Table S1. Data sets of dihydroorotate dehydrogenase inhibitors.

Molecule ChEMBL ID	SMILES	pIC50
CHEMBL1076869	Brc1ccc(cc1)c2csc(N\N=C\c3ccccc3)n2	5.48
CHEMBL1084927	CCC(=O)Nc1ccc(cc1C(=O)O)N(C)Cc2cccnc2	5.26
CHEMBL1084928	CN(Cc1cccnc1)c2ccc(NC(=O)C3CC3)c(c2)C(=O)O	7
CHEMBL1088742	OC(=O)c1ccccc1NC(=O)Nc2cc(Cl)cc(Cl)c2	6.16
CHEMBL1088743	OC(=O)c1ccccc1N\N=C\c2oc(cc2)c3ccccc3Cl	6.3
CHEMBL116206	Cc1cc(Nc2ccc(cc2)C(F)(F)F)[nH]n1	4.78
CHEMBL116946	Cc1n[nH]c(Nc2ccc(cc2)C(F)(F)F)c1C	4.65
CHEMBL118125	Cc1n[nH]c(Nc2c(F)cc(F)cc2F)c1C#N	4.65
CHEMBL118168	FC(F)(F)c1ccc(Nc2[nH]nc3CCCCc23)cc1	5.21
CHEMBL118395	Cc1n[nH]c(Nc2ccc(OC(F)(F)F)cc2)c1C#N	6.3
CHEMBL118468	CC(C)c1n[nH]c(Nc2ccc(cc2)C(F)(F)F)c1C#N	5.4
CHEMBL118894	Cc1n[nH]c(Nc2ccc(cc2)C(F)(F)F)c1CO	5.57
CHEMBL119801	Cc1n[nH]c(Nc2ccc(cc2)C#N)c1C#N	5.5
CHEMBL120640	Cc1n[nH]c(Nc2ccc(cc2)C(C)(C)C)c1C#N	5.44
CHEMBL1237007	OC(=O)c1cccnc1Nc2ccc(Cl)cc2	6.4
CHEMBL1332971	Cc1c(Cl)cccc1Nc2ncccc2C(=O)O	4.89
CHEMBL135703	Cc1cc(O)n2nc(SCc3ccccc3)nc2n1	4.05
CHEMBL1373924	COc1cccc(c1)C(=O)Nc2nc3ccccc3s2	5.17
CHEMBL141732	O\C(=C(\C#N)/C(=O)Nc1ccc(cc1)C(F)(F)F)\C2CC2	6.93
CHEMBL142996	O\C(=C(\C#N)/C(=O)Nc1ccc(cc1)c2ccccc2)\C3CC3	7.28
CHEMBL1450	OC1=C([C@@H]2CC[C@H](CC2)c3ccc(Cl)cc3)C(=O)c4ccccc4C1=O	4.84
CHEMBL1460972	CCOC(=O)c1sc(Nc2ccc(Br)cc2)nc1C	5.04
CHEMBL154121	COc1ccccc1c2cc(F)c(NC(=O)C3=C(CCC3)C(=O)O)c(F)c2	7.38
CHEMBL154151	CN(C)c1ccc(cc1)c2ccc(NC(=O)C3=C(CCC3)C(=O)O)cc2Cl	7.3
CHEMBL154214	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(cc2F)c3ccc(OC(F)(F)F)cc3	5.24
CHEMBL154336	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(cc2C#N)c3cccc(OC(F)(F)F)c3	6.43
CHEMBL154372	COc1cccc(c1)c2ccc(NC(=O)C3=C(CCC3)C(=O)O)c(OC)c2	6.77
CHEMBL154493	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(cc2F)c3cccc(OC(F)(F)F)c3	6.55
CHEMBL154513	OC(=O)C1=C(CCC1)C(=O)Nc2c(F)cc(cc2F)c3ccccc3F	7.35
CHEMBL154613	CN(C)c1ccc(cc1)c2cc(F)c(NC(=O)C3=C(CCC3)C(=O)O)c(F)c2	6.21
CHEMBL154623	OC(=O)C1=C(CCC1)C(=O)Nc2c(F)c(F)c(c(F)c2F)c3cccc(OC(F)(F)F)c3	8.15
CHEMBL154908	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(cc2Cl)c3ccc(Br)cc3	5.54
CHEMBL155530	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(cc2[N+](=O)[O-])c3cccc(OC(F)(F)F)c3	6.41
CHEMBL155548	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(cc2Cl)c3cccc(OC(F)(F)F)c3	6.54
CHEMBL155597	Cc1cc(ccc1NC(=O)C2=C(CCC2)C(=O)O)c3cccc(OC(F)(F)F)c3	6.82
CHEMBL155732	COc1cc(ccc1NC(=O)C2=C(CCC2)C(=O)O)c3ccccc3Cl	6.65
CHEMBL157004	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(cc2C(F)(F)F)c3cccc(OC(F)(F)F)c3	6.08
CHEMBL1571058	OC(=O)c1cc(nc2ccccc12)c3ccc4OCOc4c3	5.29
CHEMBL157164	CC(C)(C)c1ccc(cc1)c2ccc(NC(=O)C3=C(CCC3)C(=O)O)cc2Cl	7.1
CHEMBL157277	COc1ccccc1c2ccc(NC(=O)C3=C(CCC3)C(=O)O)c(Cl)c2	6.51
CHEMBL1596993	COc1ccc(Nc2ccccc2C(=O)O)cc1	5
CHEMBL1599552	Cc1cc(O)n2nc(SCc3ccccc3Cl)nc2n1	4.92

CHEMBL1617398	Cc1c(Nc2ncccc2C(=O)O)cccc1C(F)(F)F	5.1
CHEMBL1704856	Cc1cc(O)n2nc(SCc3ccc(Cl)cc3)nc2n1	4.41
CHEMBL1929432	CC\C(=C(/C#N)\C(=O)Nc1ccc(OS(=O)(=O)C(F)(F)F)cc1)\O	6.82
CHEMBL1929433	CC\C(=C(/C#N)\C(=O)Nc1ccc(OS(=O)(=O)C(F)(F)F)c(c1)C(=O)OC)\O	7.03
CHEMBL1929434	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2ccccc2)c(c1)C(=O)OC)\O	7.14
CHEMBL1929435	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2ccc(F)cc2)c(c1)C(=O)OC)\O	6.96
CHEMBL1929436	CC\C(=C(/C#N)\C(=O)Nc1ccc(c(c1)C(=O)OC)c2ccccc2Cl)\O	7.28
CHEMBL1929437	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2cccc(Cl)c2)c(c1)C(=O)OC)\O	7.51
CHEMBL1929438	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2ccc(Cl)cc2)c(c1)C(=O)OC)\O	7.35
CHEMBL1929439	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2cccc(OC(F)(F)F)c2)c(c1)C(=O)OC)\O	7.57
CHEMBL1929440	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2cccc(F)c2)c(c1)C(=O)OC)\O	6.7
CHEMBL1929441	CC\C(=C(/C#N)\C(=O)Nc1ccc(c(c1)C(=O)OC)c2ccc(F)cc2F)\O	7.51
CHEMBL1929442	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2cccnc2)c(c1)C(=O)OC)\O	7.4
CHEMBL1929443	CC\C(=C(/C#N)\C(=O)Nc1ccc(c(c1)C(=O)OC)c2ccc(F)cc2C)\O	7.31
CHEMBL1929444	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2ccc(F)nc2)c(c1)C(=O)OC)\O	6.82
CHEMBL1929445	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2ccc(F)c(F)c2)c(c1)C(=O)OC)\O	7.01
CHEMBL1929446	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2cc(F)c(F)c(F)c2)c(c1)C(=O)OC)\O	6.86
CHEMBL1929447	CC\C(=C(/C#N)\C(=O)Nc1ccc(c(c1)C(=O)OC)c2ccc(F)cc2OC)\O	7.18
CHEMBL1929448	CCOc1cccc(c1)c2ccc(NC(=O)\C(=C(/O)\CC)\C#N)cc2C(=O)OC	7.23
CHEMBL1929449	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2ccc3OCOc3c2)c(c1)C(=O)OC)\O	7.12
CHEMBL1929450	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2cccc(OC)c2)c(c1)C(=O)OC)\O	7.58
CHEMBL1929451	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2ccc3OCCOc3c2)c(c1)C(=O)OC)\O	7.18
CHEMBL1929452	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2cccc(OC(F)F)c2)c(c1)C(=O)OC)\O	7.47
CHEMBL1929453	CC\C(=C(/C#N)\C(=O)Nc1ccc(c2cccc(OC3CCC3)c2)c(c1)C(=O)OC)\O	7.51
CHEMBL193365	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(OCc3c(F)cccc3Cl)c(Cl)c2	7.96
CHEMBL193371	OC(=O)C1=C(COC1)C(=O)Nc2ccc(OCc3c(F)cccc3Cl)c(Cl)c2	7.39
CHEMBL194023	COc1cccc(c1)c2ccc(NC(=O)C3=C(CSC3)C(=O)O)c(F)c2	6.88
CHEMBL194075	OC(=O)C1=C(CSC1)C(=O)Nc2c(F)cc(cc2F)c3cccc(OC(F)(F)F)c3	7.82
CHEMBL194395	COc1cccc(c1)c2ccc(NC(=O)C3=C(C(O)CC3)C(=O)O)c(F)c2	6.17
CHEMBL194776	OC(=O)C1=C(CSC1)C(=O)Nc2cc(Br)c(OCc3c(F)cccc3Cl)c(Br)c2	6.98
CHEMBL194954	OC(=O)C1=C(COC1)C(=O)Nc2c(F)c(F)c(c(F)c2F)c3cccc(OC(F)(F)F)c3	7.24
CHEMBL194955	OC(=O)C1=C(CSC1)C(=O)Nc2c(F)c(F)c(c(F)c2F)c3cccc(OC(F)(F)F)c3	8.4
CHEMBL195163	OC(=O)C1=C(COC1)C(=O)Nc2c(F)cc(cc2F)c3cccc(OC(F)(F)F)c3	6.69
CHEMBL195246	OC(=O)C1=C(CSC1)C(=O)Nc2cc(Br)c(OCc3ccccc3)c(Br)c2	6.76
CHEMBL195622	COc1cccc(c1)c2cc(F)c(NC(=O)C3=C(CCC3)C(=O)O)c(F)c2	7.96
CHEMBL1956291	Cc1cc(Nc2ccc(cc2)S(F)(F)(F)(F)F)n3nc(nc3n1)C(F)(F)F	4.39
CHEMBL1957366	Oc1c(C#N)c(nc2ccncc12)c3ccc(cc3)c4ccccc4OC(F)(F)F	6.7
CHEMBL1957370	Oc1c(C#N)c(nc2ccncc12)c3ccc(cc3)c4ccncc4Cl	5.2
CHEMBL1957380	Oc1c(C#N)c(nc2ccncc12)c3ccc(cc3)c4cccnc4	5.24
CHEMBL1957460	Cc1nccc(c1Cl)c2ccc(cc2)c3nc4ccncc4c(O)c3C#N	5.89
CHEMBL1957462	Cc1nn(C)c(C)c1c2ccc(cc2)c3nc4ccncc4c(O)c3C#N	5.96
CHEMBL196173	OC(=O)C1=C(CS(=O)(=O)C1)C(=O)Nc2ccc(cc2)c3ccccc3	5.42
CHEMBL196181	OC(=O)C1=C(CCC1)C(=O)Nc2cc(Br)c(OCc3c(F)cccc3Cl)c(Br)c2	6.96
CHEMBL196256	COc1cccc(c1)c2ccc(NC(=O)C3=C(CCC3O)C(=O)O)c(F)c2	5.84

CHEMBL197194	COc1cccc(c1)c2ccc(NC(=O)C3=C(CCC3)C(=O)O)c(F)c2	6.87
CHEMBL197455	COc1cccc(c1)c2ccc(NC(=O)C3=C(COC3)C(=O)O)c(F)c2	6.44
CHEMBL197553	OC(=O)C1=C(CCC1)C(=O)Nc2cc(Br)c(OCc3ccccc3)c(Br)c2	6.9
CHEMBL199347	OC(=O)c1cscc1C(=O)Nc2c(F)cc(cc2F)c3ccccc3OC(F)(F)F	8
CHEMBL199361	COc1ccccc1c2c(F)c(F)c(NC(=O)c3ccsc3C(=O)O)c(F)c2F	9
CHEMBL199501	OC(=O)c1cscc1C(=O)Nc2ccc(cc2)c3ccccc3	6
CHEMBL199574	OC(=O)c1ccccc1NC(=O)c2ccc3cc(Br)ccc3c2	5.08
CHEMBL200536	OC(=O)c1ccccc1NC(=O)c2ccc3ccccc3c2	4.86
CHEMBL200699	CCOc1cccc(c1)c2cc(F)c(NC(=O)c3ccsc3C(=O)O)c(F)c2	8.52
CHEMBL200856	CCOc1ccccc1c2cc(F)c(NC(=O)c3ccsc3C(=O)O)c(F)c2	8.05
CHEMBL200858	COc1ccccc1c2ccc(NC(=O)c3ccsc3C(=O)O)cc2Cl	7.92
CHEMBL200895	CCOc1cccc(c1)c2cc(F)c(NC(=O)c3cocc3C(=O)O)c(F)c2	7.8
CHEMBL2012831	CCCc1nc2ccccc2n1c3ccc(s3)C(=O)NC4CC4	4.82
CHEMBL2012961	Cc1cc(F)c2ncn(c3ccc(s3)C(=O)NC4CC4)c2c1	5.51
CHEMBL2012963	Fc1cc(Cl)c2ncn(c3ccc(s3)C(=O)NC4CC4)c2c1	5.25
CHEMBL2012964	Cc1cc(F)c2c(c1)ncn2c3ccc(s3)C(=O)NC4CC4	5.14
CHEMBL2012965	FC(F)(F)c1ccc2c(c1)ncn2c3ccc(s3)C(=O)NC4CC4	4.76
CHEMBL2012966	Fc1cccc2c1ncn2c3ccc(s3)C(=O)NC4CC4	4.83
CHEMBL202431	OC(=O)c1sccc1C(=O)Nc2c(F)cc(cc2F)c3cccc(OC(F)(F)F)c3	8.7
CHEMBL2043303	OC(=O)c1ccccc1Nc2ccc(Cl)cc2	6.38
CHEMBL2177115	COC(=O)c1ccc(Nc2nc(c(C)s2)c3ccc(Cl)cc3)cc1	5.9
CHEMBL2177491	Fc1ccc(\C=C\C(=O)Nc2ccccn2)cc1	4.89
CHEMBL2177492	OC(=O)c1ccc(\C=N\c2cccc3ccccc23)cc1	4.81
CHEMBL2177493	Cc1ccccc1C(=O)Nc2cc(Cl)c(O)c(Cl)c2	4.79
CHEMBL2177494	Cc1ccc(C)c(c1)\N=C\c2cccc(O)c2O	4.75
CHEMBL2177495	N1c2ccccc2Oc3nc4ccccc4nc13	4.74
CHEMBL2177853	Cc1cc(O)n2nc(SCc3ccc(Br)cc3)nc2n1	4.5
CHEMBL2177854	COc1ccc(CSc2nc3nc(C)cc(O)n3n2)cc1	4.2
CHEMBL2177855	Cc1cc(O)n2nc(SCc3ccccc3[N+](=O)[O-])nc2n1	5.02
CHEMBL2177856	Cc1cc(O)n2nc(SCc3ccc(Cl)c(Cl)c3)nc2n1	5.19
CHEMBL2177857	Cc1cc(O)n2nc(SCc3c(Cl)cccc3Cl)nc2n1	4.75
CHEMBL2177858	Cc1cc(O)n2nc(SCc3cc(Cl)ccc3Cl)nc2n1	7.29
CHEMBL2177859	Cc1cc(C)cc(CSc2nc3nc(C)cc(O)n3n2)c1	4.52
CHEMBL2177860	CCc1cc(O)n2nc(SCc3ccc(Cl)cc3)nc2n1	4.89
CHEMBL2177861	CCc1cc(O)n2nc(SCc3cc(Cl)ccc3Cl)nc2n1	7.89
CHEMBL2178104	O=Cc1ccccc1\C=N\Nc2nc(cs2)c3ccccc3	6.96
CHEMBL2178105	ClC(Cl)(Cl)c1cccc(c1)C(=O)Nc2nc3ccccc3s2	6.47
CHEMBL2178106	CCc1cccc(NC(=O)\C=C\c2ccc(Cl)c(Cl)c2)c1	6.26
CHEMBL2178107	Oc1ccc(\C=N\c2cccc3ccccc23)c(O)c1	6.11
CHEMBL2178109	Clc1ccc(C(=O)Nc2nc3ccccc3s2)c(Cl)c1	5.74
CHEMBL2178110	CC1=NN(C(=O)/C/1=C/c2oc(cc2)c3cccc(c3)C(=O)O)c4ccccc4	5.56
CHEMBL2178111	Oc1ccc(cc1)\N=C\c2ccc3ccccc3c2	5.4
CHEMBL2178112	OC(=O)c1cc(\C=C\C(=O)c2ccc(Cl)cc2)ccc1O	5.22
CHEMBL2178513	Cc1cc(O)n2nc(SCc3cccc(Cl)c3)nc2n1	4.54

CHEMBL2178514	Cc1ccc(CSc2nc3nc(C)cc(O)n3n2)cc1	4.34
CHEMBL217918	Cc1ccc2nc(c(O)c(C(=O)O)c2c1)c3ccc(Cl)cc3	6.66
CHEMBL217919	Cc1cccc2nc(c(O)c(C(=O)O)c12)c3ccc(Cl)cc3	4.29
CHEMBL217959	Cc1ccc2c(C(=O)O)c(O)c(nc2c1)c3ccc(Cl)cc3	4.77
CHEMBL218051	Cc1cc(Br)cc2c(C(=O)O)c(O)c(nc12)c3ccc(Cl)cc3	4.39
CHEMBL218052	OC(=O)c1c(O)c(nc2ccc(OC(F)(F)F)cc12)c3ccc(Cl)cc3	5.4
CHEMBL218062	OC(=O)c1c(O)c(nc2ccccc12)c3ccc(cc3)c4ccc(O)cc4	8.22
CHEMBL218084	OC(=O)c1c(O)c(nc2ccc(F)cc12)c3ccc(Oc4ccccc4)cc3	8.22
CHEMBL218085	OC(=O)c1c(O)c(nc2ccc(F)cc12)c3ccc(Sc4ccccc4)cc3	7.75
CHEMBL218169	OC(=O)c1c(O)c(nc2ccccc12)c3ccc(Oc4ccccc4)cc3	8.15
CHEMBL218249	Nc1c(nc2ccc(F)cc2c1C(=O)O)c3ccc(cc3)c4ccccc4	7.92
CHEMBL218464	OC(=O)c1c(O)c(nc2ccc(F)cc12)c3ccc(Cl)cc3	6.51
CHEMBL218467	CCOC(=O)C(=CNc1ccc2sc3ccccc3c2c1)C(=O)OCC	4.53
CHEMBL218583	OC(=O)c1c(O)c(nc2c(cccc12)c3ccccc3)c4ccc(Cl)cc4	4.58
CHEMBL218700	OC(=O)c1c(O)c(nc2ccc(Br)cc12)c3ccc(Cl)cc3	6.68
CHEMBL219174	Cc1ccc2c(C(=O)O)c(O)c(nc2c1C)c3ccc(cc3)C(F)(F)F	4.5
CHEMBL219376	OC(=O)c1c(O)c(nc2ccccc12)c3ccccc3	4.92
CHEMBL219489	OC(=O)c1c(O)c(nc2ccc(F)cc12)c3ccc(O)cc3	5.68
CHEMBL219520	COc1ccc2nc(c(O)c(C(=O)O)c2c1)c3ccc(Cl)cc3	4.37
CHEMBL219648	OC(=O)c1c(O)c(nc2ccccc12)c3ccc(cc3)c4ccccc4	8
CHEMBL220467	Cc1c(nc2ccc(F)cc2c1C(=O)O)c3ccc(cc3)c4ccccc4	8.15
CHEMBL222556	Oc1ccc(cc1O)C2=CC(=O)c3ccccc3O2	4.91
CHEMBL2259675	OC(=O)c1cc(Cl)cnc1Nc2c(F)cc(cc2F)c3ccccc3	8.1
CHEMBL2263447	OC(=O)c1cc(cnc1Nc2c(F)cc(cc2F)c3ccccc3Cl)C4CC4	8.3
CHEMBL2263448	Cc1c(F)c(Nc2ncccc2C(=O)O)c(F)cc1c3cccc(OC(F)(F)F)c3	8.22
CHEMBL2263449	Cc1c(F)c(Nc2ncccc2C(=O)O)c(F)cc1c3ccccc3Cl	8.4
CHEMBL2263625	COc1cccc(c1)c2c(F)c(F)c(Nc3ncccc3C(=O)O)c(F)c2F	8.52
CHEMBL2263626	Cc1ccccc1c2cc(F)c(Nc3ncccc3C(=O)O)c(F)c2	7.96
CHEMBL2263627	CCOc1cccc(c1)c2ccc(Nc3ncccc3C(=O)O)c(F)c2	6.7
CHEMBL2263628	COc1cccc(c1)c2cc(F)c(Nc3ncccc3C(=O)O)cc2F	7.06
CHEMBL2263629	COc1cccc(c1)c2ccc(Nc3ncccc3C(=O)O)c(Cl)c2	6.82
CHEMBL2263630	OC(=O)c1cccnc1Nc2c(F)cc(cc2F)c3cccc(OC4CCC4)c3	7.05
CHEMBL2263631	CCOc1cccc(c1)c2cc(F)c(Nc3ncccc3C(=O)O)c(F)c2	7.72
CHEMBL2263632	COc1cccc(c1)c2cc(F)c(Nc3ncccc3C(=O)O)c(F)c2	7.82
CHEMBL2263636	Cc1cnc(Nc2ccc(cc2F)c3cccc(OC(F)(F)F)c3)c(c1)C(=O)O	6.96
CHEMBL2263637	COc1cccc(c1)c2ccc(Nc3ncc(cc3C(=O)O)C4CC4)c(F)c2	7.48
CHEMBL2263638	COc1cccc(c1)c2cc(F)c(Nc3ncc(C)cc3C(=O)O)c(F)c2	7.92
CHEMBL2263639	COc1cccc(c1)c2cc(F)c(Nc3ncccc3C(=O)O)cc2C	7
CHEMBL2263640	CCc1cnc(Nc2c(F)cc(cc2F)c3cccc(OC)c3)c(c1)C(=O)O	7.92
CHEMBL2263641	CCOc1cccc(c1)c2cc(F)c(Nc3ncc(cc3C(=O)O)C4CC4)cc2F	7.64
CHEMBL2263642	COc1cccc(c1F)c2cc(F)c(Nc3ncccc3C(=O)O)c(F)c2	7.28
CHEMBL2263643	OC(=O)c1cccnc1Nc2c(F)cc(cc2F)c3cccc(OC4CC4)c3	7.77
CHEMBL2263644	Cc1c(F)c(Nc2ncccc2C(=O)O)c(F)cc1c3ccccc3	8.3
CHEMBL2263645	OC(=O)c1cc(cnc1Nc2c(F)cc(cc2F)c3cccc(OC4CC4)c3)C5CC5	8.22

CHEMBL2263646	OC(=O)c1cc(cnc1Nc2c(F)cc(cc2F)c3cccc(OC(F)(F)F)c3)C4CC4	8.4
CHEMBL2335126	CC(C)c1ccc(cc1)c2nc3ccccc3c(C(=O)O)c2C	5.8
CHEMBL2385510	CC(C)(C)c1ccc(Oc2ccc(cc2)c3cc(C(=O)O)c4cc(F)ccc4n3)cc1	7.72
CHEMBL2385511	Cc1cc(cc(C)c1Oc2ccccc2)c3cc(C(=O)O)c4cc(F)ccc4n3	7.8
CHEMBL2385512	CC(C)c1cc(c(C)cc1Oc2ccccc2)c3cc(C(=O)O)c4cc(F)ccc4n3	9
CHEMBL2385514	OC(=O)c1cc(nc2ccc(Cl)cc12)c3ccc(Oc4ccccc4)cc3	7.02
CHEMBL2385515	OC(=O)c1cc(nc2ccc(F)cc12)c3ccc(Oc4ccccc4)cc3	7.44
CHEMBL2385715	CCCOc1ccc(cc1)c2cc(C(=O)O)c3cc(Cl)ccc3n2	6.58
CHEMBL2385719	OC(=O)c1cc(nc2ccc(Cl)cc12)c3ccc(OC(F)(F)F)cc3	6.51
CHEMBL2385720	OC(=O)c1cc(nc2ccc(Cl)cc12)c3ccc(F)cc3	5.8
CHEMBL2385721	Cc1ccc(cc1)c2cc(C(=O)O)c3cc(Cl)ccc3n2	5.23
CHEMBL2431484	CCCNC(=O)C1=C(Nc2ccc(C)c(C)c2)SCC1=O	5.2
CHEMBL2431485	CCCCNC(=O)C1=C(Nc2ccc(C)c(C)c2)SCC1=O	5.35
CHEMBL2431486	Cc1ccc(NC2=C(C(=O)NC3CC3)C(=O)CS2)cc1C	5.39
CHEMBL2431487	Cc1ccc(NC2=C(C(=O)NCC3CC3)C(=O)CS2)cc1C	5.74
CHEMBL2431513	CCOC(=O)C1=C(Nc2ccc3CCCCc3c2)SCC1=O	4.92
CHEMBL2431523	CCCOC(=O)C1=C(Nc2ccc(C)c(C)c2)SCC1=O	4.93
CHEMBL267210	Cc1ccc2c(C(=O)O)c(O)c(nc2c1C)c3ccc(Cl)cc3	4.14
CHEMBL304401	CCc1oncc1\C(=N\c2ccc(cc2)C(F)(F)F)\S	5.52
CHEMBL305215	S=C(Nc1ccc(cc1)C#N)c2cnoc2C3CC3	5.03
CHEMBL306100	Cc1oncc1\C(=N\c2ccc(cc2)C#N)\S	4.46
CHEMBL306784	CCc1oncc1\C(=N\c2ccc(OC(F)(F)F)cc2)\S	6.16
CHEMBL308141	FC(F)(F)Oc1ccc(NC(=S)c2cnoc2C3CC3)cc1	6.1
CHEMBL3183877	O=C(CCNC(=O)c1ccc(cc1)C#N)N[C@@H]2CCCc3ccccc23	5.05
CHEMBL3184096	FC(F)(F)c1ccc(cc1)C(=O)NCCC(=O)N[C@@H]2CCCc3ccccc23	6.04
CHEMBL3184132	FC(F)(F)Oc1ccc(cc1)C(=O)NCCC(=O)N[C@@H]2CCCc3ccccc23	6.25
CHEMBL3184332	Cc1ccc(cc1)C(=O)NCCC(=O)N[C@@H]2CCCc3ccccc23	5.72
CHEMBL3185911	Fc1ccc(cc1)C(=O)NCCC(=O)N[C@@H]2CCCc3ccccc23	5.02
CHEMBL3186409	Clc1cccc(c1)C(=O)NCCC(=O)N[C@@H]2CCCc3ccccc23	5.13
CHEMBL3186954	Clc1ccc(cc1)C(=O)NCCC(=O)N[C@@H]2CCCc3ccccc23	5.89
CHEMBL3187986	COc1ccc(cc1)C(=O)NCCC(=O)N[C@@H]2CCCc3ccccc23	5.44
CHEMBL3188811	FC1(F)Oc2ccc(cc2O1)C(=O)NCCC(=O)N[C@@H]3CCCc4ccccc34	5.57
CHEMBL3188954	Clc1ccc(cc1Cl)C(=O)NCCC(=O)N[C@@H]2CCCc3ccccc23	5.82
CHEMBL3286441	COc1ccc2nc(C(=O)Nc3ccc(cc3)c4ccccc4)c(C)c(O)c2c1	5.64
CHEMBL3289670	Cc1cc(Nc2ccc(c(F)c2)C(F)(F)F)n3nc(nc3n1)C(C)(F)F	4.77
CHEMBL3289671	Cc1cc(Nc2cc(F)c(c(F)c2)C(F)(F)F)n3nc(nc3n1)C(C)(F)F	5.68
CHEMBL3289672	Cc1cc(Nc2cc(F)c(c(F)c2)C(F)(F)F)n3nc(nc3n1)C(F)(F)F	5.68
CHEMBL3290833	CCc1ccc2nc(C(=O)Nc3c(F)cc(cc3F)c4cccc(F)c4)c(C)c(O)c2c1	5.49
CHEMBL3290836	COc1ccc2nc(C(=O)Nc3c(F)cc(cc3F)c4cccc(F)c4)c(C)c(O)c2c1	6.03
CHEMBL3290838	Cc1c(O)c2cc(ccc2nc1C(=O)Nc3c(F)cc(cc3F)c4cccc(F)c4)C(F)(F)F	5.21
CHEMBL3290842	Cc1c(nc2ccc(F)cc2c1C(=O)O)C(=O)Nc3c(F)cc(cc3F)c4cccc(F)c4	5.34
CHEMBL3290843	CCOc1ccc2nc(C(=O)Nc3c(F)cc(cc3F)c4cccc(F)c4)c(C)c(C(=O)O)c2c1	5.55
CHEMBL3290845	Cc1c(nc2ccc(OC(F)(F)F)cc2c1C(=O)O)C(=O)Nc3c(F)cc(cc3F)c4cccc(F)c4	5.82
CHEMBL3290846	Cc1c(nc2ccc(cc2c1C(=O)O)C(F)(F)F)C(=O)Nc3c(F)cc(cc3F)c4cccc(F)c4	5.46

CHEMBL3290847	COc1ccc2nc(C(=O)Nc3ccc(cc3)c4ccccc4)c(C)c(C(=O)O)c2c1	5.96
CHEMBL330901	Cc1ccc(Nc2[nH]nc(C)c2C#N)cc1	4.92
CHEMBL333344	Cc1n[nH]c(Nc2ccc(cc2)[N+](=O)[O-])c1C#N	5.05
CHEMBL333404	Cc1n[nH]c(Nc2ccc(F)cc2)c1C#N	4.71
CHEMBL334317	Cc1n[nH]c(Nc2ccc(cc2)C(F)(F)F)c1C#N	5.58
CHEMBL3409286	CC(C)Oc1nn(c(C)c1Cc2ccccc2F)c3ncc(cn3)C4CC4	7.9
CHEMBL3409299	CC(C)Oc1nn(c(C)c1C(O)c2ccccc2)c3ncc(cn3)C4CC4	7.8
CHEMBL3409306	CCOc1nn(c(C)c1Oc2ccccc2Br)c3ncc(CC)cn3	6.9
CHEMBL3409491	CCc1cnc(nc1)n2nc(OC(C)C)c(Oc3c(F)cccc3F)c2C	9.1
CHEMBL3410571	CC(=O)c1sc(Nc2ccc(cc2)C(C)(C)C)nc1C	5.44
CHEMBL3410572	CC(=O)c1sc(Nc2ccc(C)c(C)c2)nc1C	5.42
CHEMBL3410574	CC(=O)c1sc(Nc2ccc(Cl)c(c2)C(F)(F)F)nc1C	5.63
CHEMBL3410575	CC(=O)c1sc(Nc2ccc(Br)c(c2)C(F)(F)F)nc1C	5.71
CHEMBL3410576	CC(=O)c1sc(Nc2ccc3ccccc3c2)nc1C	6.25
CHEMBL3410578	CCOC(=O)c1sc(Nc2ccc(C)c(C)c2)nc1C	5.87
CHEMBL3410579	CCOC(=O)c1sc(Nc2ccc(C)c(F)c2)nc1C	5.7
CHEMBL3410580	CCOC(=O)c1sc(Nc2ccc(C)c(Cl)c2)nc1C	6.01
CHEMBL3410581	CCOC(=O)c1sc(Nc2ccc3ccccc3c2)nc1C	6.05
CHEMBL3410582	CCOC(=O)c1sc(Nc2ccc(C)c(C)c2)nc1N	5.68
CHEMBL3410585	CCOC(=O)c1sc(Nc2ccc(Cl)c(c2)C(F)(F)F)nc1NC(=O)C3CC3	5.22
CHEMBL3410586	CCOC(=O)c1sc(Nc2ccc(C)c(C)c2)nc1NC(=O)c3ccccc3	5.04
CHEMBL3410588	CCOC(=O)c1sc(Nc2ccc(C)c(C)c2)nc1C3CC3	6.49
CHEMBL3410589	CCOC(=O)c1sc(Nc2ccc(C)c(F)c2)nc1C3CC3	6.19
CHEMBL3410590	CCOC(=O)c1sc(Nc2ccc(C)c(Cl)c2)nc1C3CC3	6.43
CHEMBL3410591	CCOC(=O)c1sc(Nc2ccc(C)c(C)c2)nc1C(C)(C)C	6.29
CHEMBL3410592	CCOC(=O)c1sc(Nc2ccc(C)c(F)c2)nc1C(C)(C)C	6.19
CHEMBL3410593	CCOC(=O)c1sc(Nc2ccc(C)c(Cl)c2)nc1C(C)(C)C	6.26
CHEMBL3410594	CCOC(=O)c1sc(Nc2ccc(C)c(C)c2)nc1c3ccccc3	7.24
CHEMBL3410595	CCOC(=O)c1sc(Nc2ccc(C)c(F)c2)nc1c3ccccc3	7.31
CHEMBL3410596	CCOC(=O)c1sc(Nc2ccc(C)c(Cl)c2)nc1c3ccccc3	7.46
CHEMBL3410597	CCOC(=O)c1sc(Nc2ccccc2)nc1c3ccccc3	6.11
CHEMBL3410598	CCOC(=O)c1sc(Nc2ccc(OC)cc2)nc1c3ccccc3	5.84
CHEMBL3410599	CCOC(=O)c1sc(Nc2ccc(Cl)cc2)nc1c3ccccc3	6.62
CHEMBL3410600	CCOC(=O)c1sc(Nc2ccc(cc2)C(F)(F)F)nc1c3ccccc3	6.39
CHEMBL3410601	CCOC(=O)c1sc(Nc2ccc(cc2)C(C)(C)C)nc1c3ccccc3	6.55
CHEMBL3410602	CCOC(=O)c1sc(Nc2ccc(Cl)c(c2)C(F)(F)F)nc1c3ccccc3	6.88
CHEMBL3410603	CCOC(=O)c1sc(Nc2ccc(Br)c(c2)C(F)(F)F)nc1c3ccccc3	6.89
CHEMBL3410604	CCOC(=O)c1sc(Nc2ccc(Cl)c(Cl)c2)nc1c3ccccc3	6.76
CHEMBL3410605	CCOC(=O)c1sc(Nc2cc(Cl)cc(Cl)c2)nc1c3ccccc3	6.41
CHEMBL3410607	CCOC(=O)c1sc(Nc2ccc3CCCc3c2)nc1c4ccccc4	7.58
CHEMBL3410608	CCOC(=O)c1sc(Nc2ccc3OCOc3c2)nc1c4ccccc4	5.96
CHEMBL3410610	CCOC(=O)c1sc(Nc2ccc3ccccc3c2)nc1c4ccccc4	7.54
CHEMBL3410611	CCOC(=O)c1sc(Nc2ccc3cc4ccccc4cc3c2)nc1c5ccccc5	6.34
CHEMBL3410616	CCOC(=O)c1sc(Nc2c(F)cc(cc2F)c3cccc(OC)c3)nc1c4ccccc4	6.51

CHEMBL345147	OC(=O)C1=C(CCC1)C(=O)Nc2c(F)cc(cc2F)c3ccccc3Cl	7.75
CHEMBL345446	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(cc2F)c3ccc(Br)cc3	6.13
CHEMBL345464	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(c(Cl)c2)c3cccc(OC(F)(F)F)c3	7.7
CHEMBL345685	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(cc2F)c3cccc(O)c3	6.21
CHEMBL345701	COc1ccccc1c2c(F)c(F)c(NC(=O)C3=C(CCC3)C(=O)O)c(F)c2F	8.1
CHEMBL347148	COc1ccc(cc1)c2ccc(NC(=O)C3=C(CCC3)C(=O)O)c(F)c2	5.77
CHEMBL348270	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(cc2)c3ccccc3	6.39
CHEMBL348871	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(c(Cl)c2)c3ccc(Br)cc3	7.16
CHEMBL349577	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(cc2C(F)(F)F)c3cccc4ccccc34	6.75
CHEMBL351786	CCOc1cccc(c1)c2cc(F)c(NC(=O)C3=C(CCC3)C(=O)O)c(F)c2	7.77
CHEMBL358435	COc1ccc(cc1)c2ccc(NC(=O)C3=C(CCC3)C(=O)O)c(Cl)c2	5.08
CHEMBL3589752	CC(C)Oc1nn(c(C)c1Oc2c(F)cccc2F)c3ncc(cc3F)C4CC4	7.6
CHEMBL3593251	CC(=O)Nc1ccc(cc1)c2ccc(cc2)c3nc4c(cc(C)cc4[nH]3)C(=O)O	6.68
CHEMBL3593802	CC(=O)Nc1cccc(c1)c2ccc(cc2)c3nc4c(cc(C)cc4[nH]3)C(=O)O	5.86
CHEMBL3593803	CC(=O)Nc1ccccc1c2ccc(cc2)c3nc4c(cc(C)cc4[nH]3)C(=O)O	4.5
CHEMBL3593804	CC(=O)Nc1ccccc1COc2ccc(cc2)c3ccc(cc3)c4nc5c(cc(C)cc5[nH]4)C(=O)O	6.52
CHEMBL3593805	CC(=O)Nc1cccc(COc2ccc(cc2)c3ccc(cc3)c4nc5c(cc(C)cc5[nH]4)C(=O)O)c1	7.55
CHEMBL3593806	CC(=O)Nc1ccc(COc2ccc(cc2)c3ccc(cc3)c4nc5c(cc(C)cc5[nH]4)C(=O)O)cc1	7.89
CHEMBL3593807	CC(=O)Nc1cc(ccc1c2ccccc2)c3nc4c(cc(C)cc4[nH]3)C(=O)O	4.33
CHEMBL3593808	Cc1cc(C(=O)N)c2nc([nH]c2c1)c3ccc(cc3)c4ccccc4	5.11
CHEMBL3593812	NC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4ccc(N)nc4	4.7
CHEMBL3593813	NC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4cncc(c4)C(=O)N5CCCC5	4.55
CHEMBL3593981	Cc1cc(C(=O)N)c2nc([nH]c2c1)c3ccc(cc3)c4cncc(c4)C(=O)N5CCCC5	4.3
CHEMBL3593983	Cc1cc(C(=O)N)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(nc4)C(=O)N5CCCC5	4.43
CHEMBL3593984	CC(=O)Nc1ccccc1c2ccc(cc2)c3nc4c(cccc4[nH]3)C(=O)N	4.29
CHEMBL3593985	CC(=O)Nc1cccc(c1)c2ccc(cc2)c3nc4c(cccc4[nH]3)C(=O)N	4.38
CHEMBL3593986	CC(=O)Nc1ccc(cc1)c2ccc(cc2)c3nc4c(cccc4[nH]3)C(=O)N	4.25
CHEMBL3593987	NC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4ccc(cc4)C(=O)N5CCCC5	4.7
CHEMBL3593989	CC(=O)Nc1ccc(cn1)c2ccc(cc2)c3nc4c(cccc4[nH]3)C(=O)N	4.4
CHEMBL3593990	NC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4cncc(CN5CCCC5)c4	4.26
CHEMBL3593992	NC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4ccc(OCCN5CCCCC5)cc4	4.51
CHEMBL3593993	NC(=O)c1cc(F)cc2[nH]c(nc12)c3ccc(cc3F)c4ccc(NC(=O)C5CC5)cc4F	4.32
CHEMBL3593995	NC(=O)c1cc(F)cc2[nH]c(nc12)c3ccc(cc3F)c4cccc(NC(=O)C5CC5)c4	4.42
CHEMBL3593996	COc1cc(ccc1NC(=O)C2CC2)c3ccc(c(F)c3)c4nc5c(cc(F)cc5[nH]4)C(=O)N	4.64
CHEMBL3593998	OC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4ccccc4	6.12
CHEMBL3639735	Cc1ccc(Nc2cnc(c(C)c2)c3ccccc3C(F)(F)F)c(c1)C(=O)O	7.7
CHEMBL3639766	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4ccccc4F	8.46
CHEMBL3674625	OC(=O)c1cc(ccc1Nc2cnc(nc2)c3ccccc3)C4CC4	6.98
CHEMBL3674626	Cc1ccc(Nc2ccc(nc2)c3cccc(c3)C(F)(F)F)c(c1)C(=O)O	7.01
CHEMBL3674627	OC(=O)c1cc(ccc1Nc2cnc(nc2)c3c(F)cc(O)cc3F)C4CC4	7.24
CHEMBL3674628	COc1ncc(Nc2ccc(cc2C(=O)O)C3CC3)cc1c4ccccc4	7.31
CHEMBL3674629	Cc1ccc(Nc2cnc(c(F)c2)c3ccccc3)c(c1)C(=O)O	7.75
CHEMBL3674630	OC(=O)c1cc(ccc1Nc2cnc(nc2)c3ccccc3C4CC4)C5CC5	7.24
CHEMBL3674631	OC(=O)c1cc(ccc1Nc2cncc(c2)c3ccccc3)C4CC4	6.95

CHEMBL3674632	Cc1ccc(Nc2cc(Cl)cnc2c3ccccc3)c(c1)C(=O)O	7.21
CHEMBL3674633	OC(=O)c1cc(ccc1Nc2cnc(c3ccccc3)c(c2)c4ccccc4)C5CC5	8
CHEMBL3674634	OC(=O)c1cc(ccc1Nc2cnc(nc2)c3cccc(OC4CC4)c3)C5CC5	6.94
CHEMBL3674635	OC(=O)c1cc(ccc1Nc2cnc(C3CC3)c(c2)c4ccccc4)C5CC5	7.55
CHEMBL3674636	Cc1ccc(Nc2cnc(N3CCCCC3)c(C)c2)c(c1)C(=O)O	7.39
CHEMBL3674637	Cc1ccc(Nc2cnc(N3CCCCCC3)c(C)c2)c(c1)C(=O)O	6.92
CHEMBL3674638	Cc1ccc(Nc2ccc(nc2)c3ccncc3Cl)c(c1)C(=O)O	6.96
CHEMBL3674639	CCOc1cccc(c1)c2ccc(Nc3ccc(C)cc3C(=O)O)cn2	6.72
CHEMBL3674640	CCOc1cccc(c1)c2ncc(Nc3ccc(C)cc3C(=O)O)cc2C	7.52
CHEMBL3674641	CCOc1cccc(c1)c2cc(C)c(Nc3ccc(C)cc3C(=O)O)cn2	7.11
CHEMBL3674642	COc1cccc(c1)c2ncc(Nc3ccc(cc3C(=O)O)C(F)(F)F)cc2C	6.86
CHEMBL3674643	COc1cccc(c1)c2ncc(Nc3ccc(C)cc3C(=O)O)cc2C	7.68
CHEMBL3674644	CCOc1ccc(F)c(c1)c2ccc(Nc3ccc(C)cc3C(=O)O)cn2	7.72
CHEMBL3674645	Cc1ccc(Nc2ccc(nc2)c3ccccc3F)c(c1)C(=O)O	7.04
CHEMBL3674646	Cc1ccc(Nc2cnc(c(C)c2)c3ccccc3)c(c1)C(=O)O	7.28
CHEMBL3674647	CC(C)Oc1ccc(F)c(c1)c2ccc(Nc3ccc(C)cc3C(=O)O)cn2	7.55
CHEMBL3674648	CC(C)Oc1cccc(c1)c2ncc(Nc3ccc(C)cc3C(=O)O)cc2C	7.96
CHEMBL3674649	Cc1ccc(Nc2cnc(c(C)c2)c3ccccc3Cl)c(c1)C(=O)O	7.85
CHEMBL3674650	Cc1ccc(Nc2cnc(c(C)c2)c3cccc(c3)C(=O)N)c(c1)C(=O)O	6.72
CHEMBL3674651	COc1ccc(F)c(c1)c2cc(C)c(Nc3ccc(C)cc3C(=O)O)cn2	7.01
CHEMBL3674652	COc1cccc(c1)c2ncc(Nc3ccc(C)cc3C(=O)O)cc2C(F)(F)F	7.92
CHEMBL3674653	CN(C)C(=O)c1cccc(c1)c2ncc(Nc3ccc(C)cc3C(=O)O)cc2C	7.48
CHEMBL3674654	Cc1ccc(Nc2ccc(nc2)c3ccccc3Cl)c(c1)C(=O)O	7.5
CHEMBL3674655	Cc1cc(Nc2ccc(cc2C(=O)O)C3CC3)cnc1c4cccc(OC(F)(F)F)c4	8.3
CHEMBL3674656	Cc1cc(Nc2ccc(cc2C(=O)O)C3CC3)cnc1c4ccccc4	8.22
CHEMBL3674657	Cc1ccc(Nc2cnc(c(C)c2)c3cccc(Cl)c3)c(c1)C(=O)O	8
CHEMBL3674658	Cc1ccc(Nc2cnc(c(C)c2)c3ccccc3F)c(c1)C(=O)O	8.3
CHEMBL3674659	Cc1ccc(Nc2cnc(c(C)c2)c3ccncc3F)c(c1)C(=O)O	7.43
CHEMBL3674660	OC(=O)c1cc(ccc1Nc2cnc(c3ccccc3)c(c2)C(F)(F)F)C4CC4	8.7
CHEMBL3674661	COc1cccc(c1)c2ncc(Nc3ccc(cc3C(=O)O)C4CC4)cc2C(F)(F)F	8.15
CHEMBL3674662	OC(=O)c1cc(Cl)ccc1Nc2ccc(nc2)c3ccccc3Cl	6.84
CHEMBL3674663	OC(=O)c1cc(ccc1Nc2ccc(nc2)c3ccccc3Cl)C4CC4	8.4
CHEMBL3674664	Cc1ccc(Nc2ccc(nc2)c3ccncc3F)c(c1)C(=O)O	7.05
CHEMBL3674665	Cc1ccc(Nc2ccc(nc2)c3c(F)cccc3F)c(c1)C(=O)O	7.72
CHEMBL3674666	OC(=O)c1cc(ccc1Nc2cnc(nc2)c3ccccc3Cl)C4CC4	8.52
CHEMBL3674667	Cc1ccc(Nc2cnc(nc2)c3ccccc3Cl)c(c1)C(=O)O	7.24
CHEMBL3674668	Cc1ccc(Nc2cnc(c(C)c2)c3cccc(c3)C(=O)N4CCCC4)c(c1)C(=O)O	8.05
CHEMBL3674669	Cc1ccc(Nc2cnc(c(C)c2)c3cccc(c3)C(=O)NC4CC4)c(c1)C(=O)O	7.92
CHEMBL3674670	OC(=O)c1cc(ccc1Nc2cnc(nc2)c3ccccc3F)C4CC4	8
CHEMBL3674671	OC(=O)c1cc(ccc1Nc2cnc(nc2)c3ccccc3C(F)(F)F)C4CC4	8.05
CHEMBL3674672	Cc1ccccc1c2ncc(Nc3ccc(cc3C(=O)O)C4CC4)cn2	7.92
CHEMBL3674673	OC(=O)c1cc(ccc1Nc2cnc(nc2)c3cc(F)ccc3F)C4CC4	7.42
CHEMBL3674674	OC(=O)c1cc(ccc1Nc2cnc(nc2)c3cc(ccc3F)C(F)(F)F)C4CC4	7.68
CHEMBL3674675	OC(=O)c1cc(ccc1Nc2ccc(nc2)c3ccccc3F)C4CC4	8.1

CHEMBL3674676	Cc1ccc(Nc2ccc(nc2)c3c(F)ccc(F)c3F)c(c1)C(=O)O	7.11
CHEMBL3674677	COc1ccc(F)cc1c2ncc(Nc3ccc(C)cc3C(=O)O)cc2C	7.34
CHEMBL3674678	Cc1ccc(Nc2ccc(nc2)c3ccc(F)cc3F)c(c1)C(=O)O	6.84
CHEMBL3677726	OC(=O)c1cccc2[nH]c(nc12)c3ccc(OCc4ccccc4)cc3	5.3
CHEMBL3677727	COc1cccc(c1)c2ccc(c(F)c2)c3nc4c(cccc4[nH]3)C(=O)O	6.21
CHEMBL3677728	OC(=O)c1cc(Br)cc2[nH]c(nc12)c3ccc(cc3)c4ccccc4	6.24
CHEMBL3677729	Cn1c(nc2cccc(C(=O)O)c12)c3ccc(cc3)c4ccccc4	5.8
CHEMBL3677730	OC(=O)c1cccc2[nH]c(nc12)c3cccc(Oc4ccccc4)c3	5.14
CHEMBL3677731	OC(=O)c1cccc2[nH]c(nc12)c3ccc(Oc4ccccc4)cc3	5.54
CHEMBL3677732	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccccc4	6.52
CHEMBL3677733	OC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4ccccc4F	6.31
CHEMBL3677734	OC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4cccc(F)c4	5.42
CHEMBL3677735	OC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4cccc(OC(F)(F)F)c4	5.9
CHEMBL3677736	OC(=O)c1cccc2nc(oc12)c3ccc(cc3)c4ccccc4	5.52
CHEMBL3677737	COc1cc(cc(OC)c1c2ccccc2)c3nc4c(cccc4[nH]3)C(=O)O	6.01
CHEMBL3677738	OC(=O)c1cccc2[nH]c(nc12)c3c(F)c(F)c(c(F)c3F)c4ccccc4	7.42
CHEMBL3677739	OC(=O)c1cccc2nc([nH]c12)c3ccc(cc3F)c4ccccc4F	6.01
CHEMBL3677740	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(cc3F)c4ccccc4F	6.76
CHEMBL3677741	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(cc3)c4ccccc4F	6.43
CHEMBL3677742	OC(=O)c1cccc2nc([nH]c12)c3ccc(cc3F)c4ccccc4	6.04
CHEMBL3677743	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(cc3F)c4ccccc4	6.39
CHEMBL3677744	OC(=O)c1cc(F)cc2[nH]c(nc12)c3ccc(cc3F)c4ccccc4	6.21
CHEMBL3677745	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(cc3F)c4ccc(F)cc4F	6
CHEMBL3677746	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(cc3)c4ccc(F)cc4F	5.85
CHEMBL3677747	OC(=O)c1cc(Cl)cc2nc([nH]c12)c3ccc(cc3)c4ccccc4	6
CHEMBL3677748	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4ccccc4	8.17
CHEMBL3677749	OC(=O)c1cc(Cl)cc2[nH]c(nc12)c3ccc(cc3F)c4ccccc4	6.18
CHEMBL3677750	OC(=O)c1cc(Cl)cc2[nH]c(nc12)c3ccc(cc3)c4ccccc4F	6.02
CHEMBL3677751	COc1cc(ccc1c2nc3c(cc(C)cc3[nH]2)C(=O)O)c4ccccc4	5.93
CHEMBL3677752	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3c(F)cc(cc3F)c4ccccc4	6.75
CHEMBL3677753	OC(=O)c1cc(Cl)cc2CC(=Nc12)c3ccc(cc3)c4ccccc4	5.63
CHEMBL3677754	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4cccc(F)c4F	6.05
CHEMBL3677755	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cn3)c4ccccc4	5.15
CHEMBL3677756	OC(=O)c1cccc2[nH]c(nc12)c3ccc(Nc4ccccc4)cc3	4.57
CHEMBL3677757	OC(=O)c1cccc2[nH]c(nc12)c3ccc(Oc4c(F)cccc4F)cc3	5.8
CHEMBL3677758	OC(=O)c1cc(F)cc2[nH]c(nc12)c3ccc(cc3)c4cccnc4	6.36
CHEMBL3677759	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4cccnc4	6.39
CHEMBL3677760	OC(=O)c1cccc2cc([nH]c12)c3ccc(cc3)c4ccccc4	6.22
CHEMBL3677761	OC(=O)c1cccc2nc([nH]c12)c3ccc(cc3)c4c(F)cccc4F	5.74
CHEMBL3677762	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(Oc4ccccc4)cc3	5.47
CHEMBL3677763	OC(=O)c1cc(F)cc2[nH]c(nc12)c3c(F)cc(cc3F)c4ccccc4	6.56
CHEMBL3677764	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(Oc4ccccn4)cc3	5.36
CHEMBL3677765	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(nc3)c4ccccc4	5.42
CHEMBL3677766	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(cc3)c4c(F)cccc4F	6.46

CHEMBL3677767	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3c(F)c(F)c(c(F)c3F)n4c(C)ccc4C	8.25
CHEMBL3677768	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4ccc(CN5CCCCC5)cc4	7.11
CHEMBL3677769	Cc1cc(C(=O)O)c2nc(C#Cc3ccccc3)[nH]c2c1	4.94
CHEMBL3677770	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4ccc(NC(=O)C5CCCN5)cc4	7.25
CHEMBL3677771	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4cccc(NC(=O)C5CCCN5)c4	6.09
CHEMBL3677772	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(OCCCN5CCOCC5)cc4	5.52
CHEMBL3677773	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(OCCCN5CCCCC5)cc4	5.79
CHEMBL3677774	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(NC(=O)C5CCCN5)cc4	6.16
CHEMBL3677775	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(NC(=O)C5CCNCC5)cc4	5.43
CHEMBL3677776	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(cc3)c4ccc(O)c(O)c4	6.19
CHEMBL3677777	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(cc4)C(=O)NC5CCNCC5	5.18
CHEMBL3677778	Cc1cc(C(=O)O)c2nc(c3ccc(cc3)c4ccccc4)n(CCO)c2c1	5.32
CHEMBL3677779	Cc1cc(C(=O)O)c2c(c1)nc(c3c(F)c(F)c(c(F)c3F)c4ccc(O)cc4)n2CCO	7.11
CHEMBL3677780	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(cc3)c4ccc(OCCC5CCNCC5)cc4	5.22
CHEMBL3677781	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3c(F)c(F)c(c(F)c3F)c4ccc(O)cc4	7.8
CHEMBL3677782	Cc1cc(C(=O)O)c2c(c1)nc(c3ccc(cc3)c4ccc(O)cc4)n2CCO	5.67
CHEMBL3677783	CONC(=O)c1cc(C)cc2nc([nH]c12)c3c(F)c(F)c(c(F)c3F)c4ccccc4	5.66
CHEMBL3677784	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(cc3)c4ccc(OCCO)cc4	5.51
CHEMBL3677785	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3c(F)c(F)c(c(F)c3F)c4ccccc4OCc5ccccc5	7.22
CHEMBL3677787	Cc1cc(C(=O)N)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4ccccc4	6.35
CHEMBL3677788	Cc1cc(c2nnn[nH]2)c3nc([nH]c3c1)c4c(F)c(F)c(c(F)c4F)c5ccccc5	5.92
CHEMBL3677789	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3c(F)c(F)c(c(F)c3F)c4cccc(O)c4	7.87
CHEMBL3677790	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3c(F)c(F)c(c(F)c3F)c4cccc(OCc5ccccc5)c4	7.87
CHEMBL3677791	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(cc3)c4ccccc4OCc5ccccc5	5.82
CHEMBL3677792	OC(=O)c1cccc2nc([nH]c12)c3c(F)c(F)c(c(F)c3F)c4cccc(OCc5ccccc5)c4	7.58
CHEMBL3677793	Nc1nnc(s1)c2cccc3[nH]c(nc23)c4ccc(cc4)c5ccccc5	4.8
CHEMBL3677794	Cc1cc(C#N)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4ccccc4	5.78
CHEMBL3677795	Cc1ccc(C)n1c2c(F)c(F)c(c(F)c2F)c3nc4cccc(C(=O)O)c4[nH]3	6.96
CHEMBL3677796	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4cnn(Cc5ccccc5)c4	6.81
CHEMBL3677798	Cc1cc(C(=O)O)c2nc(c3c(F)c(F)c(c(F)c3F)c4ccccc4)n(C)c2c1	6.94
CHEMBL3677799	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(OCc5ccncc5)cc4	5.76
CHEMBL3677800	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4cccc(OCc5ccccc5)c4	5.92
CHEMBL3677801	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4cccc(O)c4	6.06
CHEMBL3677802	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(O)cc4	6.46
CHEMBL3677803	OC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4cccc(OCc5ccccc5)c4	5.89
CHEMBL3677804	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(OCc5ccccn5)cc4	5.65
CHEMBL3677805	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(OCc5cccnc5)cc4	6.12
CHEMBL3677806	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3ccc(cc3)n4c(C)ccc4C	6.4
CHEMBL3677807	OC(=O)c1cccn2nc(nc12)c3ccc(cc3)c4ccccc4	5.92
CHEMBL3677808	Cc1cc(C(=O)O)c2c(c1)nc(c3c(F)c(F)c(c(F)c3F)c4ccccc4)n2C	8.52
CHEMBL3677809	OC(=O)c1cccc2nc([nH]c12)c3c(F)c(F)c(c(F)c3F)c4cccs4	6.3
CHEMBL3677810	OC(=O)c1cccc2nc([nH]c12)c3c(F)c(F)c(c(F)c3F)c4cccc(F)c4	7.55
CHEMBL3677811	Cc1cc(C(=O)O)c2[nH]c(nc2c1)c3c(F)c(F)c(c(F)c3F)c4cccc(F)c4	8.05
CHEMBL3677812	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4ccc(OCc5ccccc5)cc4	7.32

CHEMBL3677813	OC(=O)c1cccc2[nH]c(nc12)c3c(F)c(F)c(c(F)c3F)c4cccc(F)c4F	6.68
CHEMBL3677814	OC(=O)c1cccc2[nH]c(nc12)c3c(F)c(F)c(c(F)c3F)c4cc(F)cc(F)c4	7.7
CHEMBL3677815	OC(=O)c1cccc2[nH]c(nc12)c3c(F)c(F)c(c(F)c3F)c4ccc(F)c(F)c4	5.91
CHEMBL3677816	OC(=O)c1cccc2[nH]c(nc12)c3c(F)c(F)c(c(F)c3F)c4ccccc4F	7.75
CHEMBL3677817	OC(=O)c1cccc2[nH]c(nc12)c3c(F)c(F)c(c(F)c3F)c4ccc(OCc5ccccc5)cc4	6.42
CHEMBL3677818	OC(=O)c1cccc2[nH]c(nc12)c3c(F)c(F)c(c(F)c3F)c4ccc(F)cc4	6.09
CHEMBL3677819	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4ccc(F)cc4	6.93
CHEMBL3677820	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(Oc5ccc(C=O)cc5)cc4	5.8
CHEMBL3677821	OC(=O)c1cccc2[nH]c(nc12)c3c(F)c(F)c(c(F)c3F)c4cccnc4	6.55
CHEMBL3677822	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(Oc5ccccc5C(=O)O)cc4	5.65
CHEMBL3677823	OC(=O)c1cccn2cc(nc12)c3ccc(cc3)c4ccccc4	5.42
CHEMBL3677824	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4ccsc4	7.3
CHEMBL3677825	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4cccnc4	7.5
CHEMBL3677826	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(Oc5ccccc5C=O)cc4	5.98
CHEMBL3677827	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4ccc(OCc5ccccc5)cc4	5.91
CHEMBL3677828	OC(=O)c1cccc2[nH]c(nc12)c3c(F)c(F)c(c(F)c3F)c4ccsc4	6.36
CHEMBL3677829	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4ccc(F)c(F)c4	6.5
CHEMBL3677830	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3c(F)c(F)c(c(F)c3F)c4cc(F)cc(F)c4	7.68
CHEMBL3677831	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4cnccn4	5.07
CHEMBL3677832	OC(=O)c1cccc2[nH]c(nc12)c3c(F)c(F)c(c(F)c3F)c4cccc(OC(F)(F)F)c4	6.66
CHEMBL3677833	Cc1cc(C(=O)O)c2nc([nH]c2c1)c3ccc(cc3)c4cccs4	5.78
CHEMBL3694254	O=C(NC1CC1)c2ccc(s2)N3CCSc4ccccc34	5.1
CHEMBL370008	OC(=O)C1=C(CCC1)C(=O)Nc2ccc(OCc3ccccc3)cc2	5.7
CHEMBL370228	COc1cccc(c1)c2ccc(NC(=O)c3cocc3C(=O)O)c(F)c2	6.47
CHEMBL370865	OC(=O)c1ccccc1NC(=O)c2ccc(cc2)c3ccccc3	5.3
CHEMBL371732	COc1cccc(c1)c2ccc(NC(=O)c3ccsc3C(=O)O)c(F)c2	7.36
CHEMBL372101	OC(=O)C1=C(CSC1)C(=O)Nc2ccc(cc2)c3ccccc3	6.18
CHEMBL374432	Cc1ccc2c(C(=O)O)c(O)c(nc2c1C)c3ccc(Br)cc3	4.25
CHEMBL375425	Cc1cc(C)c2nc(c(O)c(C(=O)O)c2c1)c3ccc(Cl)cc3	5.31
CHEMBL3808600	COc1ccccc1NC(=O)c2cccc3nc([nH]c23)c4cc(Br)nn4c5ncccc5Cl	6.75
CHEMBL3809369	Cc1ccccc1NC(=O)c2cccc3nc([nH]c23)c4cc(Br)nn4c5ncccc5Cl	6.17
CHEMBL3809712	COc1ccc(cc1NC(=O)c2cccc3nc([nH]c23)c4cc(Br)nn4c5ncccc5Cl)C(F)(F)F	5.31
CHEMBL381043	OC(=O)c1sccc1C(=O)Nc2ccc(cc2)c3ccccc3	6.52
CHEMBL3817894	CCCCOc1cccc(c1)c2cc(C(=O)O)c3ccccc3n2	5.88
CHEMBL3818031	CCC(C)c1ccc(cc1)c2nc3ccc(Br)cc3c(C(=O)O)c2C	8.01
CHEMBL3818174	COC(=O)c1cc(nc2ccccc12)c3ccc(OC)c(OC)c3	5.49
CHEMBL3818257	CC(C)c1ccc(cc1)c2cc(C(=O)O)c3cc(Br)ccc3n2	6.87
CHEMBL3818502	CCCCc1ccc(cc1)c2cc(C(=O)O)c3ccccc3n2	6.36
CHEMBL3818640	OC(=O)c1cc(nc2ccc(Br)cc12)c3ccc(Cl)c(Cl)c3	7.24
CHEMBL3819188	OC(=O)c1cc(nc2ccc(Br)cc12)c3ccc(Cl)cc3Cl	6.18
CHEMBL383165	CCOc1ccccc1c2cc(F)c(NC(=O)c3cscc3C(=O)O)c(F)c2	8
CHEMBL38434	Cc1c(C(=O)O)c2cc(F)ccc2nc1c3ccc(cc3)c4ccccc4F	7.4
CHEMBL386159	OC(=O)c1c(O)c(nc2ccc(F)cc12)c3ccc(cc3)c4ccc(O)cc4	8.15
CHEMBL386700	OC(=O)c1c(O)c(nc2ccc(cc12)C(F)(F)F)c3ccc(Cl)cc3	6.57

CHEMBL3891218	Cc1sc(N\N=C\c2ccccc2C(=O)O)nc1c3ccccc3Cl	7.18
CHEMBL3893343	CCCC(C)N(\N=C\c1ccccc1C(=O)O)c2nc(c(C)s2)c3ccccc3Cl	7.82
CHEMBL3896992	OC(=O)c1ccccc1\C=N\Nc2nc(cs2)c3ccccc3Cl	7.54
CHEMBL3900235	OCCN(\N=C\c1ccccc1C(=O)O)c2nc(cs2)c3ccccc3Cl	6.37
CHEMBL3907085	O=C(CCNC(=O)c1ccccc1)N[C@@H]2CCCc3ccccc23	4.91
CHEMBL3909259	CCCN(\N=C\c1ccccc1C(=O)O)c2nc(cs2)c3ccccc3Cl	8.05
CHEMBL3910373	CCN(\N=C\c1ccccc1C(=O)O)c2nc(cs2)c3ccccc3Cl	7.23
CHEMBL3913950	CN(\N=C\c1ccccc1C(=O)O)c2nc(cs2)c3cccc(Cl)c3	7.96
CHEMBL3914938	OC(=O)c1cccnc1Nc2ccc(OC(F)(F)F)cc2	6.3
CHEMBL3916793	OC(=O)c1cccnc1Nc2ccc(F)cc2	5.55
CHEMBL3919303	CCc1sc(N\N=C\c2ccccc2C(=O)O)nc1c3ccccc3Cl	6.45
CHEMBL3922925	CN(\N=C\c1ccc(C)cc1C(=O)O)c2nc(cs2)c3ccccc3Cl	8.1
CHEMBL3927131	CCCC(C)N(\N=C\c1ccccc1C(=O)O)c2nc(cs2)c3ccccc3Cl	7.72
CHEMBL3928205	CCC(C)N(\N=C\c1ccccc1C(=O)O)c2nc(cs2)c3ccccc3Cl	7.62
CHEMBL3931872	CN(\N=C\c1ccc(C)cc1C(=O)O)c2nc(c(C)s2)c3ccccc3	7.85
CHEMBL3937185	CC(C)N(\N=C\c1ccccc1C(=O)O)c2nc(cs2)c3ccccc3Cl	7.03
CHEMBL3941922	CN(\N=C\c1ccccc1C(=O)O)c2nc(cs2)c3cc(Cl)ccc3Cl	7.55
CHEMBL3944693	OC(=O)c1cccnc1Nc2ccccc2	4.76
CHEMBL3949527	OC(=O)c1ccccc1\C=N\Nc2nc(cs2)c3ccccc3	6.86
CHEMBL3950655	CN(\N=C\c1ccc(cc1C(=O)O)C(F)(F)F)c2nc(cs2)c3ccccc3Cl	7.06
CHEMBL3959360	CN(\N=C\c1ccc(F)cc1C(=O)O)c2nc(cs2)c3ccccc3Cl	8.7
CHEMBL3968151	Cc1sc(N\N=C\c2ccccc2C(=O)O)nc1c3ccccc3	7.09
CHEMBL3980486	CN(\N=C\c1ccccc1C(=O)O)c2nc(cs2)c3ccccc3Cl	8.1
CHEMBL41719	OC(=O)c1c(O)c(nc2ccc(F)cc12)c3ccc(cc3)c4ccccc4	8.3
CHEMBL418870	FC(F)(F)c1ccc(Nc2[nH]nc3CCCC(=O)c23)cc1	5.19
CHEMBL419631	CCc1oncc1\C(=N\c2ccc(cc2)N(C)C)\S	4.39
CHEMBL483161	COc1ccccc1c2ccc(NC(=O)\C(=C(\C)/O)\C#N)c(Cl)c2	6.7
CHEMBL483552	C\C(=C(/C#N)\C(=O)Nc1ccc(cc1Cl)c2ccccc2Cl)\O	6.75
CHEMBL483994	C\C(=C(/C#N)\C(=O)Nc1ccc(cc1Cl)c2ccccc2)\O	6.5
CHEMBL483995	CCOc1cccc(c1)c2ccc(NC(=O)\C(=C(\C)/O)\C#N)cc2	6.89
CHEMBL484531	C\C(=C(/C#N)\C(=O)Nc1ccc(cc1)c2ccccc2Cl)\O	6.89
CHEMBL484594	C\C(=C(/C#N)\C(=O)Nc1ccc(cc1Cl)c2c(Cl)cccc2Cl)\O	4.78
CHEMBL484595	C\C(=C(/C#N)\C(=O)Nc1ccc(cc1Cl)c2cccc(Cl)c2)\O	5.82
CHEMBL484602	C\C(=C(/C#N)\C(=O)Nc1ccc(cc1C(F)(F)F)c2cccc(Cl)c2)\O	4.06
CHEMBL484780	C\C(=C(/C#N)\C(=O)Nc1ccc(c(Cl)c1)c2ccccc2Cl)\O	7.66
CHEMBL505315	C\C(=C(/C#N)\C(=O)Nc1ccc(cc1)c2cccc(Cl)c2Cl)\O	6.7
CHEMBL519160	C\C(=C(/C#N)\C(=O)Nc1ccc(cc1)c2ccccc2)\O	7.05
CHEMBL520008	C\C(=C(/C#N)\C(=O)Nc1ccc(c(Cl)c1)c2cccc(Cl)c2)\O	6.72
CHEMBL520306	C\C(=C(/C#N)\C(=O)Nc1ccc(cc1C(F)(F)F)c2ccccc2Cl)\O	6.77
CHEMBL520999	C\C(=C(/C#N)\C(=O)Nc1ccc(cc1Cl)c2cccc(Cl)c2Cl)\O	6.48
CHEMBL571285	NC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4cccnc4	4.72
CHEMBL576423	NC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4ccccn4	4.55
CHEMBL578185	NC(=O)c1cccc2[nH]c(nc12)c3ccc(cc3)c4ccccc4	5.01
CHEMBL63323	OC(=O)c1cccnc1Nc2cccc(c2)C(F)(F)F	4.77

CHEMBL70261	Cc1oncc1\C(=N\c2ccc(OC(F)(F)F)cc2)\S	5.14
CHEMBL70544	CC(=O)\C(=C(\S)/Nc1ccc(cc1)C(F)(F)F)\C#N	6.1
CHEMBL70708	FC(F)(F)c1ccc(NC(=S)c2cnoc2C3CC3)cc1	5.5
CHEMBL71154	CCc1oncc1\C(=N\c2ccc(cc2)C#N)\S	4.96
CHEMBL960	Cc1oncc1C(=O)Nc2ccc(cc2)C(F)(F)F	5
CHEMBL973	C\C(=C(/C#N)\C(=O)Nc1ccc(cc1)C(F)(F)F)\O	6.86
CHEMBL999	C\C(=C(\C#N)/C(=O)Nc1ccc(cc1)C(F)(F)F)\O	6.36

Table S2. Docking score and predicted activity value for the top 200 zinc candidates.

		Predicted activity		
Name	Docking score	GIAN	GIAT	SGCA
ZINC000008577218*	64.296	7.300996	7.765394	7.234998
ZINC000015919406	63.009	6.723702	5.593675	6.857596
ZINC000002036915	62.93	7.608401	7.819659	6.585709
ZINC000003952167	62.463	6.645174	6.335661	5.166162
ZINC000043100953	61.858	4.887485	7.542762	7.400549
ZINC000003831490	61.751	6.62721	7.416915	7.190752
ZINC000004261765*	60.522	8.057562	10.81596	12.78676
ZINC000001530605	60.384	5.740261	7.979621	6.135328
ZINC000001587572	59.994	7.6084	7.81966	6.585708
ZINC000095618747*	59.621	7.532437	10.96646	12.39158
ZINC000043195321	59.17	6.07048	7.23513	5.990883
ZINC000100004249	59.033	5.674796	6.083844	5.279045
ZINC000100048501	58.625	6.299141	8.085845	6.764382
ZINC000013588928	58.578	7.530169	8.905917	10.66835
ZINC000095892888	58.467	4.630929	5.935944	5.206252
ZINC000022054044	58.284	6.194102	7.258717	6.175798
ZINC000006095847	58.118	5.294021	6.119356	6.854791
ZINC000001444556	58.108	5.074522	6.087246	5.250934
ZINC000000005423	58.018	5.96597	7.224964	6.556073
ZINC000001540228	57.612	6.668216	6.510778	7.344737
ZINC000043194409	57.499	6.707047	4.910901	5.83283
ZINC000000089688	57.233	5.00581	5.799558	5.621189
ZINC000003871698	57.183	5.491028	6.483674	5.680937
ZINC000003872687	56.959	4.598122	5.705404	5.326142
ZINC000053166256	56.936	4.977914	4.997481	5.279971
ZINC000033753205	56.9	5.868948	9.044409	10.17845
ZINC000000007455	56.757	4.696512	6.164524	5.058284
ZINC000001493878	56.466	6.399541	8.024447	7.691423
ZINC000100005073	56.312	4.23337	7.947003	5.665305
ZINC000019632628	56.269	5.228067	4.575965	5.482564
ZINC000000121541	56.257	4.744668	4.305178	3.71702
ZINC000013129998	56.23	4.986147	5.606158	5.192493
ZINC000000537795	56.195	5.679065	6.292289	6.575707
ZINC000012501706	56.083	7.57146	8.986579	11.4689
ZINC000019203855	55.963	4.09478	6.272138	5.492144
ZINC000001530935	55.905	4.633284	3.962843	4.647081
ZINC000003952881	55.842	5.451977	6.315676	6.638064
ZINC000004618208	55.713	4.633284	3.962843	4.647081
ZINC000001530604	55.606	5.740261	7.979621	6.135327
ZINC000000001342	55.487	4.446496	4.897518	4.607798
ZINC000002040778	55.399	4.971159	4.704404	5.306667

ZINC000017835656	55.256	3.994599	4.564504	3.85613
ZINC000003830847	55.14	4.240569	5.403502	4.173788
ZINC000003874496	54.744	4.696104	5.328797	5.245481
ZINC000000607910	54.623	4.598122	5.705404	5.326142
ZINC000003956788	54.564	5.213435	5.50495	5.163043
ZINC000001999441	54.309	7.473666	8.909299	7.538009
ZINC000003860441	54.142	4.760465	8.037248	6.951668
ZINC000022056375	54.133	5.262184	5.959076	5.878389
ZINC000006093393	53.857	4.281672	5.780708	5.956861
ZINC000006745272	53.717	5.595707	7.352758	7.356881
ZINC000005423072	53.699	4.642952	5.160971	5.682736
ZINC000005843546	53.657	5.580665	6.001852	5.799144
ZINC000005140767	53.651	4.668482	6.256027	4.896819
ZINC000003935481	53.651	4.439359	5.15712	5.499027
ZINC000000538174	53.631	5.713495	6.447265	6.845958
ZINC000001843099	53.585	5.767795	6.613459	4.489143
ZINC000007997905	53.318	3.994599	4.564504	3.85613
ZINC000000001567	53.313	4.715746	5.611708	5.534105
ZINC000005425173	53.285	4.349578	5.766132	4.529187
ZINC000003791775	53.242	4.410463	6.007408	4.677265
ZINC000005733652	52.942	4.79531	4.110694	5.426235
ZINC000000538163	52.926	5.043701	6.729642	5.478788
ZINC000017653974	52.92	5.4334	5.617358	5.085844
ZINC000003964126	52.916	4.845099	6.078844	6.276227
ZINC000000057466	52.859	5.778152	6.512209	4.772442
ZINC000007997966	52.811	4.578921	5.517211	5.383073
ZINC000252679615	52.811	4.57892	5.517211	5.383073
ZINC000002568036	52.811	4.21554	5.479602	5.626502
ZINC000000899824	52.81	6.183718	6.968305	6.779979
ZINC000009060429	52.787	4.410463	6.007408	4.677264
ZINC000013546270	52.778	8.218697	10.84782	11.66157
ZINC000013449412	52.76	5.485429	5.467895	6.842892
ZINC000000035804	52.746	5.749037	6.361116	6.146009
ZINC000005140766	52.66	4.950457	4.979789	5.379768
ZINC000004099200	52.523	4.849636	5.701288	5.550549
ZINC000019632614	52.519	6.488966	7.526567	6.908721
ZINC000003818726	52.508	5.65894	6.333538	5.042331
ZINC000100015491	52.447	4.661204	4.851078	5.705404
ZINC000000599734	52.355	4.895085	4.47099	4.89599
ZINC000028870000	52.253	6.107962	5.08248	5.52845
ZINC000001481956	52.145	6.695495	7.295831	7.462146
ZINC000051133897	52.084	4.6772	6.337007	4.672034
ZINC000022060383	52.08	6.080103	6.294571	6.257107
ZINC000000000865	52.021	4.592355	5.138213	4.581967

ZINC000019203852	52.011	4.09478	6.272138	5.492144
ZINC000012404515	51.945	5.975027	5.010041	5.654284
ZINC000004214700	51.876	6.695495	7.295831	7.462146
ZINC000001640621	51.81	4.510243	5.09842	4.939918
ZINC000013531944	51.778	5.88609	5.933717	6.081086
ZINC000000968326	51.773	4.828036	5.009841	5.750008
ZINC000001530811	51.772	4.433525	4.042876	4.344839
ZINC000000607986	51.659	7.473666	8.909299	7.538009
ZINC000013233295	51.592	5.339896	5.632687	5.314468
ZINC000000601305	51.543	4.68365	4.094828	5.014022
ZINC000100006429	51.337	4.933535	5.193223	4.915394
ZINC000012341529	51.318	5.886089	5.933717	6.081086
ZINC000013831791	51.317	5.438772	5.346507	5.247869
ZINC000029210629	51.312	6.777005	6.920874	6.221011
ZINC000003786192	51.295	6.115422	5.175305	5.774267
ZINC000001641925	51.29	4.729214	5.231195	4.858466
ZINC000022056370	51.25	5.262183	5.959076	5.878389
ZINC000043202140	51.188	6.82178	6.980927	6.892757
ZINC000000001003	51.149	4.847857	6.034954	5.110968
ZINC000011679756	51.109	7.149884	7.044483	6.112609
ZINC000000968328	50.955	5.15685	5.867417	5.734884
ZINC000004096488	50.94	4.927535	7.252732	8.655126
ZINC000001545565	50.853	5.395932	4.364805	4.547904
ZINC000001530940	50.834	4.326652	4.745024	4.453138
ZINC000003927870	50.825	4.183327	7.745678	8.274746
ZINC000004098610	50.796	5.824383	8.410183	7.736589
ZINC000000000017	50.728	4.138582	4.407006	3.364537
ZINC000000968327	50.627	4.828036	5.00984	5.750008
ZINC000000538538	50.545	4.491793	4.647077	4.487322
ZINC000004676424	50.413	4.849636	5.701287	5.550549
ZINC000005424275	50.39	3.85517	5.024442	3.435555
ZINC000000057461	50.346	5.594043	5.873698	4.596666
ZINC000004097476	50.343	3.716354	5.61807	4.287302
ZINC000031425359	50.334	7.051373	5.293667	8.015163
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ZINC000000643114	49.554	4.68365	4.094828	5.014022
ZINC000000089763	49.549	4.304827	4.670278	4.862598
ZINC000000057490	49.523	5.419512	5.9966	5.425169
ZINC000018185774	49.513	5.646585	4.266383	5.801611
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ZINC000000537802	48.977	5.317133	6.073922	6.325182
ZINC000001542113	48.849	6.035281	5.986148	6.59202
ZINC000000537805	48.815	6.089524	6.553387	6.552194
ZINC000001540998	48.811	6.414423	6.278392	6.592865
ZINC000000125047	48.764	5.52607	5.549182	5.075521
ZINC000019796155	48.732	5.597431	5.292646	5.245823
ZINC000003927198	48.727	4.424043	8.329219	5.211196
ZINC000001690324	48.68	4.781328	4.565401	5.347376
ZINC000005844788	48.639	7.473665	8.909299	7.538009
ZINC000021981235	48.574	5.194707	5.071111	5.237409
ZINC000003830961	48.506	3.184162	5.421502	3.932911
ZINC000036056301	48.505	5.825628	4.481654	5.086045
ZINC000003871356	48.388	3.501432	3.722906	4.610196
ZINC000053084692	48.381	4.212025	4.502934	5.369962
ZINC000000039092	48.338	4.841402	3.964946	5.051723
ZINC000001530636	48.284	5.017924	5.41182	4.599806
ZINC000005116154	48.278	4.517035	6.40187	4.764874
ZINC000000537874	48.263	4.961668	6.04738	5.822662
ZINC000000001246	48.259	5.434993	5.527972	6.044355
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ZINC000013818943	48.201	4.500135	7.787578	7.226458
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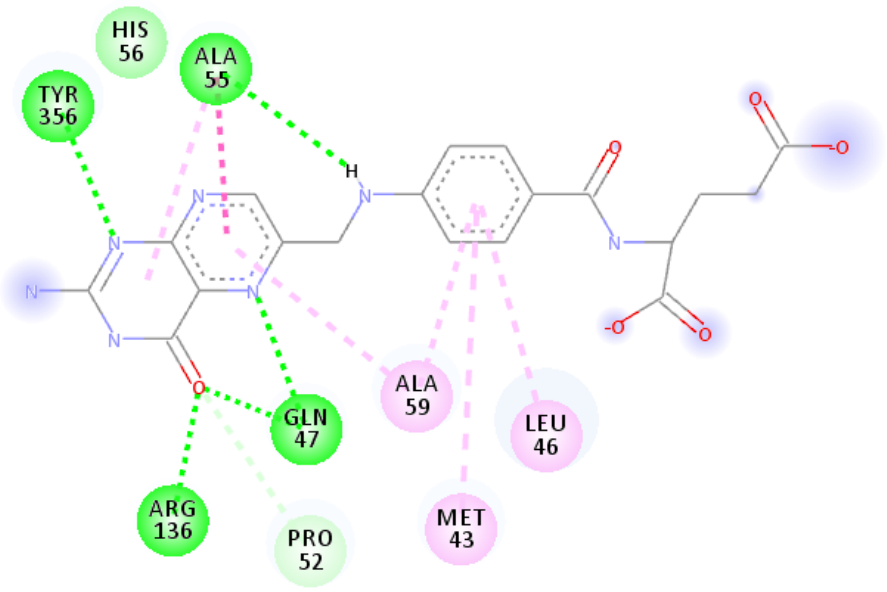
ZINC000003830933	47.907	3.956304	6.191349	4.583596
ZINC000003814784	47.904	5.975027	5.010042	5.654285
ZINC000000002097	47.876	4.750436	5.396768	5.246945
ZINC000022059926	47.808	5.49988	5.974154	5.263975
ZINC000005924265	47.762	5.09754	4.794147	5.356349

ZINC000003812865	47.704	5.815678	5.943406	5.403072
ZINC000000057537	47.64	5.431703	4.983044	5.389072
ZINC000000057494	47.539	4.579184	5.200683	4.814668
ZINC000002005305	47.482	7.351001	8.238765	7.220576
ZINC000000001490	47.463	4.907505	5.452746	4.464963
ZINC000100004231	47.438	5.775934	6.06221	5.453905
ZINC000000011012	47.418	4.493898	5.679562	5.331686
ZINC000000900543	47.372	3.13424	4.511394	3.722074
ZINC000035342789	47.369	5.131887	3.623349	5.206191
ZINC000000898237	47.342	4.191215	4.989699	4.945329
ZINC000003871576	47.328	5.756988	4.360831	5.81127
ZINC000000005191	47.315	4.770481	3.731991	4.617854
ZINC000004213946	47.234	7.473666	8.909299	7.538009
ZINC000002570817	47.222	4.322212	3.962971	5.058281
ZINC000004693574	47.216	4.655963	5.358908	4.808446
ZINC000011617039	47.173	7.046603	7.681741	6.688553
ZINC000003872177	47.115	8.41622	4.727499	7.164699
ZINC000100004227	47.113	4.712177	4.765829	4.191784
ZINC000095619124	47.066	6.739865	6.383723	7.551508
ZINC000018115268	47.034	6.856761	5.478155	4.636524
ZINC000000001382	47.018	4.378035	5.346808	4.750925
ZINC000003869608	46.997	5.860081	5.261596	5.896521
ZINC000003830986	46.987	4.895085	4.47099	4.89599
ZINC000006716957	46.969	9.029577	8.046642	8.966531
ZINC000095617673	46.882	5.123659	5.474619	6.76257
ZINC000000020221	46.86	3.75293	3.763909	4.088777
ZINC000001529323	46.856	7.434438	7.96345	7.010843

*The selected candidates

(a)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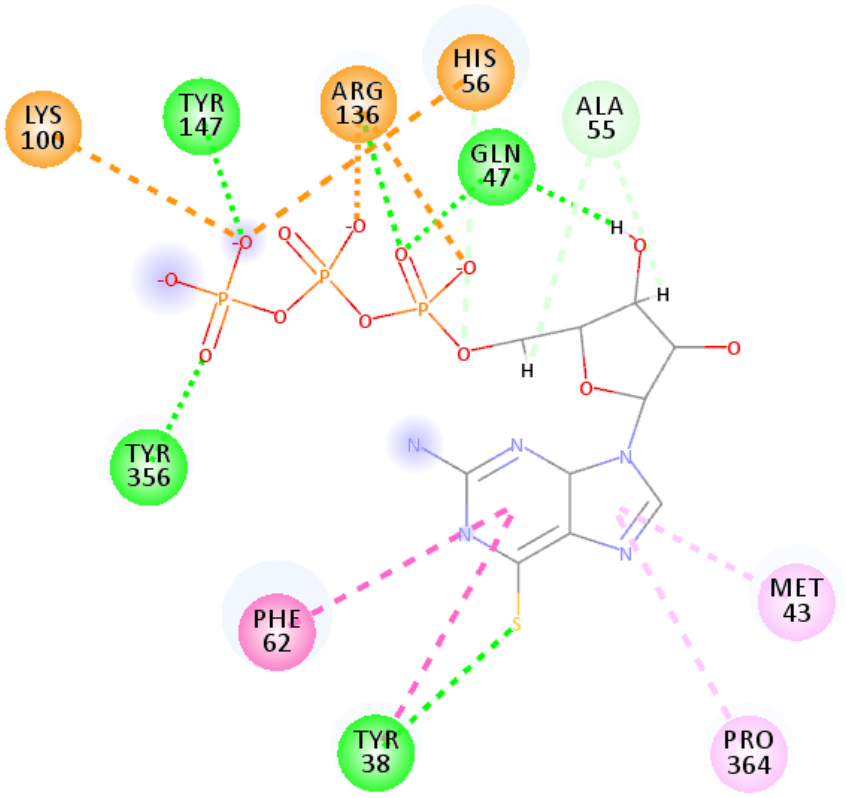
(b)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PHE
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MET
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TYR
38
PRO
364

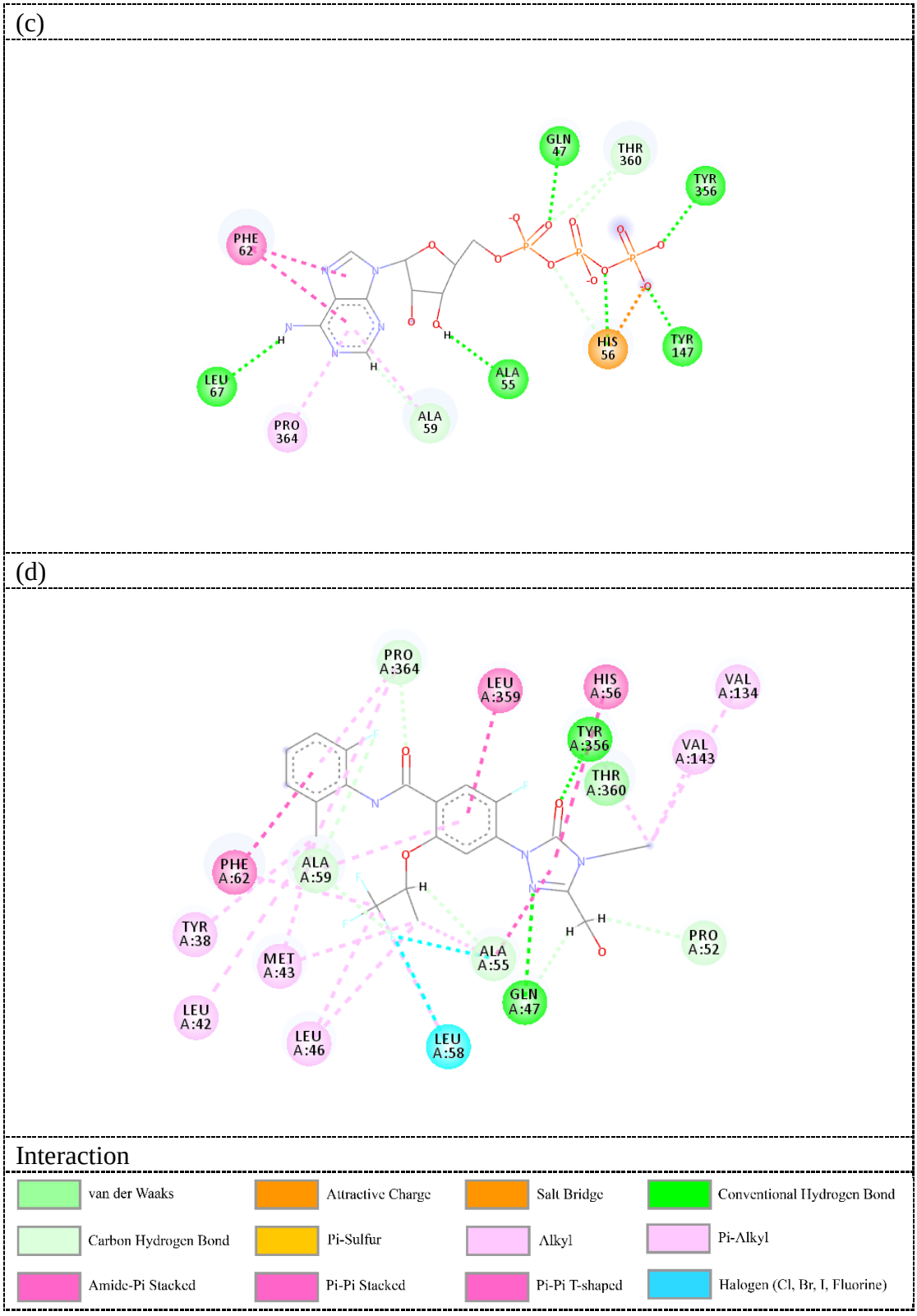
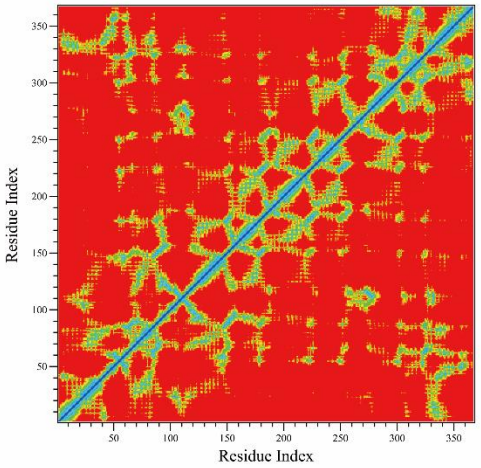
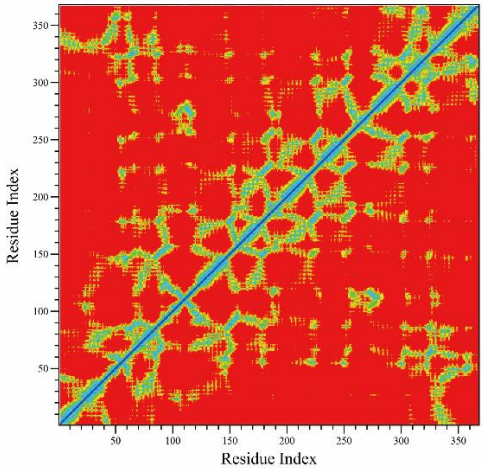


Figure S1. 2D horizon of molecular docking results. (**a**) ZINC8577218, (**b**) ZINC95618747, (**c**) ZINC4261765 and (**d**) BAY-2402234.

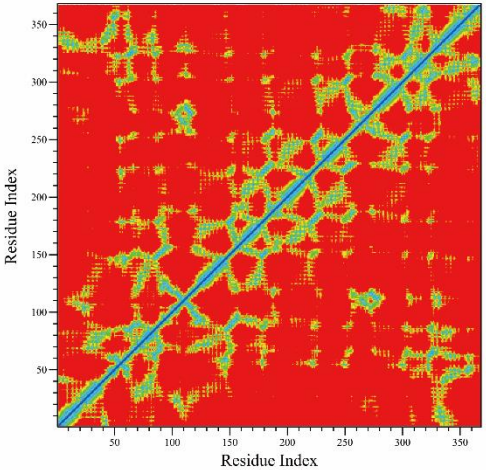
(a)


Residue Index
Residue Index
50
100
150
200
250
300
350

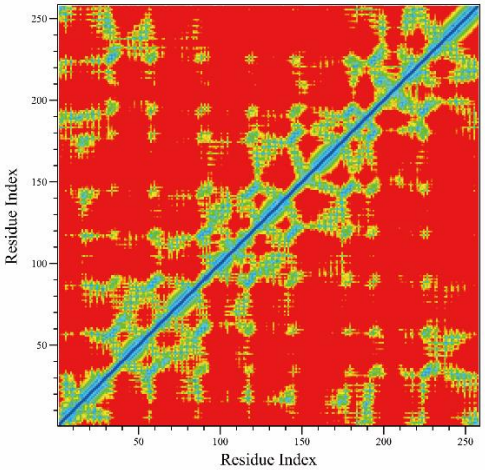
(b)


Residue Index
Residue Index
50
100
150
200
250
300
350

(c)


Residue Index
Residue Index
50
100
150
200
250
300
350

(d)


Residue Index
Residue Index
50
100
150
200
250

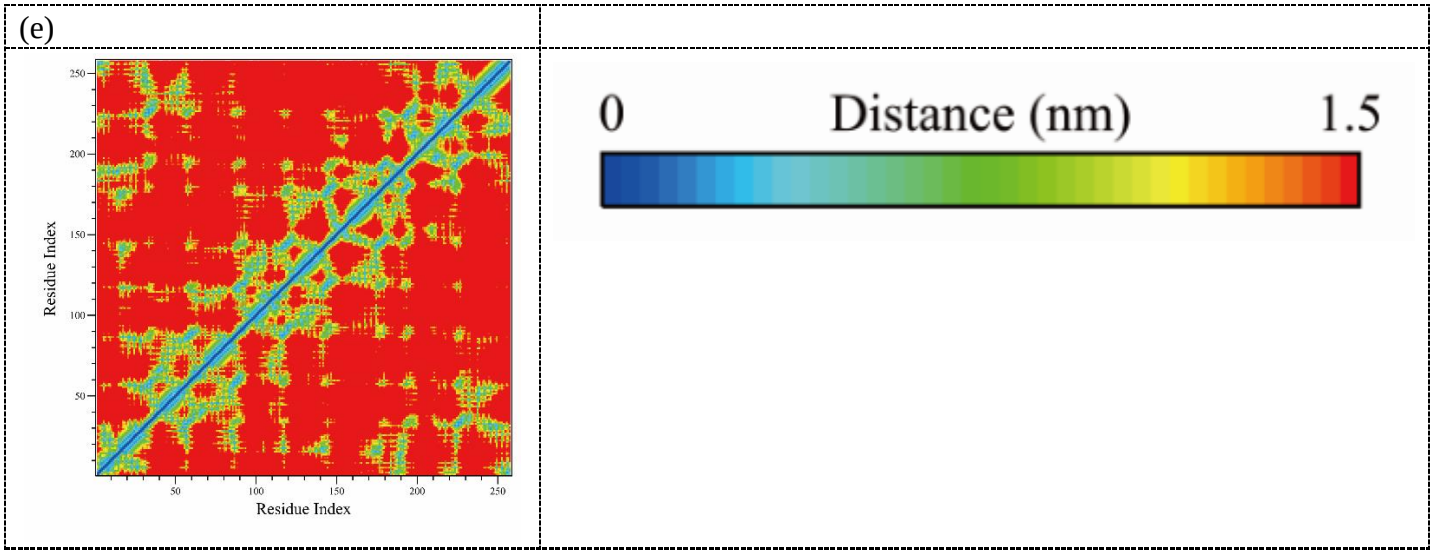


Figure S2. Residue distance matrix. (**a**) DHODH protein with ZINC8577218. (**b**) DHODH protein with ZINC95618747. (**c**) DHODH protein with ZINC4261765. (**d**) UMPS protein with ZINC95618747. (**e**) UMPS protein with ZINC4261765.