBL1277840	C=C1CC[C@H]2[C@](C)(CO)CCC[C@]2(C)[C@H]1CC/C(C)=C\CO	'='	137700	nM	3.861
CHEMBL559870	Oc1cc(O)c2oc3cc(O)c4oc5cc(O)cc(O)c5oc4c3oc2c1	'='	158300	nM	3.817

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CHEMBL1277662	CC(C)c1cc2c(cc1O)[C@@]1(C)CCC[C@@](C)(C=O)[C@@H]1CC2	'='	163200	nM	3.787
CHEMBL2391422	Oc1cc(O)cc(Oc2c(O)cc(Oc3c(O)cc(O)cc3O)cc2O)c1	'='	164700	nM	3.783
CHEMBL71893	CC(C)C1=CC2=CC[C@H]3[C@](C)(C(=O)O)CCC[C@]3(C)[C@H]2CC1	'='	189100	nM	3.723
CHEMBL473159	Oc1cc(O)cc(O)c1	'>'	200000	nM	3.699
CHEMBL12798	COC(=O)[C@]1(C)CCC[C@]2(C)c3ccc(C(C)C)cc3CC[C@H]21	'='	207000	nM	3.684
CHEMBL197310	CC(C)c1cc2c(cc1O)[C@@]1(C)CCC[C@@](C)(CO)[C@@H]1CC2	'='	220800	nM	3.656
CHEMBL1277661	CC(C)c1cc2c(cc1O)[C@@]1(C)CC[C@H](O)C(C)(C)[C@@H]1CC2	'='	233400	nM	3.632
CHEMBL28	O=c1cc(-c2ccc(O)cc2)oc2cc(O)cc(O)c12	'='	280800	nM	3.552
CHEMBL512164	C=C[C@@]1(C)CC[C@H]2C(=CC[C@H]3[C@](C)(C(=O)O)CCC[C@]23C)C1	'='	283500	nM	3.547

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Table S2. List of QSAR models used to predict 38 types of bioactivities, available at ChemoSophia web platform.

Condition	Target / mechanism
anxiolytic, anti-depressant, anti-psychotic	5-HT_{1A} receptor
anti-atherosclerosis	Acyl-co-A-cholesterol transferase
benign prostatic hyperplasia (BPH), hypertension and post-traumatic stress disorder	α1 adrenergic receptor
analgesic activity, painkiller	no specific target
conduction anesthesia	no specific target
antibacterial	DNA gyrase
anti-oxidant	alkylic action
anti-tumor	anti-mitotics
anti-tumor	DNA-anti-metabolites
anti-tumor	DNA/RNA-anti-metabolites
anti-tumor	topoisomerase I
anti-tumor	topoisomerase II
anti-tumor	breast cancer
anti-tumor	CDK4 inhibitors
anti-arrhythmic	no specific target
SARS-CoV †	main protease, 3CLpro
SARS-CoV †	RNA dependent RNA polymerase, RdRp
SARS-CoV †	no specific target
anti-inflammatory	COX1 inhibitors
anti-inflammatory	COX2 inhibitors
anti-inflammatory	LOX5 inhibitors
anti-inflammatory	p38 MAP kinase inhibitors
anti-inflammatory	*in vivo*, paw oedema
anti-inflammatory	*in vivo*, peritonitis
anti-tubercular	DHFR inhibitors
psychotropic drugs	benzodiazepine receptor
	human factor Xa inhibitors
AIDS	human immunodeficiency virus
anti-malarial	*Plasmodium*
avian flu	avian influenza virus
bird viral laryngotracheitis	no specific target
Crimean–Congo hemorrhagic fever	Crimean–Congo hemorrhagic fever virus
flu	influenza A virus
flu	influenza B virus
Issyk-Kul fever	Issyk-Kul virus
Pogosta disease	Sindbis virus
tick-borne encephalitis	tick-borne encephalitis virus
progestagens	no specific target

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† implementation in progress (currently not available)

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Table S3. Predicted bioactivities for a series of platinum complexes.

number	formula	5HT1A	acyl-co-A	α1 adrenergic	ANALGE	ANESTE	DNA gyrase	anti-oxidant	anti-mitotics	DNA-anti-metabolites	DNA/RNA-anti-metabolites
1	$[(C_2H_5)_4N]_2[PtCl_6]$	NO	NO	YES	NO	YES	NO	NO	NO	NO	NO
2	$[(C_2H_5)_2NH_2]_2[PtCl_6]$	NO	NO	NO	NO	NO	NO	YES	NO	NO	NO
3	$[(CH_3)_3NH]_2[PtCl_6]$	NO	NO	NO	NO	YES	YES	NO	NO	NO	NO
4	$[Ph_4P]_2[PtCl_6]\times CH_3CN$	NO	NO	NO	NO	NO	YES	NO	YES	NO	NO
5	$[Ph_3PCH=CHCH_3]_2[PtCl_6]$	NO	NO	NO	NO	NO	YES	NO	NO	NO	NO
6	$[Ph_3PCH_2OCH_3]_2[PtCl_6]$	NO	NO	NO	NO	YES	NO	NO	NO	NO	NO
7	$[Ph_3PC_2H_5]_2[PtBr_6]$	NO	NO	NO	NO	YES	NO	NO	YES	NO	NO
8	$[Ph_3P(cyclo\text{-}C_3H_5)]_2[PtBr_6]$	NO	NO	NO	NO	YES	NO	NO	YES	NO	NO
9	$[Ph_3PCH_2Ph]_2[PtBr_6]$	NO	NO	NO	NO	NO	YES	YES	YES	NO	NO
10	$[Ph_3PCH_3]_2[PtBr6]$	NO	NO	NO	NO	YES	NO	NO	YES	NO	NO
11	$[Ph_3PCH=CH_2]_2[PtBr_6]$	NO	NO	NO	NO	YES	NO	YES	NO	NO	NO
12	$[Ph_3PCH_2CH=CH_2]_2[PtBr_6]$	NO	NO	NO	NO	NO	NO	YES	NO	NO	NO
13	$[(C_2H_5)_4N]_2[PtCl_5(DESO\text{-}S)]$	NO	NO	NO	NO	NO	NO	YES	NO	NO	NO
14	$[Ph_3PCH_2CH=CHCH_2PPh_3][PtCl_5(DMSO\text{-}S)]$	NO	NO	NO	NO	YES	NO	YES	YES	NO	NO
15	$[Ph_3PC_2H_5][PtCl_5(DESO\text{-}S)]$	NO	NO	NO	NO	NO	NO	NO	YES	NO	NO
16	$[Ph_3PCH_2OCH_3][PtCl_3(DMSO)]$	NO	NO	NO	NO	NO	NO	NO	YES	NO	NO
17	*cis*-$[PtCl_2(DESO)(PPh_3)]$	NO	NO	NO	NO	NO	NO	NO	YES	NO	NO
18	$[Ph_3PCH_2Ph][PtBr_5(DMSO\text{-}S)]$	NO	NO	NO	NO	YES	YES	NO	YES	NO	NO

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Table S4. Predicted bioactivities for a series of platinum complexes (continuation).

number	formula	topoisomerase I	topoisomerase II	breast cancer	anti-arrhythmic	CDK4 inhibitors	SARS-CoV-2	SARS-CoV-2 3CLpro	SARS-CoV-2 RdRp	COX1	COX2
1	$[(C_2H_5)_4N]_2[PtCl_6]$	NO	NO	NO	YES	NO	NO	NO	YES	NO	NO
2	$[(C_2H_5)_2NH_2]_2[PtCl_6]$	NO	NO	NO	NO	NO	NO	NO	NO	NO	NO
3	$[(CH_3)_3NH]_2[PtCl_6]$	NO	NO	NO	NO	NO	NO	NO	NO	NO	NO
4	$[Ph_4P]_2[PtCl_6]\times CH_3CN$	NO	NO	NO	NO	NO	YES	NO	YES	NO	0
5	$[Ph_3PCH=CHCH_3]_2[PtCl_6]$	YES	NO	NO	NO	NO	YES	NO	YES	NO	NO
6	$[Ph_3PCH_2OCH_3]_2[PtCl_6]$	NO	NO	NO	NO	NO	NO	NO	YES	NO	YES
7	$[Ph_3PC_2H_5]_2[PtBr_6]$	YES	NO	NO	NO	NO	NO	NO	YES	YES	NO
8	$[Ph_3P(cyclo\text{-}C_3H_5)]_2[PtBr_6]$	NO	NO	NO	NO	NO	NO	NO	YES	NO	NO
9	$[Ph_3PCH_2Ph]_2[PtBr_6]$	NO	NO	NO	NO	NO	NO	NO	YES	NO	NO
10	$[Ph_3PCH_3]_2[PtBr6]$	NO	NO	NO	YES	NO	YES	YES	YES	NO	YES
11	$[Ph_3PCH=CH_2]_2[PtBr_6]$	NO	NO	NO	YES	NO	YES	NO	YES	NO	YES
12	$[Ph_3PCH_2CH=CH_2]_2[PtBr_6]$	NO	NO	NO	NO	NO	YES	NO	YES	YES	YES
13	$[(C_2H_5)_4N]_2[PtCl_5(DESO\text{-}S)]$	NO	NO	NO	NO	YES	YES	NO	YES	NO	NO
14	$[Ph_3PCH_2CH=CHCH_2PPh_3][PtCl_5(DMSO\text{-}S)]$	NO	NO	NO	NO	YES	NO	NO	YES	YES	NO
15	$[Ph_3PC_2H_5][PtCl_5(DESO\text{-}S)]$	NO	NO	NO	YES	NO	YES	NO	YES	NO	NO
16	$[Ph_3PCH_2OCH_3][PtCl_3(DMSO)]$	NO	NO	NO	YES	NO	YES	NO	YES	NO	NO
17	*cis*-$[PtCl_2(DESO)(PPh_3)]$	YES	NO	NO	YES	NO	YES	NO	NO	NO	NO
18	$[Ph_3PCH_2Ph][PtBr_5(DMSO\text{-}S)]$	NO	NO	NO	NO	NO	NO	NO	NO	NO	NO

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Table S4. Predicted bioactivities for a series of platinum complexes (continuation).

number	formula	DHFR inhibitors	benzodiazepine receptor	human factor Xa	HIV	LOX5	anti-malarial	p38 MAP kinase inhibitors	paw oedema	avian influenza virus	bird viral laryngotracheitis
1	$[(C_2H_5)_4N]_2[PtCl_6]$	NO	YES	NO	NO	NO	NO	NO	NO	NO	NO
2	$[(C_2H_5)_2NH_2]_2[PtCl_6]$	NO	NO	NO	NO	YES	NO	NO	NO	NO	NO
3	$[(CH_3)_3NH]_2[PtCl_6]$	NO	NO	NO	YES	YES	NO	NO	NO	NO	NO
4	$[Ph_4P]_2[PtCl_6]\times CH_3CN$	NO	NO	NO	NO	YES	NO	NO	NO	NO	NO
5	$[Ph_3PCH=CHCH_3]_2[PtCl_6]$	NO	NO	NO	YES	YES	NO	NO	NO	NO	NO
6	$[Ph_3PCH_2OCH_3]_2[PtCl_6]$	NO	NO	NO	YES	YES	NO	NO	NO	NO	NO
7	$[Ph_3PC_2H_5]_2[PtBr_6]$	NO	NO	NO	NO	NO	NO	NO	NO	NO	NO
8	$[Ph_3P(cyclo\text{-}C_3H_5)]_2[PtBr_6]$	NO	NO	YES	YES	NO	NO	NO	NO	NO	NO
9	$[Ph_3PCH_2Ph]_2[PtBr_6]$	NO	NO	YES	YES	YES	NO	NO	NO	NO	NO
10	$[Ph_3PCH_3]_2[PtBr6]$	NO	NO	NO	YES	YES	NO	NO	NO	NO	NO
11	$[Ph_3PCH=CH_2]_2[PtBr_6]$	NO	YES	NO	NO	YES	NO	NO	YES	NO	NO
12	$[Ph_3PCH_2CH=CH_2]_2[PtBr_6]$	NO	YES	NO	YES	YES	NO	NO	NO	NO	NO
13	$[(C_2H_5)_4N]_2[PtCl_5(DESO\text{-}S)]$	NO	NO	NO	YES	NO	NO	NO	NO	NO	NO
14	$[Ph_3PCH_2CH=CHCH_2PPh_3][PtCl_5(DMSO\text{-}S)]$	NO	YES	NO	NO	NO	NO	NO	NO	NO	NO
15	$[Ph_3PC_2H_5][PtCl_5(DESO\text{-}S)]$	NO	NO	NO	YES	NO	NO	NO	NO	NO	NO
16	$[Ph_3PCH_2OCH_3][PtCl_3(DMSO)]$	NO	NO	NO	YES	YES	NO	NO	NO	NO	NO
17	*cis*-$[PtCl_2(DESO)(PPh_3)]$	NO	NO	NO	NO	NO	NO	NO	NO	NO	YES
18	$[Ph_3PCH_2Ph][PtBr_5(DMSO\text{-}S)]$	NO	NO	NO	NO	YES	NO	NO	NO	NO	NO

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Table S5. Predicted bioactivities for a series of platinum complexes (continuation).

number	formula	Crimean–Congo hemorrhagic fever	influenza A	influenza B	Issyk-Kul virus	Sindbis virus	peritonitis	tick-borne encephalitis	progestagens
1	$[(C_2H_5)_4N]_2[PtCl_6]$	NO	YES	NO	NO	NO	NO	NO	NO
2	$[(C_2H_5)_2NH_2]_2[PtCl_6]$	NO	YES	NO	YES	NO	NO	NO	NO
3	$[(CH_3)_3NH]_2[PtCl_6]$	NO	NO	YES	NO	NO	NO	NO	NO
4	$[Ph_4P]_2[PtCl_6]\times CH_3CN$	NO	NO	NO	NO	NO	NO	NO	NO
5	$[Ph_3PCH=CHCH_3]_2[PtCl_6]$	NO	NO	NO	NO	NO	NO	NO	NO
6	$[Ph_3PCH_2OCH_3]_2[PtCl_6]$	NO	NO	NO	NO	NO	NO	NO	NO
7	$[Ph_3PC_2H_5]_2[PtBr_6]$	NO	NO	NO	NO	NO	NO	NO	NO
8	$[Ph_3P(cyclo\text{-}C_3H_5)]_2[PtBr_6]$	NO	NO	NO	NO	NO	NO	NO	NO
9	$[Ph_3PCH_2Ph]_2[PtBr_6]$	NO	NO	NO	NO	NO	NO	NO	NO
10	$[Ph_3PCH_3]_2[PtBr6]$	NO	NO	NO	NO	NO	NO	NO	NO
11	$[Ph_3PCH=CH_2]_2[PtBr_6]$	NO	NO	NO	NO	NO	NO	NO	NO
12	$[Ph_3PCH_2CH=CH_2]_2[PtBr_6]$	NO	NO	NO	NO	NO	NO	NO	NO
13	$[(C_2H_5)_4N]_2[PtCl_5(DESO\text{-}S)]$	NO	YES	NO	NO	NO	NO	NO	NO
14	$[Ph_3PCH_2CH=CHCH_2PPh_3][PtCl_5(DMSO\text{-}S)]$	NO	YES	NO	NO	NO	NO	NO	NO
15	$[Ph_3PC_2H_5][PtCl_5(DESO\text{-}S)]$	NO	YES	NO	NO	NO	NO	NO	NO
16	$[Ph_3PCH_2OCH_3][PtCl_3(DMSO)]$	NO	NO	NO	NO	NO	NO	NO	NO
17	*cis*-$[PtCl_2(DESO)(PPh_3)]$	NO	NO	NO	NO	NO	NO	NO	NO
18	$[Ph_3PCH_2Ph][PtBr_5(DMSO\text{-}S)]$	NO	YES	NO	NO	NO	NO	NO	NO