Supplemental Information

COMPARE analysis, a bioinformatic approach to accelerate drug repurposing against Covid-19 and other emerging epidemics

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Lists of correlated "fished" compounds extracted using COMPARE algorithm after seeding compounds with ostensible anti SARS-CoV-2 effects

Suppl. Table 1- List of compounds correlated to Chloroquine. Highlighted rows indicate drugs that are approved or in clinical development

pearsonCo	spearmanC	rank	correlation	seed ident	target iden	seed descr	target desc	count com	seed molti	seed gene	seed provi	seed probe	seed miR	Seed SMILI	seed nsc	seed logHi	seed endp	seed targe	target molt	target prov	target gene	target prot	target miR	Target SMI	target nsc	target logH	target end	target target
1	1	1	1	NSC_S_140	NSC_S_140	NSC S1405	NSC S1405	65						CCN(CC)CC	14050	-4	GI50							CCN(CC)CC	14050	-4	GI50	
0.69	0.75	2	0.69	NSC_S_140	NSC_S_624	NSC S1405	NSC S6246	50						CCN(CC)CC	14050	-4	GI50							COc1cc2CC	624660	-4	GI50	
0.68	0.66	3	0.68	NSC_S_140	NSC_S_670	NSC S1405	NSC S6702	57						CCN(CC)CC	14050	-4	GI50							CN(C)CCO(	670226	-4	GI50	
0.68	0.73	4	0.68	NSC_S_140	NSC_S_169	NSC S1405	NSC S1698	51						CCN(CC)CC	14050	-4	GI50							FC(F)(F)c1c	169877	-4	GI50	
0.66	0.67	5	0.66	NSC_S_140	NSC_S_708	NSC S1405	NSC S7080	57						CCN(CC)CC	14050	-4	GI50							CNCCCNC1	708074	-4	GI50	
0.66	0.63	6	0.66	NSC_S_140	NSC_S_670	NSC S1405	NSC S6702	55						CCN(CC)CC	14050	-4	GI50							CN(C)CCO(	670229	-4	GI50	
0.65	0.65	7	0.65	NSC_S_140	NSC_S_670	NSC S1405	NSC S6702	55						CCN(CC)CC	14050	-4	GI50							CN(C)CCO[	670225	-4	GI50	
0.64	0.55	8	0.64	NSC_S_140	NSC_S_676	NSC S1405	NSC S6760	57						CCN(CC)CC	14050	-4	GI50							COc1cc2C[(	676002	-4	GI50	
0.62	0.49	9	0.62	NSC_S_140	NSC_S_134	NSC S1405	NSC S1347	51						CCN(CC)CC	14050	-4	GI50							COc1cc2CC	134759	-4	GI50	
0.62	0.65	10	0.62	NSC_S_140	NSC_S_628	NSC S1405	NSC S6283	49						CCN(CC)CC	14050	-4	GI50							CCOC(=O)N	628303	-4	GI50	
0.62	0.64	11	0.62	NSC_S_140	NSC_S_381	NSC S1405	NSC S3811	52						CCN(CC)CC	14050	-4	GI50							CC(O)CN(C	38114	-4	GI50	
0.61	0.58	12	0.61	NSC_S_140	NSC_S_743	NSC S1405	NSC S7430	54						CCN(CC)CC	14050	-4	GI50							CN(CCCN1(	743058	-4	GI50	
0.61	0.61	13	0.61	NSC_S_140	NSC_S_715	NSC S1405	NSC S7154	56						CCN(CC)CC	14050	-4	GI50							CC(C)(C)[Si	715470	-4	GI50	
0.61	0.58	14	0.61	NSC_S_140	NSC_S_716	NSC S1405	NSC S7168	57						CCN(CC)CC	14050	-4	GI50							Nc1c2CCCN	716850	-4	GI50	
0.61	0.73	15	0.61	NSC_S_140	NSC_S_141	NSC S1405	NSC S1415	52						CCN(CC)CC	14050	-4	GI50							CC1=NCCc2	141527	-3.3	GI50	
0.6	0.63	16	0.6	NSC_S_140	NSC_S_367	NSC S1405	NSC S3670	55						CCN(CC)CC	14050	-4	GI50							CCCCCCC1(	36704	-4	GI50	
0.6	0.64	17	0.6	NSC_S_140	NSC_S_670	NSC S1405	NSC S6703	56						CCN(CC)CC	14050	-4	GI50							CCCCCC[n+	670390	2	GI50	
0.6	0.6	18	0.6	NSC_S_140	NSC_S_105	NSC S1405	NSC S1051	54						CCN(CC)CC	14050	-4	GI50							COc1ccc2C	105130	-4	GI50	Pheanthine antimalarial and antiviral from plants
0.6	0.62	19	0.6	NSC_S_140	NSC_S_645	NSC S1405	NSC S6450	65						CCN(CC)CC	14050	-4	GI50							Clc1ccc(cc1	645033	-4	GI50	
0.6	0.61	20	0.6	NSC_S_140	NSC_S_671	NSC S1405	NSC S6717	57						CCN(CC)CC	14050	-4	GI50							CCCCN1C(=	671765	-4	GI50	
0.6	0.58	21	0.6	NSC_S_140	NSC_S_766	NSC S1405	NSC S7664	51						CCN(CC)CC	14050	-4	GI50							CC1CCN(Cc	766431	-4	GI50	
0.59	0.43	22	0.59	NSC_S_140	NSC_S_650	NSC S1405	NSC S6507	53						CCN(CC)CC	14050	-4	GI50							COc1cc(CN	650768	-4	GI50	
0.59	0.5	23	0.59	NSC_S_140	NSC_S_681	NSC S1405	NSC S6810	53						CCN(CC)CC	14050	-4	GI50							Cc1ccc(cc1	681083	-4	GI50	
0.59	0.62	24	0.59	NSC_S_140	NSC_S_134	NSC S1405	NSC S1348	40						CCN(CC)CC	14050	-4	GI50							CCN(CC)CC	13484	-4	GI50	
0.59	0.49	25	0.59	NSC_S_140	NSC_S_720	NSC S1405	NSC S7204	57						CCN(CC)CC	14050	-4	GI50							CN(C)CCN(	720486	-4	GI50	
0.59	0.54	26	0.59	NSC_S_140	NSC_S_665	NSC S1405	NSC S6658	44						CCN(CC)CC	14050	-4	GI50							CN1CCN(C(	665801	-4	GI50	
0.59	0.64	27	0.59	NSC_S_140	NSC_S_715	NSC S1405	NSC S7155	54						CCN(CC)CC	14050	-4	GI50							CN1C2CCC	715580	-4	GI50	
0.59	0.63	28	0.59	NSC_S_140	NSC_S_646	NSC S1405	NSC S6460	49						CCN(CC)CC	14050	-4	GI50							CCN(CC)CC	646030	-4	GI50	
0.59	0.57	29	0.59	NSC_S_140	NSC_S_685	NSC S1405	NSC S6859	52						CCN(CC)CC	14050	-4	GI50							O=C(NCCC(	685965	-4	GI50	
0.59	0.76	30	0.59	NSC_S_140	NSC_S_854	NSC S1405	NSC S8544	52						CCN(CC)CC	14050	-4	GI50							CCCCc1oc2	85442	-3.6	GI50	Amiodarone
0.58	0.62	31	0.58	NSC_S_140	NSC_S_665	NSC S1405	NSC S6656	52						CCN(CC)CC	14050	-4	GI50							CN(C)\C=N	665666	-4	GI50	
0.58	0.47	32	0.58	NSC_S_140	NSC_S_652	NSC S1405	NSC S6528	45						CCN(CC)CC	14050	-4	GI50							NC(=O)N1N	652807	-4	GI50	
0.58	0.57	33	0.58	NSC_S_140	NSC_S_766	NSC S1405	NSC S7665	51						CCN(CC)CC	14050	-4	GI50							CCN(CC)CC	766565	-4	GI50	
0.58	0.69	34	0.58	NSC_S_140	NSC_S_645	NSC S1405	NSC S6450	56						CCN(CC)CC	14050	-4	GI50							Clc1ccc(cc1	645026	-4	GI50	
0.58	0.63	35	0.58	NSC_S_140	NSC_S_633	NSC S1405	NSC S6334	55						CCN(CC)CC	14050	-4	GI50							Clc1cccc(c1	633413	-5	GI50	
0.57	0.6	36	0.57	NSC_S_140	NSC_S_687	NSC S1405	NSC S6870	51						CCN(CC)CC	14050	-4	GI50							O=C1N(C(=	687032	-4	GI50	
0.57	0.59	37	0.57	NSC_S_140	NSC_S_680	NSC S1405	NSC S6800	56						CCN(CC)CC	14050	-4	GI50							COc1ccc2[(	680095	-4	GI50	
0.57	0.65	38	0.57	NSC_S_140	NSC_S_146	NSC S1405	NSC S1462	56						CCN(CC)CC	14050	-4	GI50							COc1cc(CC	146267	-4	GI50	
0.57	0.6	39	0.57	NSC_S_140	NSC_S_766	NSC S1405	NSC S7666	54						CCN(CC)CC	14050	-4	GI50							COc1ccc2n	766603	-4	GI50	
0.57	0.56	40	0.57	NSC_S_140	NSC_S_683	NSC S1405	NSC S6838	57						CCN(CC)CC	14050	-4	GI50							COc1ccc2[(	683880	-4	GI50	
0.57	0.59	41	0.57	NSC_S_140	NSC_S_703	NSC S1405	NSC S7031	56						CCN(CC)CC	14050	-4	GI50							COc1ccc2N	703163	-4	GI50	
0.57	0.63	42	0.57	NSC_S_140	NSC_S_766	NSC S1405	NSC S7660	55						CCN(CC)CC	14050	-4	GI50							Fc1ccc(Nc2	766055	-4	GI50	
0.56	0.51	43	0.56	NSC_S_140	NSC_S_717	NSC S1405	NSC S7178	57						CCN(CC)CC	14050	-4	GI50							OCCN1CCN	717853	-4	GI50	
0.56	0.39	44	0.56	NSC_S_140	NSC_S_654	NSC S1405	NSC S6546	50						CCN(CC)CC	14050	-4	GI50							CC(C)(Oc1c	654628	-4	GI50	
0.56	0.33	45	0.56	NSC_S_140	NSC_S_654	NSC S1405	NSC S6546	50						CCN(CC)CC	14050	-4	GI50							CC(C)(Oc1c	654629	-4	GI50	
0.56	0.43	46	0.56	NSC_S_140	NSC_S_717	NSC S1405	NSC S7178	57						CCN(CC)CC	14050	-4	GI50							Cc1nc2c(n(	717851	-4	GI50	
0.56	0.42	47	0.56	NSC_S_140	NSC_S_716	NSC S1405	NSC S7163	54						CCN(CC)CC	14050	-4	GI50							CSc1ccc(cc	716338	-4	GI50	
0.56	0.61	48	0.56	NSC_S_140	NSC_S_736	NSC S1405	NSC S7363	54						CCN(CC)CC	14050	-4	GI50							O[C@@H]1	736380	-4	GI50	
0.56	0.61	49	0.56	NSC_S_140	NSC_S_644	NSC S1405	NSC S6446	57						CCN(CC)CC	14050	-4	GI50							NCCOc1ccc	644617	-4	GI50	
0.56	0.47	50	0.56	NSC_S_140	NSC_S_672	NSC S1405	NSC S6720	44						CCN(CC)CC	14050	-4	GI50							CC1CN=C(N	672014	-4	GI50	
0.56	0.44	51	0.56	NSC_S_140	NSC_S_209	NSC S1405	NSC S2097	56						CCN(CC)CC	14050	-4	GI50							COc1cc2CC	209759	-4	GI50	
0.56	0.57	52	0.56	NSC_S_140	NSC_S_931	NSC S1405	NSC S9313	55						CCN(CC)CC	14050	-4	GI50							COc1cc2CC	93135	-4	GI50	Oxycanthine from fruits
0.56	0.58	53	0.56	NSC_S_140	NSC_S_108	NSC S1405	NSC S1081	55						CCN(CC)CC	14050	-4	GI50							CN(C)S(=O)	108165	-4	GI50	Thiothixene is used to treat certain mental/mood disorders (such as schizophrenia)
0.56	0.44	54	0.56	NSC_S_140	NSC_S_647	NSC S1405	NSC S6473	49						CCN(CC)CC	14050	-4	GI50							COc1ccc2n	647317	-4	GI50	
0.56	0.59	55	0.56	NSC_S_140	NSC_S_633	NSC S1405	NSC S6333	52						CCN(CC)CC	14050	-4	GI50							Clc1cccc(c1	633398	-4	GI50	
0.56	0.48	56	0.56	NSC_S_140	NSC_S_381	NSC S1405	NSC S3811	55						CCN(CC)CC	14050	-4	GI50							CCN(CC)CC	38110	-4	GI50	
0.55	0.39	57	0.55	NSC_S_140	NSC_S_603	NSC S1405	NSC S6039	51						CCN(CC)CC	14050	-4	GI50							OCCN1CCN	603976	-4	GI50	
0.55	0.43	58	0.55	NSC_S_140	NSC_S_635	NSC S1405	NSC S6359	54						CCN(CC)CC	14050	-4	GI50							CN(C)Cc1c(	635926	-4	GI50	
0.55	0.46	59	0.55	NSC_S_140	NSC_S_355	NSC S1405	NSC S3558	55						CCN(CC)CC	14050	-4	GI50							CCN(CC)CC	35587	-4	GI50	Lucanthone antiparasite investigation
0.55	0.72	60	0.55	NSC_S_140	NSC_S_566	NSC S1405	NSC S5662	56						CCN(CC)CC	14050	-4	GI50							Clc1ccc2c(N	56624	-4	GI50	
0.55	0.58	61	0.55	NSC_S_140	NSC_S_638	NSC S1405	NSC S6386	64						CCN(CC)CC	14050	-4	GI50							CCN(CC)Cc	6386	-4	GI50	
0.55	0.62	62	0.55	NSC_S_140	NSC_S_619	NSC S1405	NSC S6191	56						CCN(CC)CC	14050	-4	GI50							C\C=C(\CC(	619167	-4	GI50	

Suppl. Table 2- List of compounds correlated to Hydroxychloroquine. Highlighted rows indicate drugs that are approved or in clinical development

pearsonCorrelation	spearmanCorrelation	rank	correlation	seed identString	target identString	seed descriptorForDisplay	target descriptorForDisplay	count common cell lines	seed moltId	seed geneSymbol	seed provider	seed probeSetId	seed miR	Seed SMILES	seed nsc	seed logHiConc	seed endpoint	seed target	target moltId	target provider	target geneSymbol	target probeSetId	target miR	Target SMILES	target nsc	target logHiConc	target endpoint	target target
0.66	0.34	1	0.66	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_645150_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S645150 2 GI50 AVGD	44						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							COc1ccc2nc3cc(Cl)ccc3c(Sc4ccc(cc4C)[N+](=O)[O-])c2c1	645150	-4.0	GI50	
0.65	0.34	2	0.65	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_695786_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S695786 2 GI50 AVGD	51						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CO[C@]12CC3C[C@H]4CC5CCC6=CC(=O)CC[C@]6(OC(=O)C)C5C[C@]4(C)C3(C7C[C@H]8[C@@H]9CCC%10=CC(=O)CC[C@]%10(OC(=O)C)[C@H]9CC[C@]8(C)C17)C(=O)C2	695786	-4.0	GI50	
0.65	0.32	3	0.65	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_648375_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S648375 2 GI50 AVGD	42						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CC1(C)CC(=C(C(=O)N)C(=O)O1)\C=C/2\OC(=O)c3ccccc23	648375	-4.0	GI50	
0.62	0.33	4	0.62	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_661935_-5.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S661935 2 GI50 AVGD	52						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CCOC(=O)\C(=N/c1c(O)c2c(O)ccc(O)c2c(O)c1Cl)\CO	661935	-5.0	GI50	
0.61	0.45	5	0.61	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_695646_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S695646 2 GI50 AVGD	46						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							Clc1cccc(c1)N2CCN(CCCN3N=C4CSc5c(ccc6ccccc56)N4C3=O)CC2	695646	-4.0	GI50	
0.6	0.27	6	0.6	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_618631_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S618631 2 GI50 AVGD	53						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CC(=C)c1cc(cc(C(=C)C)c1S(=O)(=O)C)C(C)(C)C	618631	-4.0	GI50	
0.6	0.26	7	0.6	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_125177_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S125177 2 GI50 AVGD	42						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CC(=C)\C=C\c1c(O)c(O)c2ccccc2c1O	125177	-4.0	GI50	Lapachol
0.6	0.26	8	0.6	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_626992_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S626992 2 GI50 AVGD	44						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							OC(=O)CN(c1ccc(Cl)cc1)S(=O)(=O)c2ccccc2	626992	-4.0	GI50	
0.6	0.27	9	0.6	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_640038_-2.2_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S640038 2 GI50 AVGD	41						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT								640038	-2.2	GI50	
0.6	0.31	10	0.6	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_628967_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S628967 2 GI50 AVGD	43						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CC(=O)OC[C@H]1[C@@H](C[C@@H]2OC(=O)C[C@H]12)OC(=O)C	628967	-4.0	GI50	
0.59	0.26	11	0.59	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_628996_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S628996 2 GI50 AVGD	44						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							C[C@@H]1CC(=O)C2CCCC1C2=O	628996	-4.0	GI50	
0.58	0.46	12	0.58	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_17746_-4.0_2_GI50_AVGDA	NSC S758663 3 GIPRCNT AVGD	NSC S17746 2 GI50 AVGDA	56						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CCCCCCCC\C=C\CCCCCCCC1=NC(C)(C)CN1C(C)C	17746	-4.0	GI50	
0.58	0.12	13	0.58	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_623728_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S623728 2 GI50 AVGD	45						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							Cc1ccc(C)c(c1)N2C(=O)C(=O)C(\C(=N/c3cccc4c(O)nnc(O)c34)\C2=O)c5nc6ccccc6s5	623728	-4.0	GI50	
0.57	0.36	14	0.57	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_601980_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S601980 2 GI50 AVGD	56						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							Cc1nc2ccccc2nc1NNc3ccccc3	601980	-4.0	GI50	
0.57	0.37	15	0.57	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_629110_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S629110 2 GI50 AVGD	44						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							OC(CCNC12CC3CC(CC(C3)C1)C2)c4ccccc4	629110	-4.0	GI50	
0.57	0.35	16	0.57	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_644498_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S644498 2 GI50 AVGD	50						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CN(C)CCOc1ccc(c2cccnc12)[N+](=O)[O-]	644498	-4.0	GI50	
0.56	0.34	17	0.56	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_645023_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S645023 2 GI50 AVGD	47						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							[O-][N+](=O)c1ccc(cc1)n2nnc(C3=NCCN3)c2c4ccc(Cl)cc4	645023	-4.0	GI50	
0.56	0.19	18	0.56	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_753389_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S753389 2 GI50 AVGD	47						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							Cc1ccc2[nH]cc(c3nc(cs3)c4c[nH]c5ncccc45)c2c1	753389	-4.0	GI50	
0.56	0.22	19	0.56	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_680185_-8.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S680185 2 GI50 AVGD	47						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CCOc1cc2[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@@H]3C\C(=N\O)\c2cc1O	680185	-8.0	GI50	
0.56	0.16	20	0.56	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_732177_-4.3_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S732177 2 GI50 AVGD	44						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							NC(=N)N\N=C\c1c(nc2SCCn12)c3cc(Cl)sc3Cl	732177	-4.3	GI50	
0.55	-0.01	21	0.55	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_652551_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S652551 2 GI50 AVGD	46						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CN1c2ccccc2C(=O)c3c(O)cc(OCCCCOC(C)(C)C#C)cc13	652551	-4.0	GI50	
0.55	0.09	22	0.55	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_702692_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S702692 2 GI50 AVGD	45						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							NS(=O)(=O)c1cc(c(NC(=O)Nc2ccc(Cl)c(Cl)c2)c(Cl)c1Cl)S(=O)(=O)N	702692	-4.0	GI50	
0.54	0.47	23	0.54	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_9772_-4.0_2_GI50_AVGDAT	NSC S758663 3 GIPRCNT AVGD	NSC S9772 2 GI50 AVGDAT	56						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							Oc1ccc2cc(Br)ccc2c1c3c(O)ccc4cc(Br)ccc34	9772	-4.0	GI50	
0.54	0.44	24	0.54	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_660431_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S660431 2 GI50 AVGD	45						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							Cc1ccc(C)n2c3cc4ccccc4cc3nc12	660431	-4.0	GI50	
0.54	0.21	25	0.54	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_651731_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S651731 2 GI50 AVGD	44						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CCOC1=CP(=O)(CC(=C1Cl)C)OCC	651731	-4.0	GI50	
0.54	0.25	26	0.54	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_697770_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S697770 2 GI50 AVGD	46						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							COCN1C(=O)[C@@H]2CCCN2C(=O)c3cc(N)ccc13	697770	-4.0	GI50	
0.54	0.14	27	0.54	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_658260_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S658260 2 GI50 AVGD	51						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							Cc1nc(C)c(cc1C(=O)Nc2cccc3C(=O)NC(=O)c23)C(=O)Nc4cccc5c(O)[nH]c(O)c45	658260	-4.0	GI50	
0.53	0.23	28	0.53	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_642501_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S642501 2 GI50 AVGD	47						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							Cc1ncc([N+](=O)[O-])n1CCNC(=O)CCCCn2ccnc2[N+](=O)[O-]	642501	-4.0	GI50	
0.53	0.28	29	0.53	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_697507_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S697507 2 GI50 AVGD	40						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CC12ON=C(N1C=CN3C2ON=C3c4ccccc4)c5ccccc5	697507	-4.0	GI50	
0.53	0.23	30	0.53	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_59941_-4.0_2_GI50_AVGDA	NSC S758663 3 GIPRCNT AVGD	NSC S59941 2 GI50 AVGDA	43						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							Cc1cccc(C(=O)c2cccc3ccccc23)c1C(=O)O	59941	-4.0	GI50	
0.53	0.15	31	0.53	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_695645_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S695645 2 GI50 AVGD	47						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							O=C1N(CCCN2CCOCC2)N=C3CSc4c(ccc5ccccc45)N13	695645	-4.0	GI50	
0.53	0.4	32	0.53	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_671397_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S671397 2 GI50 AVGD	46						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							COc1ccc(cc1)\N=C\2/C(/N(C(N2c3ccc(OC)cc3)=S)c4ccccc4[N+](=O)[O-])=N\c5ccc(OC)cc5	671397	-4.0	GI50	
0.52	0.45	33	0.52	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_67025_-4.0_2_GI50_AVGDA	NSC S758663 3 GIPRCNT AVGD	NSC S67025 2 GI50 AVGDA	47						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							C\C(=C\C(=N\N=C(N)N)\c1ccccc1)\c2ccccc2	67025	-4.0	GI50	
0.52	0.25	34	0.52	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_642500_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S642500 2 GI50 AVGD	48						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							Cc1ncc([N+](=O)[O-])n1CCNC(=O)CCCCCn2ccnc2[N+](=O)[O-]	642500	-4.0	GI50	
0.52	0.45	35	0.52	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_720193_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S720193 2 GI50 AVGD	54						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							N(\N=C(/c1ccccc1)\c2ccccn2)c3nc4ccccc4[nH]3	720193	-4.0	GI50	
0.52	0.41	36	0.52	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_647037_-5.7_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S647037 2 GI50 AVGD	44						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CCOC(=O)CNC(=O)C(CSC(=O)N(C)O)NC(=O)CCC(N)C(=O)O	647037	-5.7	GI50	
0.52	0.4	37	0.52	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_756898_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S756898 2 GI50 AVGD	53						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							COc1ccc2c(cn(C)c2c1)C3(C(=O)Nc4ccc(Cl)cc34)c5cn(C)c6cc(OC)ccc56	756898	-4.0	GI50	
0.52	0.12	38	0.52	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_693410_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S693410 2 GI50 AVGD	51						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							C[C@@]12O[C@@]3([C@H]4O[C@@H]14)[C@@H]([C@H]2Cl)C(=O)N5CCOC35C	693410	-4.0	GI50	
0.52	0.12	39	0.52	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_655295_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S655295 2 GI50 AVGD	45						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							COc1cc(CCCC(O)COc2cccc3C4CCCCCC4(O)c23)cc(OC)c1	655295	-4.0	GI50	
0.52	0.38	40	0.52	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_720341_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S720341 2 GI50 AVGD	54						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							COC(=O)c1c(O)ccc2c1c3C(=O)c4ccccc4C(=O)c3n2c5ccc(OC)cc5	720341	-4.0	GI50	
0.52	0.29	41	0.52	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_719181_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S719181 2 GI50 AVGD	47						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							Cc1nnc2nc(cc(c3ccc(Cl)cc3)n12)c4ccc(Cl)cc4Cl	719181	-4.0	GI50	
0.52	0.24	42	0.52	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_94265_-4.0_2_GI50_AVGDA	NSC S758663 3 GIPRCNT AVGD	NSC S94265 2 GI50 AVGDA	55						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							COc1ccc2c(c1)[nH]c3c(\C=C\c4ccccc4)nccc23	94265	-4.0	GI50	
0.52	0.17	43	0.52	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_656456_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S656456 2 GI50 AVGD	42						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							O=C(N(C1CCCCC1)C(=S)N2CCN(CC2)c3ccccc3)c4occc4	656456	-4.0	GI50	
0.51	0.05	44	0.51	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_767951_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S767951 2 GI50 AVGD	53						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CCc1cc(Nc2nccc(n2)c3c(nc4ccccn34)c5ccc(OC)c(c5)C(=O)Nc6c(F)cccc6F)c(OC)cc1N7CCC(CC7)N8CCN(CC8)S(=O)(=O)C	767951	-4.0	GI50	IGF1R
0.51	0.16	45	0.51	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_632871_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S632871 2 GI50 AVGD	43						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							[Cl-][Pt+2]([Cl-])([NH2+]c1ccc(\C=C\C(=O)[O-])cc1)[NH2+]c2ccc(\C=C\C(=O)[O-])cc2	632871	-4.0	GI50	
0.51	0.35	46	0.51	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_662574_-5.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S662574 2 GI50 AVGD	42						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CCOC(=O)c1c(c(C)cn1C)c2ccccc2	662574	-5.0	GI50	
0.51	0.27	47	0.51	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_700653_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S700653 2 GI50 AVGD	52						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							CC1OC(OC2C(O)COC(OC3C(C)OC(OC4C(O)C(O)COC4OC(=O)[C@]56CCC(C)(C)C[C@@H]5C7=CCC8[C@@]9(C)C[C@H](O)[C@H](OC%10OC(CO)C(O)C(O)C%10O)[C@@](C)(CO)[C@@H]9CC[C@@]8(C)[C@]7(C)CC	700653	-4.0	GI50	
-0.5	-0.18	3	-0.5	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_279503_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S279503 2 GI50 AVGD	47						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							COC(=O)C12OCC34C(CC5C(=CC(=O)C(O)C5(C)C3C(O)C1O)C)OC(=O)C(OC(=O)CC(C)C)C24	279503	-4.0	GI50	Isobrucine A
-0.5	-0.37	2	-0.5	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_673464_-4.0_2_GI50_AVGD	NSC S758663 3 GIPRCNT AVGD	NSC S673464 2 GI50 AVGD	52						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							Oc1cc(Br)cc2cc(Br)cnc12	673464	-4.0	GI50	
-0.51	-0.04	1	-0.51	NSC_S_758663_-5.0_3_GIPRCNT_AVGD	NSC_S_94739_-5.0_2_GI50_AVGDA	NSC S758663 3 GIPRCNT AVGD	NSC S94739 2 GI50 AVGDA	55						CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc	758663	-5.0	GIPRCNT							COc1cc2c3CN4CCC[C@H]4[C@H](O)c3c5ccc(O)cc5c2cc1OC	94739	-5.0	GI50	

Suppl. Table 3- List of compounds correlated to Ritonavir. Highlighted rows indicate drugs that are approved or in clinical development

0.77	0.59	1	0.77	NSC_S_7	NSC_S_7	NSC S76	NSC S71	43	CC(C)[C@	760369	-5	GIPRCNT	CC1=NN	713649	-4	GI50	
0.76	0.44	2	0.76	NSC_S_7	NSC_S_6	NSC S76	NSC S65	40	CC(C)[C@	760369	-5	GIPRCNT	FC(F)(F)C	654728	-4	GI50	
0.76	0.49	3	0.76	NSC_S_7	NSC_S_6	NSC S76	NSC S65	45	CC(C)[C@	760369	-5	GIPRCNT	ClC1C(N	650007	-4	GI50	
0.75	0.31	4	0.75	NSC_S_7	NSC_S_6	NSC S76	NSC S65	42	CC(C)[C@	760369	-5	GIPRCNT	Cc1ccc(\	655144	-4	GI50	
0.75	0.5	5	0.75	NSC_S_7	NSC_S_6	NSC S76	NSC S65	41	CC(C)[C@	760369	-5	GIPRCNT	Nc1ccc2	652760	-4	GI50	
0.74	0.39	6	0.74	NSC_S_7	NSC_S_6	NSC S76	NSC S65	46	CC(C)[C@	760369	-5	GIPRCNT	CCSCCC	650641	-4	GI50	
0.74	0.34	7	0.74	NSC_S_7	NSC_S_6	NSC S76	NSC S65	50	CC(C)[C@	760369	-5	GIPRCNT	CSC1NC(	659341	-4	GI50	
0.74	0.33	8	0.74	NSC_S_7	NSC_S_6	NSC S76	NSC S62	43	CC(C)[C@	760369	-5	GIPRCNT	Clc1cc(C	627583	-4	GI50	
0.74	0.56	9	0.74	NSC_S_7	NSC_S_6	NSC S76	NSC S65	46	CC(C)[C@	760369	-5	GIPRCNT	SCCSCC	650639	-4	GI50	
0.74	0.55	10	0.74	NSC_S_7	NSC_S_1	NSC S76	NSC S17	45	CC(C)[C@	760369	-5	GIPRCNT	O=C1OC	177881	-4	GI50	
0.73	0.46	11	0.73	NSC_S_7	NSC_S_6	NSC S76	NSC S63	41	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	632023	-4	GI50	
0.72	0.47	12	0.72	NSC_S_7	NSC_S_6	NSC S76	NSC S66	49	CC(C)[C@	760369	-5	GIPRCNT	CCCCC1(	660676	-4	GI50	
0.72	0.55	13	0.72	NSC_S_7	NSC_S_6	NSC S76	NSC S64	45	CC(C)[C@	760369	-5	GIPRCNT	CCOc1cc	642571	-4	GI50	
0.72	0.43	14	0.72	NSC_S_7	NSC_S_7	NSC S76	NSC S71	47	CC(C)[C@	760369	-5	GIPRCNT	CC1=NN	713290	-4	GI50	
0.72	0.47	15	0.72	NSC_S_7	NSC_S_7	NSC S76	NSC S78	54	CC(C)[C@	760369	-5	GIPRCNT	Nc1ncn(	78674	-4	GI50	
0.71	0.38	16	0.71	NSC_S_7	NSC_S_6	NSC S76	NSC S65	46	CC(C)[C@	760369	-5	GIPRCNT	CSCCCN	650638	-4	GI50	
0.71	0.5	17	0.71	NSC_S_7	NSC_S_8	NSC S76	NSC S85	56	CC(C)[C@	760369	-5	GIPRCNT	OC(=O)C	85372	-4	GI50	
0.7	0.27	18	0.7	NSC_S_7	NSC_S_7	NSC S76	NSC S72	51	CC(C)[C@	760369	-5	GIPRCNT	CC(C)(C)	723394	-4	GI50	
0.7	0.47	19	0.7	NSC_S_7	NSC_S_6	NSC S76	NSC S67	52	CC(C)[C@	760369	-5	GIPRCNT	[O-][N+](	670134	-4	GI50	
0.7	0.28	20	0.7	NSC_S_7	NSC_S_6	NSC S76	NSC S69	52	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	697392	-4	GI50	
0.7	0.45	21	0.7	NSC_S_7	NSC_S_6	NSC S76	NSC S63	48	CC(C)[C@	760369	-5	GIPRCNT	[O-][N+](	632950	-4	GI50	
0.7	0.26	22	0.7	NSC_S_7	NSC_S_6	NSC S76	NSC S63	43	CC(C)[C@	760369	-5	GIPRCNT	NC(=S)N	631519	-4	GI50	
0.7	0.48	23	0.7	NSC_S_7	NSC_S_7	NSC S76	NSC S71	55	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	714390	-4	GI50	
0.69	0.39	24	0.69	NSC_S_7	NSC_S_7	NSC S76	NSC S71	50	CC(C)[C@	760369	-5	GIPRCNT	Clc1ccc(	713685	-4	GI50	
0.69	0.53	25	0.69	NSC_S_7	NSC_S_7	NSC S76	NSC S71	55	CC(C)[C@	760369	-5	GIPRCNT	CC1CC[C	710091	-5	GI50	
0.69	0.59	26	0.69	NSC_S_7	NSC_S_6	NSC S76	NSC S68	51	CC(C)[C@	760369	-5	GIPRCNT	CCC(C1N	684387	-4	GI50	
0.69	0.47	27	0.69	NSC_S_7	NSC_S_8	NSC S76	NSC S85	56	CC(C)[C@	760369	-5	GIPRCNT	Cc1nc(N	85069	-4	GI50	
0.69	0.34	28	0.69	NSC_S_7	NSC_S_7	NSC S76	NSC S72	56	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	722739	-4	GI50	
0.69	0.34	29	0.69	NSC_S_7	NSC_S_7	NSC S76	NSC S71	55	CC(C)[C@	760369	-5	GIPRCNT	CC1(C)C	714392	-4	GI50	
0.69	0.41	30	0.69	NSC_S_7	NSC_S_7	NSC S76	NSC S72	57	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	727958	-4	GI50	
0.69	0.32	31	0.69	NSC_S_7	NSC_S_6	NSC S76	NSC S65	44	CC(C)[C@	760369	-5	GIPRCNT	CC(C)(C)	652596	-4	GI50	
0.69	0.41	32	0.69	NSC_S_7	NSC_S_6	NSC S76	NSC S64	44	CC(C)[C@	760369	-5	GIPRCNT	N\N=C(/	641440	-4	GI50	
0.69	0.47	33	0.69	NSC_S_7	NSC_S_1	NSC S76	NSC S19	45	CC(C)[C@	760369	-5	GIPRCNT	Fc1cccc	191382	-4	GI50	
0.69	0.32	34	0.69	NSC_S_7	NSC_S_6	NSC S76	NSC S62	41	CC(C)[C@	760369	-5	GIPRCNT	CC(Sc1cc	627448	-4	GI50	
0.69	0.39	35	0.69	NSC_S_7	NSC_S_1	NSC S76	NSC S15	55	CC(C)[C@	760369	-5	GIPRCNT	Cc1cc(C	157469	-4	GI50	
0.69	0.57	36	0.69	NSC_S_7	NSC_S_6	NSC S76	NSC S68	54	CC(C)[C@	760369	-5	GIPRCNT	CCO\C(=	684851	-4	GI50	
0.69	0.41	37	0.69	NSC_S_7	NSC_S_6	NSC S76	NSC S69	51	CC(C)[C@	760369	-5	GIPRCNT	CC(NNC(	698277	-4	GI50	
0.68	0.35	38	0.68	NSC_S_7	NSC_S_7	NSC S76	NSC S71	49	CC(C)[C@	760369	-5	GIPRCNT	O=C1N(	713687	-4	GI50	
0.68	0.47	39	0.68	NSC_S_7	NSC_S_5	NSC S76	NSC S59	42	CC(C)[C@	760369	-5	GIPRCNT	Nc1ccc(\	59065	-4	GI50	
0.68	0.41	40	0.68	NSC_S_7	NSC_S_6	NSC S76	NSC S65	51	CC(C)[C@	760369	-5	GIPRCNT	CC1(C)C	657421	-4	GI50	
0.68	0.54	41	0.68	NSC_S_7	NSC_S_6	NSC S76	NSC S68	54	CC(C)[C@	760369	-5	GIPRCNT	Oc1ccc(	683634	-4	GI50	
0.68	0.61	42	0.68	NSC_S_7	NSC_S_6	NSC S76	NSC S69	53	CC(C)[C@	760369	-5	GIPRCNT	C[C@H]	699834	-4	GI50	
0.68	0.33	43	0.68	NSC_S_7	NSC_S_1	NSC S76	NSC S16	54	CC(C)[C@	760369	-5	GIPRCNT	C(Cc1ccn	163398	-4	GI50	
0.68	0.52	44	0.68	NSC_S_7	NSC_S_7	NSC S76	NSC S73	52	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	732974	-4	GI50	
0.68	0.35	45	0.68	NSC_S_7	NSC_S_6	NSC S76	NSC S65	48	CC(C)[C@	760369	-5	GIPRCNT	CN1C\C(	657708	-4	GI50	
0.68	0.4	46	0.68	NSC_S_7	NSC_S_7	NSC S76	NSC S70	50	CC(C)[C@	760369	-5	GIPRCNT	CCN1C\(	709500	-4	GI50	
0.68	0.47	47	0.68	NSC_S_7	NSC_S_1	NSC S76	NSC S10	41	CC(C)[C@	760369	-5	GIPRCNT	OC(=O)c	101492	-4	GI50	
0.68	0.42	48	0.68	NSC_S_7	NSC_S_6	NSC S76	NSC S68	49	CC(C)[C@	760369	-5	GIPRCNT	COc1c(C	687149	-4	GI50	
0.68	0.39	49	0.68	NSC_S_7	NSC_S_6	NSC S76	NSC S66	57	CC(C)[C@	760369	-5	GIPRCNT	[O-][N+](	665081	-4	GI50	
0.67	0.39	50	0.67	NSC_S_7	NSC_S_1	NSC S76	NSC S15	55	CC(C)[C@	760369	-5	GIPRCNT	OC(=O)C	157725	-4	GI50	
0.67	0.42	51	0.67	NSC_S_7	NSC_S_3	NSC S76	NSC S35	55	CC(C)[C@	760369	-5	GIPRCNT	CN1CCN	356363	-4	GI50	
0.67	0.41	52	0.67	NSC_S_7	NSC_S_6	NSC S76	NSC S64	45	CC(C)[C@	760369	-5	GIPRCNT	N#Cc1cc	644579	-4	GI50	
0.67	0.26	53	0.67	NSC_S_7	NSC_S_6	NSC S76	NSC S65	43	CC(C)[C@	760369	-5	GIPRCNT	CCC(C)C	651760	-4	GI50	
0.67	0.27	54	0.67	NSC_S_7	NSC_S_6	NSC S76	NSC S65	40	CC(C)[C@	760369	-5	GIPRCNT	CC(=O)C	657712	-4	GI50	
0.67	0.38	55	0.67	NSC_S_7	NSC_S_7	NSC S76	NSC S72	56	CC(C)[C@	760369	-5	GIPRCNTBrucine	COc1cc2	72917	-4	GI50	Brucine
0.67	0.64	56	0.67	NSC_S_7	NSC_S_6	NSC S76	NSC S67	43	CC(C)[C@	760369	-5	GIPRCNT	CCOC(=C	671475	-4	GI50	
0.67	0.48	57	0.67	NSC_S_7	NSC_S_7	NSC S76	NSC S73	50	CC(C)[C@	760369	-5	GIPRCNT	CO\N=C	735312	-4	GI50	
0.67	0.38	58	0.67	NSC_S_7	NSC_S_7	NSC S76	NSC S74	57	CC(C)[C@	760369	-5	GIPRCNT	COc1cc(	740129	-4	GI50	
0.67	0.35	59	0.67	NSC_S_7	NSC_S_6	NSC S76	NSC S68	49	CC(C)[C@	760369	-5	GIPRCNT	Nc1ccc(	685807	-4	GI50	
0.67	0.49	60	0.67	NSC_S_7	NSC_S_6	NSC S76	NSC S69	50	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	690760	-4	GI50	
0.67	0.36	61	0.67	NSC_S_7	NSC_S_7	NSC S76	NSC S71	52	CC(C)[C@	760369	-5	GIPRCNT	CCOc1cc	716199	-4	GI50	
0.67	0.33	62	0.67	NSC_S_7	NSC_S_7	NSC S76	NSC S71	48	CC(C)[C@	760369	-5	GIPRCNT	CN(C)c1	713023	-4	GI50	
0.67	0.43	63	0.67	NSC_S_7	NSC_S_1	NSC S76	NSC S15	52	CC(C)[C@	760369	-5	GIPRCNT	OC(=O)C	154652	-4	GI50	
0.67	0.35	64	0.67	NSC_S_7	NSC_S_7	NSC S76	NSC S76	57	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	768584	-4	GI50	
0.67	0.28	65	0.67	NSC_S_7	NSC_S_7	NSC S76	NSC S73	51	CC(C)[C@	760369	-5	GIPRCNT	Cc1cc(c(	731389	-4	GI50	
0.67	0.32	66	0.67	NSC_S_7	NSC_S_2	NSC S76	NSC S21	55	CC(C)[C@	760369	-5	GIPRCNT	Cc1ccc(c	211193	-4	GI50	
0.67	0.45	67	0.67	NSC_S_7	NSC_S_6	NSC S76	NSC S68	53	CC(C)[C@	760369	-5	GIPRCNT	CN(C)n1	685033	-4	GI50	
0.67	0.45	68	0.67	NSC_S_7	NSC_S_6	NSC S76	NSC S62	40	CC(C)[C@	760369	-5	GIPRCNT	CCOC(=C	628254	-4	GI50	
0.67	0.24	69	0.67	NSC_S_7	NSC_S_1	NSC S76	NSC S16	55	CC(C)[C@	760369	-5	GIPRCNT	CC1=[N+	169930	-4	GI50	
0.66	0.41	70	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S68	49	CC(C)[C@	760369	-5	GIPRCNT	CSc1cc(C	681181	-4	GI50	
0.66	0.24	71	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S66	51	CC(C)[C@	760369	-5	GIPRCNT	CC1(C)N	663920	-4	GI50	
0.66	0.24	72	0.66	NSC_S_7	NSC_S_7	NSC S76	NSC S74	57	CC(C)[C@	760369	-5	GIPRCNT	CCCCCC	742849	-4	GI50	
0.66	0.31	73	0.66	NSC_S_7	NSC_S_3	NSC S76	NSC S32	56	CC(C)[C@	760369	-5	GIPRCNT	C\C=C(/C	329695	-4	GI50	
0.66	0.67	74	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S67	43	CC(C)[C@	760369	-5	GIPRCNT	CC1CN=	672015	-4	GI50	
0.66	0.13	75	0.66	NSC_S_7	NSC_S_7	NSC S76	NSC S70	55	CC(C)[C@	760369	-5	GIPRCNT	Oc1[nH]	707059	-4	GI50	
0.66	0.44	76	0.66	NSC_S_7	NSC_S_8	NSC S76	NSC S85	56	CC(C)[C@	760369	-5	GIPRCNT	CC(C)CC	85260	-4	GI50	
0.66	0.33	77	0.66	NSC_S_7	NSC_S_1	NSC S76	NSC S16	53	CC(C)[C@	760369	-5	GIPRCNT	CCOC(=C	163798	-4	GI50	
0.66	0.32	78	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S65	44	CC(C)[C@	760369	-5	GIPRCNT	CC(=O)N	654786	-4	GI50	
0.66	0.31	79	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S64	46	CC(C)[C@	760369	-5	GIPRCNT	CC(CC(O	642300	-4.3	GI50	
0.66	0.36	80	0.66	NSC_S_7	NSC_S_7	NSC S76	NSC S71	53	CC(C)[C@	760369	-5	GIPRCNT	Oc1c(\C	711848	-4	GI50	
0.66	0.46	81	0.66	NSC_S_7	NSC_S_2	NSC S76	NSC S22	57	CC(C)[C@	760369	-5	GIPRCNT	[O-][N+](	228099	-4	GI50	
0.66	0.38	82	0.66	NSC_S_7	NSC_S_7	NSC S76	NSC S72	50	CC(C)[C@	760369	-5	GIPRCNT	COc1cc2	723412	-4	GI50	
0.66	0.41	83	0.66	NSC_S_7	NSC_S_7	NSC S76	NSC S72	57	CC(C)[C@	760369	-5	GIPRCNT	c1ccc(C#	728063	-4	GI50	
0.66	0.46	84	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S68	49	CC(C)[C@	760369	-5	GIPRCNT	Clc1ccc(	684145	-4	GI50	
0.66	0.51	85	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S63	41	CC(C)[C@	760369	-5	GIPRCNT	Cc1ccc(c	633550	-4	GI50	
0.66	0.49	86	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S69	55	CC(C)[C@	760369	-5	GIPRCNT	CC1(C)O	692403	-4	GI50	
0.66	0.42	87	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S69	52	CC(C)[C@	760369	-5	GIPRCNT	Brc1ccc(	698967	-4	GI50	
0.66	0.28	88	0.66	NSC_S_7	NSC_S_7	NSC S76	NSC S70	48	CC(C)[C@	760369	-5	GIPRCNT	ClC1=CC	709508	-4	GI50	
0.66	0.6	89	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S62	40	CC(C)[C@	760369	-5	GIPRCNT	CCc1ccc	627724	-4	GI50	
0.66	0.39	90	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S63	41	CC(C)[C@	760369	-5	GIPRCNT	CN(C)CC	630698	-4	GI50	
0.66	0.33	91	0.66	NSC_S_7	NSC_S_8	NSC S76	NSC S85	54	CC(C)[C@	760369	-5	GIPRCNT	Cc1nnc2	85323	-4	GI50	
0.66	0.53	92	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S64	44	CC(C)[C@	760369	-5	GIPRCNT	CC(C)c1c	646156	-4	GI50	
0.66	0.43	93	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S63	44	CC(C)[C@	760369	-5	GIPRCNT	CN1C(=C	634645	-4	GI50	
0.66	0.32	94	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S68	51	CC(C)[C@	760369	-5	GIPRCNT	CN(CC(=	688108	-4	GI50	
0.66	0.35	95	0.66	NSC_S_7	NSC_S_7	NSC S76	NSC S74	56	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	740083	-4	GI50	
0.66	0.46	96	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S69	55	CC(C)[C@	760369	-5	GIPRCNT	CCOC(=C	694960	-4	GI50	
0.66	0.39	97	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S65	49	CC(C)[C@	760369	-5	GIPRCNT	COC(C)(C	658698	-4	GI50	
0.66	0.27	98	0.66	NSC_S_7	NSC_S_6	NSC S76	NSC S63	48	CC(C)[C@	760369	-5	GIPRCNT	CC(=O)N	634931	-4	GI50	
0.65	0.56	99	0.65	NSC_S_7	NSC_S_7	NSC S76	NSC S74	57	CC(C)[C@	760369	-5	GIPRCNT	CCSC[C@	743045	-4	GI50	
0.65	0.52	100	0.65	NSC_S_7	NSC_S_7	NSC S76	NSC S71	55	CC(C)[C@	760369	-5	GIPRCNT	COc1nnc	711312	-4	GI50	
0.65	0.49	101	0.65	NSC_S_7	NSC_S_7	NSC S76	NSC S74	57	CC(C)[C@	760369	-5	GIPRCNT	CN(C)c1c	740120	-4	GI50	
0.65	0.4	102	0.65	NSC_S_7	NSC_S_6	NSC S76	NSC S69	56	CC(C)[C@	760369	-5	GIPRCNT	ONC(=O	692763	-4	GI50	
0.65	0.38	103	0.65	NSC_S_7	NSC_S_6	NSC S76	NSC S65	49	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	657020	-4	GI50	
0.65	0.52	104	0.65	NSC_S_7	NSC_S_6	NSC S76	NSC S61	46	CC(C)[C@	760369	-5	GIPRCNT	OC(=O)C	619423	-4	GI50	
0.65	0.32	105	0.65	NSC_S_7	NSC_S_1	NSC S76	NSC S16	56	CC(C)[C@	760369	-5	GIPRCNT	NCCc1cc	166395	-4	GI50	
0.65	0.32	106	0.65	NSC_S_7	NSC_S_7	NSC S76	NSC S73	56	CC(C)[C@	760369	-5	GIPRCNT	Cc1nc2c	736045	-4	GI50	
0.65	0.43	107	0.65	NSC_S_7	NSC_S_7	NSC S76	NSC S72	55	CC(C)[C@	760369	-5	GIPRCNT	Clc1ccc(	725674	-4	GI50	
0.65	0.41	108	0.65	NSC_S_7	NSC_S_3	NSC S76	NSC S32	55	CC(C)[C@	760369	-5	GIPRCNT	OP(=O)(	328005	-4	GI50	
0.65	0.28	109	0.65	NSC_S_7	NSC_S_6	NSC S76	NSC S68	55	CC(C)[C@	760369	-5	GIPRCNT	Cc1ccc(c	684810	-4	GI50	
0.65	0.46	110	0.65	NSC_S_7	NSC_S_6	NSC S76	NSC S66	53	CC(C)[C@	760369	-5	GIPRCNT	Clc1ccc(	669336	-4	GI50	
0.65	0.34	111	0.65	NSC_S_7	NSC_S_7	NSC S76	NSC S74	53	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	740261	-4	GI50	
0.65	0.47	112	0.65	NSC_S_7	NSC_S_2	NSC S76	NSC S22	45	CC(C)[C@	760369	-5	GIPRCNT	Oc1ccc2	22842	-3.9	GI50	Coumesterol natural compound fro
0.65	0.61	113	0.65	NSC_S_7	NSC_S_6	NSC S76	NSC S66	54	CC(C)[C@	760369	-5	GIPRCNT	O=C1C2	666513	-4	GI50	
0.65	0.32	114	0.65	NSC_S_7	NSC_S_6	NSC S76	NSC S69	47	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	699106	-4	GI50	
0.65	0.38	115	0.65	NSC_S_7	NSC_S_1	NSC S76	NSC S10	54	CC(C)[C@	760369	-5	GIPRCNT	Oc1cccc	103832	-4	GI50	
0.65	0.32	116	0.65	NSC_S_7	NSC_S_6	NSC S76	NSC S69	55	CC(C)[C@	760369	-5	GIPRCNT	[O-][N+](	697714	-4	GI50	
0.65	0.36	117	0.65	NSC_S_7	NSC_S_6	NSC S76	NSC S68	53	CC(C)[C@	760369	-5	GIPRCNT	Nc1nc(c	683627	-4	GI50	
0.65	0.26	118	0.65	NSC_S_7	NSC_S_6	NSC S76	NSC S66	53	CC(C)[C@	760369	-5	GIPRCNT	COC12C	668917	-4	GI50	
0.64	0.42	119	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S71	54	CC(C)[C@	760369	-5	GIPRCNT	COc1cc(	711846	-4	GI50	
0.64	0.34	120	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S64	42	CC(C)[C@	760369	-5	GIPRCNT	COC(=O)	648845	-4	GI50	
0.64	0.28	121	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S71	49	CC(C)[C@	760369	-5	GIPRCNT	CCO\C(=	710861	-4	GI50	
0.64	0.24	122	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S69	49	CC(C)[C@	760369	-5	GIPRCNT	CN1N(\C	693124	-4	GI50	
0.64	0.43	123	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S68	57	CC(C)[C@	760369	-5	GIPRCNT	CCO\C=N	684397	-4	GI50	
0.64	0.38	124	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S64	42	CC(C)[C@	760369	-5	GIPRCNT	[Cl-][Pd+	648084	-4	GI50	
0.64	0.29	125	0.64	NSC_S_7	NSC_S_1	NSC S76	NSC S12	57	CC(C)[C@	760369	-5	GIPRCNT	COc1c(C	123389	-4	GI50	
0.64	0.53	126	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S68	52	CC(C)[C@	760369	-5	GIPRCNT	CC(=O)N	687803	-4	GI50	
0.64	0.26	127	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S71	54	CC(C)[C@	760369	-5	GIPRCNT	Cn1c2c(	719503	-4	GI50	
0.64	0.33	128	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S62	41	CC(C)[C@	760369	-5	GIPRCNT	[Cl-][Pt+	623316	-4	GI50	
0.64	0.36	129	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S71	53	CC(C)[C@	760369	-5	GIPRCNT	CC1=CC	718919	-4	GI50	
0.64	0.24	130	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S69	56	CC(C)[C@	760369	-5	GIPRCNT	OC(=O)[	698256	-4	GI50	
0.64	0.4	131	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S63	48	CC(C)[C@	760369	-5	GIPRCNT	CC(C)c1c	634415	-4	GI50	
0.64	0.39	132	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S73	53	CC(C)[C@	760369	-5	GIPRCNT	S=C1SN=	732632	-4	GI50	
0.64	0.33	133	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S72	57	CC(C)[C@	760369	-5	GIPRCNT	CCOC(=C	722989	-4	GI50	
0.64	0.34	134	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S61	53	CC(C)[C@	760369	-5	GIPRCNT	Nc1ccc2	618177	-4	GI50	
0.64	0.57	135	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S68	53	CC(C)[C@	760369	-5	GIPRCNT	COC(=O)	689401	-4	GI50	
0.64	0.44	136	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S71	54	CC(C)[C@	760369	-5	GIPRCNT	Clc1ccc(	711844	-4	GI50	
0.64	0.4	137	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S65	56	CC(C)[C@	760369	-5	GIPRCNT	CC1=CC(	657458	-4	GI50	
0.64	0.35	138	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S74	57	CC(C)[C@	760369	-5	GIPRCNT	CCCCCC	742851	-4	GI50	
0.64	0.65	139	0.64	NSC_S_7	NSC_S_1	NSC S76	NSC S14	58	CC(C)[C@	760369	-5	GIPRCNT	NNc1c2c	14977	-4	GI50	
0.64	0.43	140	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S68	50	CC(C)[C@	760369	-5	GIPRCNT	CC(=O)C	682869	-4	GI50	
0.64	0.45	141	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S76	57	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	768585	-4	GI50	
0.64	0.32	142	0.64	NSC_S_7	NSC_S_3	NSC S76	NSC S30	56	CC(C)[C@	760369	-5	GIPRCNT	CC1C(C)	301491	-4	GI50	
0.64	0.37	143	0.64	NSC_S_7	NSC_S_8	NSC S76	NSC S84	56	CC(C)[C@	760369	-5	GIPRCNT	Cc1ccnc	84464	-4	GI50	
0.64	0.4	144	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S65	54	CC(C)[C@	760369	-5	GIPRCNT	CCOC(=C	657825	-4	GI50	
0.64	0.25	145	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S71	51	CC(C)[C@	760369	-5	GIPRCNT	Nc1ccc(c	712671	-4	GI50	
0.64	0.33	146	0.64	NSC_S_7	NSC_S_4	NSC S76	NSC S40	53	CC(C)[C@	760369	-5	GIPRCNT	CC(C)OC	408050	-4	GI50	
0.64	0.31	147	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S73	54	CC(C)[C@	760369	-5	GIPRCNT	COC(=O)	734905	-4	GI50	
0.64	0.11	148	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S72	51	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	722869	-4	GI50	
0.64	0.47	149	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S70	50	CC(C)[C@	760369	-5	GIPRCNT	CC(SC(=S	709981	-4	GI50	
0.64	0.46	150	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S75	57	CC(C)[C@	760369	-5	GIPRCNT	CN1CCN	754172	-4.3	GI50	
0.64	0.38	151	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S65	44	CC(C)[C@	760369	-5	GIPRCNT	CCOC(=C	653945	-4	GI50	
0.64	0.27	152	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S71	50	CC(C)[C@	760369	-5	GIPRCNT	C[C@]12	718179	-4	GI50	
0.64	0.54	153	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S65	42	CC(C)[C@	760369	-5	GIPRCNT	C1C(N(N	656630	-4	GI50	
0.64	0.46	154	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S65	55	CC(C)[C@	760369	-5	GIPRCNT	CC1=CC(	657588	-4	GI50	
0.64	0.38	155	0.64	NSC_S_7	NSC_S_6	NSC S76	NSC S69	48	CC(C)[C@	760369	-5	GIPRCNT	Oc1c(CN	699960	-4	GI50	
0.64	0.53	156	0.64	NSC_S_7	NSC_S_7	NSC S76	NSC S73	54	CC(C)[C@	760369	-5	GIPRCNT	Nc1cccc(	733257	-4	GI50	
0.63	0.4	157	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S66	56	CC(C)[C@	760369	-5	GIPRCNT	C1CCC2	661962	-5	GI50	
0.63	0.33	158	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S71	55	CC(C)[C@	760369	-5	GIPRCNT	CSc1ccc(	711932	-4	GI50	
0.63	0.03	159	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S70	51	CC(C)[C@	760369	-5	GIPRCNT	S=C=N[C	708096	-4	GI50	
0.63	0.38	160	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S62	45	CC(C)[C@	760369	-5	GIPRCNT	COC(=O)	625818	-4	GI50	
0.63	0.21	161	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S74	57	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	740128	-4	GI50	
0.63	0.35	162	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S72	55	CC(C)[C@	760369	-5	GIPRCNT	Cc1cc(c(	725844	-4	GI50	
0.63	0.38	163	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S70	57	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	704244	-4	GI50	
0.63	0.34	164	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S63	47	CC(C)[C@	760369	-5	GIPRCNT	CC12c3c	635925	-4	GI50	
0.63	0.37	165	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S71	57	CC(C)[C@	760369	-5	GIPRCNT	ClC1=C(N	716984	-4	GI50	
0.63	0.35	166	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S72	56	CC(C)[C@	760369	-5	GIPRCNT	CCOC(=C	722572	-4	GI50	
0.63	0.52	167	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S69	57	CC(C)[C@	760369	-5	GIPRCNT	COc1cc(\	691564	-4	GI50	
0.63	0.29	168	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S63	43	CC(C)[C@	760369	-5	GIPRCNT	Cc1ccc(c	637533	-4	GI50	
0.63	0.17	169	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S69	46	CC(C)[C@	760369	-5	GIPRCNT	COC(=O)	697382	-4	GI50	
0.63	0.52	170	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S66	52	CC(C)[C@	760369	-5	GIPRCNT	Sc1nnc(n	665950	-4	GI50	
0.63	0.39	171	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S68	54	CC(C)[C@	760369	-5	GIPRCNT	Oc1nnc(	684060	-4	GI50	
0.63	0.19	172	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S68	56	CC(C)[C@	760369	-5	GIPRCNT	Brc1nn(	681324	-4	GI50	
0.63	0.46	173	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S68	53	CC(C)[C@	760369	-5	GIPRCNT	CCN(C(=	688372	-4	GI50	
0.63	0.16	174	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S72	50	CC(C)[C@	760369	-5	GIPRCNT	CS\C(=N	724284	-4	GI50	
0.63	0.37	175	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S69	54	CC(C)[C@	760369	-5	GIPRCNT	CC(C)OC	699799	-4	GI50	
0.63	0.41	176	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S66	49	CC(C)[C@	760369	-5	GIPRCNT	O=C(NC	668023	-4	GI50	
0.63	0.54	177	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S65	42	CC(C)[C@	760369	-5	GIPRCNT	[O-][N+](	655058	-4	GI50	
0.63	0.22	178	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S70	57	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	704393	-4	GI50	
0.63	0.34	179	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S70	53	CC(C)[C@	760369	-5	GIPRCNT	CC(=O)O	702990	-4	GI50	
0.63	0.38	180	0.63	NSC_S_7	NSC_S_3	NSC S76	NSC S30	54	CC(C)[C@	760369	-5	GIPRCNT	OC(=O)C	309939	-4	GI50	
0.63	0.49	181	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S68	52	CC(C)[C@	760369	-5	GIPRCNT	CCOC(=C	683340	-4	GI50	
0.63	0.31	182	0.63	NSC_S_7	NSC_S_1	NSC S76	NSC S10	54	CC(C)[C@	760369	-5	GIPRCNT	CC(=O)O	109128	-4	GI50	
0.63	0.44	183	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S73	54	CC(C)[C@	760369	-5	GIPRCNT	COc1cc2	737707	-4	GI50	
0.63	0.27	184	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S71	55	CC(C)[C@	760369	-5	GIPRCNT	COc1cc2	715841	-4	GI50	
0.63	0.41	185	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S64	47	CC(C)[C@	760369	-5	GIPRCNT	CO\C(=C	649012	-4	GI50	
0.63	0.32	186	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S73	48	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	730586	-4	GI50	
0.63	0.41	187	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S62	41	CC(C)[C@	760369	-5	GIPRCNT	O=C1c2c	627386	-4	GI50	
0.63	0.26	188	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S69	55	CC(C)[C@	760369	-5	GIPRCNT	Cc1c(C)c	697035	-4	GI50	
0.63	0.33	189	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S68	53	CC(C)[C@	760369	-5	GIPRCNT	OCC1OC	685467	-4	GI50	
0.63	0.21	190	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S70	54	CC(C)[C@	760369	-5	GIPRCNT	Fc1ccc2n	701008	-4	GI50	
0.63	0.29	191	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S70	55	CC(C)[C@	760369	-5	GIPRCNT	CC(Oc1c	704791	-4	GI50	
0.63	0.55	192	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S65	57	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	658883	-4	GI50	
0.63	0.49	193	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S63	41	CC(C)[C@	760369	-5	GIPRCNT	C=C(N1N	633669	-4	GI50	
0.63	0.43	194	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S74	57	CC(C)[C@	760369	-5	GIPRCNT	CCCCON	742462	-4	GI50	
0.63	0.38	195	0.63	NSC_S_7	NSC_S_7	NSC S76	NSC S72	47	CC(C)[C@	760369	-5	GIPRCNT	Oc1cccc	727736	-4	GI50	
0.63	0.35	196	0.63	NSC_S_7	NSC_S_6	NSC S76	NSC S68	51	CC(C)[C@	760369	-5	GIPRCNT	O=S(=O)	685893	-4	GI50	
0.62	0.36	197	0.62	NSC_S_7	NSC_S_6	NSC S76	NSC S67	57	CC(C)[C@	760369	-5	GIPRCNT	c1ccc2c(	677941	-4	GI50	
0.62	0.16	198	0.62	NSC_S_7	NSC_S_7	NSC S76	NSC S71	56	CC(C)[C@	760369	-5	GIPRCNT	COc1ccc	718553	-4	GI50	
0.62	0.35	199	0.62	NSC_S_7	NSC_S_6	NSC S76	NSC S62	42	CC(C)[C@	760369	-5	GIPRCNT	CCOC(=C	623756	-4	GI50	
0.62	0.47	200	0.62	NSC_S_7	NSC_S_6	NSC S76	NSC S63	44	CC(C)[C@	760369	-5	GIPRCNT	CC(=O)\(	634658	-4	GI50	
-0.6	-0.3	4	-0.6	NSC_S_7	NSC_S_1	NSC S76	NSC S16	54	CC(C)[C@	760369	-5	GIPRCNT	OCCNCC	169676	-4	GI50	
-0.61	-0.52	3	-0.61	NSC_S_7	NSC_S_6	NSC S76	NSC S66	55	CC(C)[C@	760369	-5	GIPRCNT	NC(Cc1c	668885	-4	GI50	
-0.65	-0.16	2	-0.65	NSC_S_7	NSC_S_6	NSC S76	NSC S64	45	CC(C)[C@	760369	-5	GIPRCNT	COC(=O)	646019	-4	GI50	
-0.65	-0.32	1	-0.65	NSC_S_7	NSC_S_7	NSC S76	NSC S71	54	CC(C)[C@	760369	-5	GIPRCNT	Cc1ccc(c	718589	-4	GI50	

Suppl. Table 4- List of compounds correlated to Lapachol. Highlighted rows indicate drugs that are approved or in clinical development

pearson	spearma	rank	correlati	seed ide	target id	seed des	target de	count co	seed mo	seed gen	seed pro	seed pro	seed mif	Seed SM	seed nsc	seed log	seed enc	seed tar	target m	target pr	target ge	target pr	target m	Target SI	target ns	target lo	target er	target target
0.74	0.77	1	0.74	NSC_S_1	NSC_S_6	NSC S11	NSC S65	42						CC(=C)\C	11905	-5	GIPRCNT							Cc1nc2C	651774	-4.1	GI50	Lapachol
0.73	0.69	2	0.73	NSC_S_1	NSC_S_1	NSC S11	NSC S13	54						CC(=C)\C	11905	-5	GIPRCNT							ClC(=CC	136592	-4	GI50	
0.72	0.73	3	0.72	NSC_S_1	NSC_S_1	NSC S11	NSC S12	53						CC(=C)\C	11905	-5	GIPRCNT							BrC(=CC	123511	-4	GI50	
0.71	0.72	4	0.71	NSC_S_1	NSC_S_7	NSC S11	NSC S75	56						CC(=C)\C	11905	-5	GIPRCNT							FC(F)(F)c	755423	-4.3	GI50	
0.71	0.71	5	0.71	NSC_S_1	NSC_S_7	NSC S11	NSC S75	56						CC(=C)\C	11905	-5	GIPRCNT							FC(F)(F)c	755427	-4.3	GI50	
0.7	0.72	6	0.7	NSC_S_1	NSC_S_6	NSC S11	NSC S65	47						CC(=C)\C	11905	-5	GIPRCNT							Oc1ccc(\	653260	-4	GI50	
0.7	0.71	7	0.7	NSC_S_1	NSC_S_7	NSC S11	NSC S74	55						CC(=C)\C	11905	-5	GIPRCNT							CCCN1C	746351	-4	GI50	
0.7	0.72	8	0.7	NSC_S_1	NSC_S_6	NSC S11	NSC S65	43						CC(=C)\C	11905	-5	GIPRCNT							Cc1ccc(C	651777	-4	GI50	
0.69	0.73	9	0.69	NSC_S_1	NSC_S_6	NSC S11	NSC S66	56						CC(=C)\C	11905	-5	GIPRCNT							CC(=O)C	667545	-4	GI50	
0.69	0.7	10	0.69	NSC_S_1	NSC_S_7	NSC S11	NSC S77	54						CC(=C)\C	11905	-5	GIPRCNT							O=C(Nc1	772887	-4	GI50	JAK
0.69	0.73	11	0.69	NSC_S_1	NSC_S_6	NSC S11	NSC S64	47						CC(=C)\C	11905	-5	GIPRCNT							CC(C)(c1	646240	-4	GI50	
0.69	0.72	12	0.69	NSC_S_1	NSC_S_6	NSC S11	NSC S65	43						CC(=C)\C	11905	-5	GIPRCNT							COc1ccc	651775	-4.1	GI50	
0.68	0.67	13	0.68	NSC_S_1	NSC_S_7	NSC S11	NSC S74	53						CC(=C)\C	11905	-5	GIPRCNT							O=C(COC	743402	-4	GI50	
0.67	0.68	14	0.67	NSC_S_1	NSC_S_7	NSC S11	NSC S75	56						CC(=C)\C	11905	-5	GIPRCNT							CCOC(=C	755267	-4	GI50	
0.67	0.65	15	0.67	NSC_S_1	NSC_S_6	NSC S11	NSC S67	56						CC(=C)\C	11905	-5	GIPRCNT							NC1=Nc2	671319	-4	GI50	
0.67	0.68	16	0.67	NSC_S_1	NSC_S_5	NSC S11	NSC S58	55						CC(=C)\C	11905	-5	GIPRCNT							ClCCn1c	58906	-4	GI50	
0.67	0.65	17	0.67	NSC_S_1	NSC_S_1	NSC S11	NSC S12	56						CC(=C)\C	11905	-5	GIPRCNT							ClC(=CC	126771	-4	GI50	
0.67	0.66	18	0.67	NSC_S_1	NSC_S_4	NSC S11	NSC S44	56						CC(=C)\C	11905	-5	GIPRCNT							CCCn1cn	44580	-4	GI50	Anti virus
0.67	0.64	19	0.67	NSC_S_1	NSC_S_7	NSC S11	NSC S74	56						CC(=C)\C	11905	-5	GIPRCNT							CN(Cc1c	740	-5	GI50	Dihydrofolate reductase Methotrexate
0.67	0.63	20	0.67	NSC_S_1	NSC_S_7	NSC S11	NSC S73	53						CC(=C)\C	11905	-5	GIPRCNT							Cc1cc(Cl	736563	-4	GI50	
0.66	0.68	21	0.66	NSC_S_1	NSC_S_7	NSC S11	NSC S73	53						CC(=C)\C	11905	-5	GIPRCNT							CCOCNc	736567	-4	GI50	
0.66	0.7	22	0.66	NSC_S_1	NSC_S_6	NSC S11	NSC S64	47						CC(=C)\C	11905	-5	GIPRCNT							CC(C)(C)	646248	-4	GI50	
0.66	0.65	23	0.66	NSC_S_1	NSC_S_7	NSC S11	NSC S74	55						CC(=C)\C	11905	-5	GIPRCNT							Cc1nn(c	746418	-4	GI50	
0.66	0.6	24	0.66	NSC_S_1	NSC_S_6	NSC S11	NSC S63	43						CC(=C)\C	11905	-5	GIPRCNT							CC[O-][T	637815	-4	GI50	
0.65	0.65	25	0.65	NSC_S_1	NSC_S_7	NSC S11	NSC S75	56						CC(=C)\C	11905	-5	GIPRCNT							FC(F)(F)c	755417	-4	GI50	
0.65	0.68	26	0.65	NSC_S_1	NSC_S_7	NSC S11	NSC S75	56						CC(=C)\C	11905	-5	GIPRCNT							COC(=O)	755265	-4	GI50	
0.65	0.69	27	0.65	NSC_S_1	NSC_S_3	NSC S11	NSC S33	55						CC(=C)\C	11905	-5	GIPRCNT							Cc1c(nc2	339768	-4	GI50	
0.65	0.68	28	0.65	NSC_S_1	NSC_S_6	NSC S11	NSC S67	41						CC(=C)\C	11905	-5	GIPRCNT							O=S1(=O	679042	-4	GI50	
0.65	0.66	29	0.65	NSC_S_1	NSC_S_7	NSC S11	NSC S74	55						CC(=C)\C	11905	-5	GIPRCNT							CN(C)c1c	741594	-4	GI50	
0.64	0.65	30	0.64	NSC_S_1	NSC_S_1	NSC S11	NSC S12	55						CC(=C)\C	11905	-5	GIPRCNT							COc1c(C	129185	-4	GI50	mycophenolic acid antiviral
0.64	0.63	31	0.64	NSC_S_1	NSC_S_7	NSC S11	NSC S75	56						CC(=C)\C	11905	-5	GIPRCNT							CCOC(=C	756662	-4	GI50	Survivan
0.64	0.61	32	0.64	NSC_S_1	NSC_S_7	NSC S11	NSC S73	56						CC(=C)\C	11905	-5	GIPRCNT							COc1cc(	73735	-4	GI50	
0.64	0.61	33	0.64	NSC_S_1	NSC_S_6	NSC S11	NSC S63	46						CC(=C)\C	11905	-5	GIPRCNT							O=C1Oc	638441	-4	GI50	
0.64	0.65	34	0.64	NSC_S_1	NSC_S_6	NSC S11	NSC S63	45						CC(=C)\C	11905	-5	GIPRCNT							CCN(CC)	635922	-4	GI50	
0.64	0.63	35	0.64	NSC_S_1	NSC_S_7	NSC S11	NSC S70	56						CC(=C)\C	11905	-5	GIPRCNT							COc1ccc	707904	-4	GI50	
0.64	0.66	36	0.64	NSC_S_1	NSC_S_6	NSC S11	NSC S62	45						CC(=C)\C	11905	-5	GIPRCNT							BrC1=CC	627687	-4	GI50	
0.64	0.61	37	0.64	NSC_S_1	NSC_S_6	NSC S11	NSC S65	55						CC(=C)\C	11905	-5	GIPRCNT							COc1ccc	655310	-4	GI50	
0.63	0.68	38	0.63	NSC_S_1	NSC_S_6	NSC S11	NSC S64	47						CC(=C)\C	11905	-5	GIPRCNT							CCOc1cc	647120	-4	GI50	
0.63	0.62	39	0.63	NSC_S_1	NSC_S_6	NSC S11	NSC S62	42						CC(=C)\C	11905	-5	GIPRCNT							COc1ccc	624228	-4	GI50	
0.63	0.61	40	0.63	NSC_S_1	NSC_S_7	NSC S11	NSC S75	56						CC(=C)\C	11905	-5	GIPRCNT							FC(F)(F)c	755429	-4	GI50	
0.63	0.63	41	0.63	NSC_S_1	NSC_S_1	NSC S11	NSC S14	56						CC(=C)\C	11905	-5	GIPRCNT							OCC1OC	146268	-4	GI50	2-Thio-6-azauridine antiviral
0.63	0.66	42	0.63	NSC_S_1	NSC_S_6	NSC S11	NSC S65	43						CC(=C)\C	11905	-5	GIPRCNT							CC(C)CC	651758	-4	GI50	
0.63	0.66	43	0.63	NSC_S_1	NSC_S_7	NSC S11	NSC S72	56						CC(=C)\C	11905	-5	GIPRCNT							CC1(C)O	720529	-4	GI50	
0.62	0.63	44	0.62	NSC_S_1	NSC_S_6	NSC S11	NSC S60	55						CC(=C)\C	11905	-5	GIPRCNT							OCC1OC	603335	-4	GI50	
0.62	0.62	45	0.62	NSC_S_1	NSC_S_1	NSC S11	NSC S11	56						CC(=C)\C	11905	-5	GIPRCNT							CC(=C)\C	11905	-4	GI50	
0.62	0.59	46	0.62	NSC_S_1	NSC_S_1	NSC S11	NSC S12	56						CC(=C)\C	11905	-5	GIPRCNT							ClC(=CC	126771	-3.6	GI50	
0.62	0.66	47	0.62	NSC_S_1	NSC_S_6	NSC S11	NSC S69	53						CC(=C)\C	11905	-5	GIPRCNT							CN(Cc1c	696558	-4	GI50	
0.62	0.66	48	0.62	NSC_S_1	NSC_S_7	NSC S11	NSC S75	56						CC(=C)\C	11905	-5	GIPRCNT							NCC(=O)	756657	-4	GI50	PDK-1
0.62	0.69	49	0.62	NSC_S_1	NSC_S_6	NSC S11	NSC S63	41						CC(=C)\C	11905	-5	GIPRCNT							Cc1cccc2	636098	-4	GI50	
0.61	0.54	50	0.61	NSC_S_1	NSC_S_6	NSC S11	NSC S68	56						CC(=C)\C	11905	-5	GIPRCNT							COc1cc(	681710	-4	GI50	
0.61	0.64	51	0.61	NSC_S_1	NSC_S_6	NSC S11	NSC S62	42						CC(=C)\C	11905	-5	GIPRCNT							OC1C2C	625123	-4	GI50	
0.61	0.57	52	0.61	NSC_S_1	NSC_S_7	NSC S11	NSC S76	51						CC(=C)\C	11905	-5	GIPRCNT							CSC1=N\	766440	-4	GI50	
0.61	0.55	53	0.61	NSC_S_1	NSC_S_6	NSC S11	NSC S66	54						CC(=C)\C	11905	-5	GIPRCNT							CN1C\C(	666037	-4	GI50	
0.61	0.7	54	0.61	NSC_S_1	NSC_S_7	NSC S11	NSC S75	56						CC(=C)\C	11905	-5	GIPRCNT							Clc1ccc(	755425	-4	GI50	
0.61	0.64	55	0.61	NSC_S_1	NSC_S_2	NSC S11	NSC S21	55						CC(=C)\C	11905	-5	GIPRCNT							Nc1nc(N	212446	-4	GI50	
0.61	0.56	56	0.61	NSC_S_1	NSC_S_6	NSC S11	NSC S60	44						CC(=C)\C	11905	-5	GIPRCNT							CCCNCC	606498	-4	GI50	
0.61	0.62	57	0.61	NSC_S_1	NSC_S_7	NSC S11	NSC S72	51						CC(=C)\C	11905	-5	GIPRCNT							COc1cc2	727621	-4	GI50	
0.61	0.59	58	0.61	NSC_S_1	NSC_S_6	NSC S11	NSC S67	47						CC(=C)\C	11905	-5	GIPRCNT							CC(=O)O	67239	-4	GI50	
0.61	0.58	59	0.61	NSC_S_1	NSC_S_6	NSC S11	NSC S62	43						CC(=C)\C	11905	-5	GIPRCNT							[O-][N+](	621387	-4	GI50	
0.61	0.62	60	0.61	NSC_S_1	NSC_S_3	NSC S11	NSC S36	49						CC(=C)\C	11905	-5	GIPRCNT							Cc1c(C(=	368390	-4	GI50	
0.61	0.65	61	0.61	NSC_S_1	NSC_S_6	NSC S11	NSC S65	43						CC(=C)\C	11905	-5	GIPRCNT							Cc1nc2C	651776	-4	GI50	
0.61	0.62	62	0.61	NSC_S_1	NSC_S_6	NSC S11	NSC S63	42						CC(=C)\C	11905	-5	GIPRCNT							Clc1ccc(\	635961	-4	GI50	
0.61	0.61	63	0.61	NSC_S_1	NSC_S_7	NSC S11	NSC S71	54						CC(=C)\C	11905	-5	GIPRCNT							Cc1ccc2(	711014	-4	GI50	
0.61	0.6	64	0.61	NSC_S_1	NSC_S_7	NSC S11	NSC S70	55						CC(=C)\C	11905	-5	GIPRCNT							COc1ccc	707909	-4	GI50	
0.61	0.68	65	0.61	NSC_S_1	NSC_S_6	NSC S11	NSC S62	40						CC(=C)\C	11905	-5	GIPRCNT							Cc1ccc(\	629824	-4	GI50	
0.6	0.59	66	0.6	NSC_S_1	NSC_S_7	NSC S11	NSC S74	54						CC(=C)\C	11905	-5	GIPRCNT							Nc1c(cc(	744116	-4	GI50	
0.6	0.64	67	0.6	NSC_S_1	NSC_S_7	NSC S11	NSC S74	56						CC(=C)\C	11905	-5	GIPRCNT							Oc1nnc(	744209	-4	GI50	
0.6	0.63	68	0.6	NSC_S_1	NSC_S_6	NSC S11	NSC S69	56						CC(=C)\C	11905	-5	GIPRCNT							CC(C)CO	694483	-4	GI50	

Suppl. Table 5- List of compounds correlated to Ethacizine. Highlighted rows indicate drugs that are approved or in clinical development

0.79	0.34	9	0.79	NSC_S_6	NSC_S_6	NSC S62	NSC S67	40	CCOC(=C	621878	-3.3	GI50	C(CN1CC	671123	-4	GI50	
0.79	0.27	10	0.79	NSC_S_6	NSC_S_6	NSC S62	NSC S66	40	CCOC(=C	621878	-3.3	GI50	OP(=O)(	666679	-4	GI50	
0.79	0.27	11	0.79	NSC_S_6	NSC_S_6	NSC S62	NSC S66	41	CCOC(=C	621878	-3.3	GI50	COC1(CC	666681	-4	GI50	
0.79	0.36	12	0.79	NSC_S_6	NSC_S_6	NSC S62	NSC S69	40	CCOC(=C	621878	-3.3	GI50	Oc1oc2c	690653	-4	GI50	
0.79	0.37	13	0.79	NSC_S_6	NSC_S_6	NSC S62	NSC S66	44	CCOC(=C	621878	-3.3	GI50	CC\C=C/	665744	-4	GI50	
0.79	0.31	14	0.79	NSC_S_6	NSC_S_6	NSC S62	NSC S64	44	CCOC(=C	621878	-3.3	GI50	COC(=O)	648209	-3.7	GI50	
0.79	0.1	15	0.79	NSC_S_6	NSC_S_6	NSC S62	NSC S69	43	CCOC(=C	621878	-3.3	GI50	COc1ccc	69600	-4	GI50	
0.79	0.27	16	0.79	NSC_S_6	NSC_S_6	NSC S62	NSC S69	40	CCOC(=C	621878	-3.3	GI50	CN1C(=C	691108	-4	GI50	
0.79	0.33	17	0.79	NSC_S_6	NSC_S_6	NSC S62	NSC S64	45	CCOC(=C	621878	-3.3	GI50	COC(=O)	648093	-3.4	GI50	
0.79	0.41	18	0.79	NSC_S_6	NSC_S_6	NSC S62	NSC S66	43	CCOC(=C	621878	-3.3	GI50	[O-][N+](	666130	-4	GI50	
0.79	0.27	19	0.79	NSC_S_6	NSC_S_2	NSC S62	NSC S27	40	CCOC(=C	621878	-3.3	GI50	Cc1onc(c	277175	-4	GI50	Flucloxacillin
0.79	0.26	20	0.79	NSC_S_6	NSC_S_3	NSC S62	NSC S38	42	CCOC(=C	621878	-3.3	GI50	CN(C)CC	38852	-4	GI50	
0.79	0.35	21	0.79	NSC_S_6	NSC_S_6	NSC S62	NSC S66	43	CCOC(=C	621878	-3.3	GI50	COc1ccc	660667	-4	GI50	
0.79	0.4	22	0.79	NSC_S_6	NSC_S_7	NSC S62	NSC S71	44	CCOC(=C	621878	-3.3	GI50	COC(=O)	717072	-4	GI50	
0.78	0.27	23	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S68	41	CCOC(=C	621878	-3.3	GI50	O=C1Oc	682615	-4	GI50	
0.78	0.27	24	0.78	NSC_S_6	NSC_S_2	NSC S62	NSC S29	41	CCOC(=C	621878	-3.3	GI50	NC(CSc1	294149	-4	GI50	
0.78	0.26	25	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	42	CCOC(=C	621878	-3.3	GI50	C1CCCC(	666684	-4	GI50	
0.78	0.35	26	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S67	44	CCOC(=C	621878	-3.3	GI50	Oc1nnc(	676716	-4	GI50	
0.78	0.36	27	0.78	NSC_S_6	NSC_S_1	NSC S62	NSC S17	45	CCOC(=C	621878	-3.3	GI50	COc1ccc	176656	-5	GI50	
0.78	0.26	28	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	43	CCOC(=C	621878	-3.3	GI50	Cc1ccc(c	666427	-4	GI50	
0.78	0.19	29	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	40	CCOC(=C	621878	-3.3	GI50	Cc1cc(C)	666358	-4	GI50	
0.78	0.29	30	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	44	CCOC(=C	621878	-3.3	GI50	CCCCCC(	664024	-5	GI50	
0.78	0.31	31	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	40	CCOC(=C	621878	-3.3	GI50	Clc1snc(	665114	-4	GI50	
0.78	0.26	32	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S68	44	CCOC(=C	621878	-3.3	GI50	O=C(NC(	682235	-4	GI50	
0.78	0.26	33	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S67	43	CCOC(=C	621878	-3.3	GI50	COc1ccc	674287	-4	GI50	
0.78	0.35	34	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S69	43	CCOC(=C	621878	-3.3	GI50	Nc1nnc(	695602	-4	GI50	
0.78	0.27	35	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	41	CCOC(=C	621878	-3.3	GI50	C(Cc1ccc	663634	-5	GI50	
0.78	0.26	36	0.78	NSC_S_6	NSC_S_3	NSC S62	NSC S38	43	CCOC(=C	621878	-3.3	GI50	OC(=O)C	38777	-4	GI50	
0.78	0.35	37	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S68	43	CCOC(=C	621878	-3.3	GI50	COc1ccc	686943	-4	GI50	
0.78	0.26	38	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	42	CCOC(=C	621878	-3.3	GI50	C[N+](C)	663626	-5	GI50	
0.78	0.26	39	0.78	NSC_S_6	NSC_S_7	NSC S62	NSC S76	43	CCOC(=C	621878	-3.3	GI50	O=C1OC	767277	-4.6	GI50	
0.78	0.26	40	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S68	42	CCOC(=C	621878	-3.3	GI50	CC(=O)N	685813	-4	GI50	
0.78	0.27	41	0.78	NSC_S_6	NSC_S_5	NSC S62	NSC S58	41	CCOC(=C	621878	-3.3	GI50	Oc1ccc2	58047	-4	GI50	
0.78	0.26	42	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S68	42	CCOC(=C	621878	-3.3	GI50	Cc1csc(N	686654	-4	GI50	
0.78	0.26	43	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S68	43	CCOC(=C	621878	-3.3	GI50	CC1=Nc2	682126	-4	GI50	
0.78	0.26	44	0.78	NSC_S_6	NSC_S_7	NSC S62	NSC S72	42	CCOC(=C	621878	-3.3	GI50	C[C@]12	729371	-4	GI50	
0.78	0.27	45	0.78	NSC_S_6	NSC_S_7	NSC S62	NSC S70	40	CCOC(=C	621878	-3.3	GI50	COc1ccc	701376	-4	GI50	
0.78	0.26	46	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	44	CCOC(=C	621878	-3.3	GI50	Oc1cccc(	666361	-4	GI50	
0.78	0.26	47	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	42	CCOC(=C	621878	-3.3	GI50	CC1C(C)(	665123	-4	GI50	
0.78	0.26	48	0.78	NSC_S_6	NSC_S_7	NSC S62	NSC S70	42	CCOC(=C	621878	-3.3	GI50	Cc1[nH]c	706036	-4	GI50	
0.78	0.27	49	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S61	41	CCOC(=C	621878	-3.3	GI50	OCC1CC(	612049	-3	GI50	Didanosine anti HIV reverse-transcriptase inhibitor
0.78	0.35	50	0.78	NSC_S_6	NSC_S_7	NSC S62	NSC S70	43	CCOC(=C	621878	-3.3	GI50	O=C1N2(	701614	-4	GI50	
0.78	0.25	51	0.78	NSC_S_6	NSC_S_7	NSC S62	NSC S70	44	CCOC(=C	621878	-3.3	GI50	CN1P(OC	705954	-4	GI50	
0.78	0.35	52	0.78	NSC_S_6	NSC_S_7	NSC S62	NSC S70	41	CCOC(=C	621878	-3.3	GI50	Clc1cccc	709515	-4	GI50	
0.78	0.36	53	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	45	CCOC(=C	621878	-3.3	GI50	C\N=C\N	664953	-4	GI50	
0.78	0.26	54	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S68	44	CCOC(=C	621878	-3.3	GI50	OC(=O)c	682230	-4	GI50	
0.78	0.26	55	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	44	CCOC(=C	621878	-3.3	GI50	CCN(CC)	664221	-4	GI50	
0.78	0.26	56	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	43	CCOC(=C	621878	-3.3	GI50	OC(=O)c	669318	-4	GI50	
0.78	0.31	57	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	44	CCOC(=C	621878	-3.3	GI50	CC(=O)O	667561	-4	GI50	
0.78	0.26	58	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	42	CCOC(=C	621878	-3.3	GI50	COC(=O)	660148	-4	GI50	
0.78	0.26	59	0.78	NSC_S_6	NSC_S_3	NSC S62	NSC S30	43	CCOC(=C	621878	-3.3	GI50	Cc1nn(c2	306711	-4	GI50	
0.78	0.26	60	0.78	NSC_S_6	NSC_S_1	NSC S62	NSC S16	44	CCOC(=C	621878	-3.3	GI50	COc1cc(	166679	-5	GI50	
0.78	0.26	61	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	43	CCOC(=C	621878	-3.3	GI50	CNNC1=	661094	-5	GI50	
0.78	0.26	62	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	42	CCOC(=C	621878	-3.3	GI50	CCOP(=C	660150	-4	GI50	
0.78	0.26	63	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	44	CCOC(=C	621878	-3.3	GI50	CC1=NN	661083	-5	GI50	
0.78	0.26	64	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S66	44	CCOC(=C	621878	-3.3	GI50	CC(=O)O	662816	-5	GI50	
0.78	0.26	65	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S63	43	CCOC(=C	621878	-3.3	GI50	CNS(=O)	637070	-4	GI50	
0.78	0.26	66	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S67	44	CCOC(=C	621878	-3.3	GI50	COC(=O)	673627	-4	GI50	
0.78	0.26	67	0.78	NSC_S_6	NSC_S_6	NSC S62	NSC S68	44	CCOC(=C	621878	-3.3	GI50	CC(=O)c1	687782	-4	GI50	
0.77	0.26	68	0.77	NSC_S_6	NSC_S_1	NSC S62	NSC S16	44	CCOC(=C	621878	-3.3	GI50	Cc1cc(Cl	164640	-4	GI50	
0.77	0.26	69	0.77	NSC_S_6	NSC_S_6	NSC S62	NSC S68	43	CCOC(=C	621878	-3.3	GI50	OCCc1cc	686931	-4	GI50	
0.77	0.34	70	0.77	NSC_S_6	NSC_S_6	NSC S62	NSC S66	45	CCOC(=C	621878	-3.3	GI50	CCOC(=C	667077	-4	GI50	
0.77	0.26	71	0.77	NSC_S_6	NSC_S_6	NSC S62	NSC S65	45	CCOC(=C	621878	-3.3	GI50	CO\N=[N	653049	-4	GI50	
0.77	0.26	72	0.77	NSC_S_6	NSC_S_6	NSC S62	NSC S66	45	CCOC(=C	621878	-3.3	GI50	O=C(CCC	665727	-4	GI50	
0.77	0.26	73	0.77	NSC_S_6	NSC_S_6	NSC S62	NSC S66	45	CCOC(=C	621878	-3.3	GI50	CC(NNC(	662457	-5	GI50	
0.77	0.26	74	0.77	NSC_S_6	NSC_S_6	NSC S62	NSC S66	42	CCOC(=C	621878	-3.3	GI50	Clc1ccc(	665959	-4	GI50	
0.77	0.26	75	0.77	NSC_S_6	NSC_S_6	NSC S62	NSC S66	44	CCOC(=C	621878	-3.3	GI50	CCOP(=C	660153	-4	GI50	
0.77	0.26	76	0.77	NSC_S_6	NSC_S_6	NSC S62	NSC S66	43	CCOC(=C	621878	-3.3	GI50	CC1=Nc2	663327	-5	GI50	
0.77	0.57	77	0.77	NSC_S_6	NSC_S_6	NSC S62	NSC S62	40	CCOC(=C	621878	-3.3	GI50	Clc1ccc(	621100	-4	GI50	
0.77	0.23	78	0.77	NSC_S_6	NSC_S_6	NSC S62	NSC S67	42	CCOC(=C	621878	-3.3	GI50	COC(=O)	676708	-4	GI50	
0.77	0.26	79	0.77	NSC_S_6	NSC_S_6	NSC S62	NSC S61	47	CCOC(=C	621878	-3.3	GI50	NC1CCC(	613661	-3.3	GI50	
0.77	0.16	80	0.77	NSC_S_6	NSC_S_6	NSC S62	NSC S66	42	CCOC(=C	621878	-3.3	GI50	C1C2CC3	665957	-4	GI50	
0.76	0.25	81	0.76	NSC_S_6	NSC_S_9	NSC S62	NSC S97	44	CCOC(=C	621878	-3.3	GI50	Cc1ccc(c	97371	-4	GI50	
0.76	0.12	82	0.76	NSC_S_6	NSC_S_6	NSC S62	NSC S67	44	CCOC(=C	621878	-3.3	GI50	CCOC(=C	671978	-4	GI50	
0.76	0.25	83	0.76	NSC_S_6	NSC_S_7	NSC S62	NSC S73	42	CCOC(=C	621878	-3.3	GI50	CC(C)C[C	735210	-4	GI50	
0.76	0.4	84	0.76	NSC_S_6	NSC_S_6	NSC S62	NSC S62	45	CCOC(=C	621878	-3.3	GI50	CCc1oc2	624793	-4	GI50	
0.76	0.32	85	0.76	NSC_S_6	NSC_S_7	NSC S62	NSC S70	44	CCOC(=C	621878	-3.3	GI50	CC(C)(C)	703456	-4	GI50	
0.76	0.22	86	0.76	NSC_S_6	NSC_S_6	NSC S62	NSC S67	40	CCOC(=C	621878	-3.3	GI50	CC1CN=(	672021	-4	GI50	
0.76	0.31	87	0.76	NSC_S_6	NSC_S_6	NSC S62	NSC S66	41	CCOC(=C	621878	-3.3	GI50	CCOC(=C	667535	-4	GI50	
0.76	0.48	88	0.76	NSC_S_6	NSC_S_6	NSC S62	NSC S64	48	CCOC(=C	621878	-3.3	GI50	Oc1c2or	640244	-4	GI50	
0.76	0.3	89	0.76	NSC_S_6	NSC_S_3	NSC S62	NSC S38	44	CCOC(=C	621878	-3.3	GI50	OC(=O)C	38743	-4	GI50	
0.76	0.19	90	0.76	NSC_S_6	NSC_S_6	NSC S62	NSC S66	44	CCOC(=C	621878	-3.3	GI50	CO\N=C(	660854	-5	GI50	
0.76	0.32	91	0.76	NSC_S_6	NSC_S_1	NSC S62	NSC S11	44	CCOC(=C	621878	-3.3	GI50	[Cl-][Pt+	119875	-5.6	GI50	DNA crosslinker
0.75	0.18	92	0.75	NSC_S_6	NSC_S_7	NSC S62	NSC S71	42	CCOC(=C	621878	-3.3	GI50		719240	2.6	GI50	
0.75	0.27	93	0.75	NSC_S_6	NSC_S_6	NSC S62	NSC S62	40	CCOC(=C	621878	-3.3	GI50	COc1ccc	624733	-4	GI50	
0.75	0.45	94	0.75	NSC_S_6	NSC_S_6	NSC S62	NSC S62	48	CCOC(=C	621878	-3.3	GI50	CCCC1C(	620502	-4	GI50	
0.75	0.12	95	0.75	NSC_S_6	NSC_S_7	NSC S62	NSC S71	42	CCOC(=C	621878	-3.3	GI50	FC(F)(F)c	713550	-4	GI50	
0.75	0.11	96	0.75	NSC_S_6	NSC_S_7	NSC S62	NSC S70	43	CCOC(=C	621878	-3.3	GI50	Clc1ccc(	703470	-4	GI50	
0.75	0.35	97	0.75	NSC_S_6	NSC_S_6	NSC S62	NSC S68	43	CCOC(=C	621878	-3.3	GI50	COc1ccc	686941	-4	GI50	
0.75	0.2	98	0.75	NSC_S_6	NSC_S_6	NSC S62	NSC S66	42	CCOC(=C	621878	-3.3	GI50	CCOP(=C	660160	-4	GI50	
0.75	0.06	99	0.75	NSC_S_6	NSC_S_7	NSC S62	NSC S70	41	CCOC(=C	621878	-3.3	GI50	c1ccc(cc	709512	-4	GI50	
0.75	0.11	100	0.75	NSC_S_6	NSC_S_6	NSC S62	NSC S66	41	CCOC(=C	621878	-3.3	GI50	COc1ccc	667550	-4	GI50	
0.75	0.3	101	0.75	NSC_S_6	NSC_S_6	NSC S62	NSC S67	41	CCOC(=C	621878	-3.3	GI50	CCN1C(=	671468	-4	GI50	
0.75	0.25	102	0.75	NSC_S_6	NSC_S_7	NSC S62	NSC S75	45	CCOC(=C	621878	-3.3	GI50	Fc1ccc(c	756252	-4.6	GI50	
0.74	0.35	103	0.74	NSC_S_6	NSC_S_7	NSC S62	NSC S70	44	CCOC(=C	621878	-3.3	GI50	COc1ccc	703469	-4	GI50	
0.74	0.39	104	0.74	NSC_S_6	NSC_S_6	NSC S62	NSC S68	42	CCOC(=C	621878	-3.3	GI50	CSc1nc(S	685836	-4	GI50	
0.74	0.16	105	0.74	NSC_S_6	NSC_S_6	NSC S62	NSC S66	42	CCOC(=C	621878	-3.3	GI50	CC1(C)C(	664345	-4	GI50	
0.74	0.37	106	0.74	NSC_S_6	NSC_S_7	NSC S62	NSC S71	41	CCOC(=C	621878	-3.3	GI50	CCOC(=C	710487	-4	GI50	
0.74	0.16	107	0.74	NSC_S_6	NSC_S_7	NSC S62	NSC S70	45	CCOC(=C	621878	-3.3	GI50	CCOC(=C	708047	-4	GI50	
0.74	0.22	108	0.74	NSC_S_6	NSC_S_6	NSC S62	NSC S66	44	CCOC(=C	621878	-3.3	GI50	CC1=NO	665733	-4	GI50	
0.74	0.35	109	0.74	NSC_S_6	NSC_S_6	NSC S62	NSC S67	44	CCOC(=C	621878	-3.3	GI50	CC(NCc1	673333	-4	GI50	
0.74	0.33	110	0.74	NSC_S_6	NSC_S_6	NSC S62	NSC S61	48	CCOC(=C	621878	-3.3	GI50	CCC(C(=(	617283	-4	GI50	
0.73	0.08	111	0.73	NSC_S_6	NSC_S_7	NSC S62	NSC S71	43	CCOC(=C	621878	-3.3	GI50	CCO\C(=	710860	-4	GI50	
0.73	0.31	112	0.73	NSC_S_6	NSC_S_7	NSC S62	NSC S70	44	CCOC(=C	621878	-3.3	GI50	COc1cc(	703457	-4	GI50	
0.73	0.18	113	0.73	NSC_S_6	NSC_S_7	NSC S62	NSC S71	42	CCOC(=C	621878	-3.3	GI50	[O-][N+](	716804	-4	GI50	
0.73	0.3	114	0.73	NSC_S_6	NSC_S_7	NSC S62	NSC S71	40	CCOC(=C	621878	-3.3	GI50	CCO\C(=	710865	-4	GI50	
0.73	0.33	115	0.73	NSC_S_6	NSC_S_6	NSC S62	NSC S62	44	CCOC(=C	621878	-3.3	GI50	CC1=CC(	62131	-4	GI50	
0.72	0.03	116	0.72	NSC_S_6	NSC_S_6	NSC S62	NSC S69	41	CCOC(=C	621878	-3.3	GI50	Cc1c(C)c	697041	-4	GI50	
0.72	0.18	117	0.72	NSC_S_6	NSC_S_6	NSC S62	NSC S66	41	CCOC(=C	621878	-3.3	GI50	O=C1C(=	666697	-4	GI50	
0.72	0.03	118	0.72	NSC_S_6	NSC_S_6	NSC S62	NSC S68	43	CCOC(=C	621878	-3.3	GI50	CC1(C)O	682544	-4	GI50	
0.72	0.17	119	0.72	NSC_S_6	NSC_S_6	NSC S62	NSC S64	42	CCOC(=C	621878	-3.3	GI50	OC1=C(\	649029	-4	GI50	
0.72	0.31	120	0.72	NSC_S_6	NSC_S_7	NSC S62	NSC S70	41	CCOC(=C	621878	-3.3	GI50	COc1ccc	704595	-4.3	GI50	
0.72	0.36	121	0.72	NSC_S_6	NSC_S_1	NSC S62	NSC S15	44	CCOC(=C	621878	-3.3	GI50	CN1CCC(	150080	-4	GI50	
0.72	0.16	122	0.72	NSC_S_6	NSC_S_6	NSC S62	NSC S62	41	CCOC(=C	621878	-3.3	GI50	Cc1cccc(	625476	-4	GI50	
0.72	0.18	123	0.72	NSC_S_6	NSC_S_2	NSC S62	NSC S20	41	CCOC(=C	621878	-3.3	GI50	OCC1OC	20256	-5	GI50	Uridine
0.72	0.27	124	0.72	NSC_S_6	NSC_S_6	NSC S62	NSC S62	47	CCOC(=C	621878	-3.3	GI50	OC1(CC(	621170	-4	GI50	
0.72	0.27	125	0.72	NSC_S_6	NSC_S_6	NSC S62	NSC S62	41	CCOC(=C	621878	-3.3	GI50	COC(=O)	621870	-4	GI50	
0.72	0.34	126	0.72	NSC_S_6	NSC_S_6	NSC S62	NSC S67	43	CCOC(=C	621878	-3.3	GI50	CCCCCC(	676862	-4	GI50	
0.72	0.04	127	0.72	NSC_S_6	NSC_S_7	NSC S62	NSC S71	43	CCOC(=C	621878	-3.3	GI50	CCO\C(=	710859	-4	GI50	
0.71	0.27	128	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S63	41	CCOC(=C	621878	-3.3	GI50	CCCC(=C	630810	-4	GI50	
0.71	0.13	129	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S66	40	CCOC(=C	621878	-3.3	GI50	CCOC(=C	663971	-4	GI50	
0.71	0.41	130	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S67	43	CCOC(=C	621878	-3.3	GI50	COc1cc2	673602	-4	GI50	
0.71	0.28	131	0.71	NSC_S_6	NSC_S_7	NSC S62	NSC S73	40	CCOC(=C	621878	-3.3	GI50	Nc1nc(N	735369	-4	GI50	
0.71	0.35	132	0.71	NSC_S_6	NSC_S_7	NSC S62	NSC S76	42	CCOC(=C	621878	-3.3	GI50	Clc1cc2(	767477	-6.2	GI50	
0.71	-0.08	133	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S64	42	CCOC(=C	621878	-3.3	GI50	COc1ccc	64945	-4	GI50	
0.71	0.24	134	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S62	44	CCOC(=C	621878	-3.3	GI50	Clc1ccc(	624916	-4	GI50	
0.71	0.12	135	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S64	41	CCOC(=C	621878	-3.3	GI50	COc1ccc	642951	-4	GI50	
0.71	0.27	136	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S64	40	CCOC(=C	621878	-3.3	GI50	Cc1ccc(c	648303	-4	GI50	
0.71	0.16	137	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S68	44	CCOC(=C	621878	-3.3	GI50	CC(C)CC(	683878	-4.3	GI50	
0.71	0.28	138	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S62	41	CCOC(=C	621878	-3.3	GI50	Cc1cc2C	621869	-4	GI50	
0.71	0.05	139	0.71	NSC_S_6	NSC_S_3	NSC S62	NSC S37	41	CCOC(=C	621878	-3.3	GI50	Cc1[nH]c	371884	-4	GI50	
0.71	0.26	140	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S63	42	CCOC(=C	621878	-3.3	GI50		633661	2.2	GI50	
0.71	0.35	141	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S62	45	CCOC(=C	621878	-3.3	GI50	COC(=O)	624782	-4	GI50	
0.71	0.23	142	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S67	43	CCOC(=C	621878	-3.3	GI50	CN1C=N(	675885	-4	GI50	
0.71	0.35	143	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S68	42	CCOC(=C	621878	-3.3	GI50	CC1CCC2	682343	-4	GI50	
0.71	0.34	144	0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S69	44	CCOC(=C	621878	-3.3	GI50	CN(C)c1(	698025	-4	GI50	
0.7	0.31	145	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S64	45	CCOC(=C	621878	-3.3	GI50	CNC(=S)(	649048	-4	GI50	
0.7	0.26	146	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S62	43	CCOC(=C	621878	-3.3	GI50	NC(=O)C	629052	-4	GI50	
0.7	0.26	147	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S65	42	CCOC(=C	621878	-3.3	GI50	C[s+]1c2	656585	-4	GI50	
0.7	0.35	148	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S64	41	CCOC(=C	621878	-3.3	GI50	[O-][N+](	647958	-4	GI50	
0.7	-0.02	149	0.7	NSC_S_6	NSC_S_7	NSC S62	NSC S73	40	CCOC(=C	621878	-3.3	GI50	Nc1nc(N	735368	-4	GI50	
0.7	0.25	150	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S64	46	CCOC(=C	621878	-3.3	GI50	O=C(Nc1	645891	-4	GI50	
0.7	0.27	151	0.7	NSC_S_6	NSC_S_7	NSC S62	NSC S72	45	CCOC(=C	621878	-3.3	GI50	CCN(CC)	727083	-4	GI50	
0.7	0.28	152	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S62	47	CCOC(=C	621878	-3.3	GI50	Cc1cc(cc	629827	-4	GI50	
0.7	0.15	153	0.7	NSC_S_6	NSC_S_7	NSC S62	NSC S70	45	CCOC(=C	621878	-3.3	GI50	FC(F)(F)c	706172	-4	GI50	
0.7	0.24	154	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S62	47	CCOC(=C	621878	-3.3	GI50	['C18H29	621808	-4	GI50	
0.7	0.25	155	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S64	46	CCOC(=C	621878	-3.3	GI50	CN1C(=C	649050	-4	GI50	
0.7	0.26	156	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S67	43	CCOC(=C	621878	-3.3	GI50	CCOC(=C	672010	-4	GI50	
0.7	0.15	157	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S63	43	CCOC(=C	621878	-3.3	GI50	CC(C)CO	638210	-4	GI50	
0.7	0.25	158	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S64	46	CCOC(=C	621878	-3.3	GI50	Cc1ccc(c	643047	-4	GI50	
0.7	0.21	159	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S66	41	CCOC(=C	621878	-3.3	GI50	CC(=O)O	667563	-4	GI50	
0.7	0.26	160	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S64	45	CCOC(=C	621878	-3.3	GI50	CC1(C)C(	648485	-4	GI50	
0.7	0.12	161	0.7	NSC_S_6	NSC_S_7	NSC S62	NSC S72	41	CCOC(=C	621878	-3.3	GI50	CC(C)(C)	722432	-4	GI50	
0.7	0.25	162	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S64	48	CCOC(=C	621878	-3.3	GI50		644458	1.9	GI50	
0.7	0.25	163	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S62	47	CCOC(=C	621878	-3.3	GI50	CCOP(=C	629864	-4	GI50	
0.7	-0.02	164	0.7	NSC_S_6	NSC_S_5	NSC S62	NSC S58	41	CCOC(=C	621878	-3.3	GI50	C1CN(CC	58255	-4	GI50	
0.7	0.23	165	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S64	46	CCOC(=C	621878	-3.3	GI50	CC1CC2=	640326	-4	GI50	
0.7	0.22	166	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S67	45	CCOC(=C	621878	-3.3	GI50	N#Cc1c(	670865	-4	GI50	
0.7	0.02	167	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S67	44	CCOC(=C	621878	-3.3	GI50	NC(=O)C	672433	-4	GI50	
0.7	0.42	168	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S65	41	CCOC(=C	621878	-3.3	GI50	CCO\C(=	658508	-4	GI50	
0.7	0.25	169	0.7	NSC_S_6	NSC_S_6	NSC S62	NSC S68	42	CCOC(=C	621878	-3.3	GI50	Cc1ccc(N	681819	-4	GI50	
0.7	0.17	170	0.7	NSC_S_6	NSC_S_7	NSC S62	NSC S70	40	CCOC(=C	621878	-3.3	GI50	COc1ccc	706178	-4	GI50	
0.69	0.27	171	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S64	44	CCOC(=C	621878	-3.3	GI50	CN(C)C(=	646962	-4	GI50	
0.69	0.25	172	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S62	48	CCOC(=C	621878	-3.3	GI50	CCOC(=C	625230	-4	GI50	
0.69	0.32	173	0.69	NSC_S_6	NSC_S_7	NSC S62	NSC S70	42	CCOC(=C	621878	-3.3	GI50	COc1cc(	706017	-4	GI50	
0.69	0.25	174	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S64	45	CCOC(=C	621878	-3.3	GI50	COc1ccc	644730	-4	GI50	
0.69	0.43	175	0.69	NSC_S_6	NSC_S_3	NSC S62	NSC S36	53	CCOC(=C	621878	-3.3	GI50	NCCCCC(	363232	-2.8	GI50	
0.69	0.25	176	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S65	48	CCOC(=C	621878	-3.3	GI50	FC(F)(F)C	653510	-4	GI50	
0.69	0.31	177	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S68	42	CCOC(=C	621878	-3.3	GI50	COC(=O)	682340	-4	GI50	
0.69	0.26	178	0.69	NSC_S_6	NSC_S_7	NSC S62	NSC S72	43	CCOC(=C	621878	-3.3	GI50	CCOc1cc	720188	-4	GI50	
0.69	0.05	179	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S67	44	CCOC(=C	621878	-3.3	GI50	CS(=O)(=	673911	-4	GI50	
0.69	0.2	180	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S68	42	CCOC(=C	621878	-3.3	GI50	COC1CC(	684431	-4.9	GI50	
0.69	0.04	181	0.69	NSC_S_6	NSC_S_7	NSC S62	NSC S70	43	CCOC(=C	621878	-3.3	GI50	CS(=O)(=	705813	-4	GI50	
0.69	0.31	182	0.69	NSC_S_6	NSC_S_7	NSC S62	NSC S70	41	CCOC(=C	621878	-3.3	GI50	CCN(CC)	709553	-4	GI50	
0.69	0.15	183	0.69	NSC_S_6	NSC_S_5	NSC S62	NSC S59	42	CCOC(=C	621878	-3.3	GI50	Nc1nc(S(	59486	-4	GI50	
0.69	0.29	184	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S64	47	CCOC(=C	621878	-3.3	GI50	COc1ccc	641615	-4	GI50	
0.69	0.16	185	0.69	NSC_S_6	NSC_S_1	NSC S62	NSC S13	44	CCOC(=C	621878	-3.3	GI50	CC(C)c1[	131261	-4	GI50	
0.69	0.21	186	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S68	41	CCOC(=C	621878	-3.3	GI50	COC1CC(	684426	-4.9	GI50	
0.69	0.34	187	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S62	45	CCOC(=C	621878	-3.3	GI50	Cc1cc2C	625961	-4	GI50	
0.69	0.36	188	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S66	43	CCOC(=C	621878	-3.3	GI50	COc1ccc	667556	-4	GI50	
0.69	0.27	189	0.69	NSC_S_6	NSC_S_7	NSC S62	NSC S71	45	CCOC(=C	621878	-3.3	GI50	Oc1[nH](	715812	-4	GI50	
0.69	0.39	190	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S67	40	CCOC(=C	621878	-3.3	GI50	CCCCOC	671989	-4	GI50	
0.69	0.24	191	0.69	NSC_S_6	NSC_S_6	NSC S62	NSC S67	44	CCOC(=C	621878	-3.3	GI50	CCOC(=C	671144	-4	GI50	
0.68	-0.01	192	0.68	NSC_S_6	NSC_S_7	NSC S62	NSC S71	40	CCOC(=C	621878	-3.3	GI50	CCO\C(=	710863	-4	GI50	
0.68	0.26	193	0.68	NSC_S_6	NSC_S_7	NSC S62	NSC S75	45	CCOC(=C	621878	-3.3	GI50	Nc1nccc	756415	-4.6	GI50	
0.68	0.06	194	0.68	NSC_S_6	NSC_S_7	NSC S62	NSC S71	43	CCOC(=C	621878	-3.3	GI50	COc1ccc	710071	-4	GI50	
0.68	0.51	195	0.68	NSC_S_6	NSC_S_6	NSC S62	NSC S63	41	CCOC(=C	621878	-3.3	GI50	CCN(CC)	635598	-4	GI50	
0.68	0.53	196	0.68	NSC_S_6	NSC_S_6	NSC S62	NSC S64	44	CCOC(=C	621878	-3.3	GI50	Cc1ccc2(	646495	-4	GI50	
0.68	0.03	197	0.68	NSC_S_6	NSC_S_7	NSC S62	NSC S70	42	CCOC(=C	621878	-3.3	GI50	Cc1ccc2(	706464	-4	GI50	
0.68	0.27	198	0.68	NSC_S_6	NSC_S_7	NSC S62	NSC S71	41	CCOC(=C	621878	-3.3	GI50	FC(F)(F)c	713546	-4	GI50	
0.68	0.03	199	0.68	NSC_S_6	NSC_S_5	NSC S62	NSC S54	43	CCOC(=C	621878	-3.3	GI50	Cc1cc2c(	54278	-4	GI50	
0.68	0.32	200	0.68	NSC_S_6	NSC_S_7	NSC S62	NSC S74	45	CCOC(=C	621878	-3.3	GI50	COc1ccc	740132	-4	GI50	
-0.5	-0.1	16	-0.5	NSC_S_6	NSC_S_6	NSC S62	NSC S64	51	CCOC(=C	621878	-3.3	GI50	COc1cc2	648790	-6	GI50	
-0.5	-0.18	15	-0.5	NSC_S_6	NSC_S_6	NSC S62	NSC S62	49	CCOC(=C	621878	-3.3	GI50	CCCCCC(	625460	-4	GI50	
-0.51	-0.07	14	-0.51	NSC_S_6	NSC_S_6	NSC S62	NSC S64	51	CCOC(=C	621878	-3.3	GI50	COc1cc2	648774	-4	GI50	
-0.51	-0.09	13	-0.51	NSC_S_6	NSC_S_7	NSC S62	NSC S75	44	CCOC(=C	621878	-3.3	GI50	Nc1c(sc2	754670	-4	GI50	
-0.51	-0.29	12	-0.51	NSC_S_6	NSC_S_7	NSC S62	NSC S71	45	CCOC(=C	621878	-3.3	GI50	O[C@@]	716516	-4	GI50	
-0.52	0.06	11	-0.52	NSC_S_6	NSC_S_2	NSC S62	NSC S26	49	CCOC(=C	621878	-3.3	GI50	C[C@@H	269757	-4	GI50	Antigenotoxicity of Baccharin, an Important Constituent of Baccharis dracunculifolia DC (Asteraceae)
-0.52	-0.2	10	-0.52	NSC_S_6	NSC_S_3	NSC S62	NSC S33	44	CCOC(=C	621878	-3.3	GI50	CC1COC	332596	-4	GI50	
-0.53	-0.13	9	-0.53	NSC_S_6	NSC_S_6	NSC S62	NSC S64	47	CCOC(=C	621878	-3.3	GI50	COc1cc2	648789	-4	GI50	
-0.54	0.01	8	-0.54	NSC_S_6	NSC_S_2	NSC S62	NSC S26	51	CCOC(=C	621878	-3.3	GI50	CC(O)\C	269754	-5	GI50	
-0.55	-0.01	7	-0.55	NSC_S_6	NSC_S_6	NSC S62	NSC S61	51	CCOC(=C	621878	-3.3	GI50	COC1=C(	618049	-4	GI50	
-0.57	0.1	6	-0.57	NSC_S_6	NSC_S_1	NSC S62	NSC S12	44	CCOC(=C	621878	-3.3	GI50	CCC1=C(	129414	-4	GI50	Emetin
-0.58	0.15	5	-0.58	NSC_S_6	NSC_S_2	NSC S62	NSC S24	46	CCOC(=C	621878	-3.3	GI50	CC[C@@	243022	-4	GI50	
-0.61	-0.25	4	-0.61	NSC_S_6	NSC_S_6	NSC S62	NSC S63	44	CCOC(=C	621878	-3.3	GI50	COc1cc2	638718	1.7	GI50	
-0.67	-0.31	3	-0.67	NSC_S_6	NSC_S_1	NSC S62	NSC S11	42	CCOC(=C	621878	-3.3	GI50		114573	2.2	GI50	
-0.68	-0.16	2	-0.68	NSC_S_6	NSC_S_3	NSC S62	NSC S37	47	CCOC(=C	621878	-3.3	GI50	CC[C@@	376128	-5.4	GI50	Dolastatin 10 has been used in trials studying the treatment of Sarcoma, Leukemia, Lymphoma, Liver Cancer, and Kidney Cancer, among others.
-0.71	-0.16	1	-0.71	NSC_S_6	NSC_S_6	NSC S62	NSC S64	43	CCOC(=C	621878	-3.3	GI50	OCCN(C(	645806	-4	GI50	

Suppl. Table 6- List of compounds correlated to Dexamethasone. Highlighted rows indicate drugs that are approved or in clinical development

1	1	1	1	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_34521_-4.0_2_GI50_AVG	NSC S34521 2 GI50 AVG	NSC S34521 2 GI50 AVGD	52
1	0.47	2	1	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_642602_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S642602 2 GI50 AVG	49
1	0.52	3	1	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_700718_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S700718 2 GI50 AVG	40
1	0.52	4	1	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_699800_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S699800 2 GI50 AVG	40
1	0.52	5	1	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_699418_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S699418 2 GI50 AVG	42
1	0.52	6	1	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_697583_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S697583 2 GI50 AVG	42
1	0.52	7	1	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_699394_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S699394 2 GI50 AVG	43
1	0.47	8	1	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_617248_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S617248 2 GI50 AVG	46
0.99	0.4	9	0.99	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_115855_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S115855 2 GI50 AVG	40
0.98	0.26	10	0.98	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_87229_-4.0_2_GI50_AVG	NSC S34521 2 GI50 AVG	NSC S87229 2 GI50 AVGD	41
0.97	0.17	11	0.97	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_293061_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S293061 2 GI50 AVG	42
0.97	0.64	12	0.97	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_10483_-4.0_2_GI50_AVG	NSC S34521 2 GI50 AVG	NSC S10483 2 GI50 AVGD	45
0.95	0.06	13	0.95	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_107680_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S107680 2 GI50 AVG	48
0.92	0.34	14	0.92	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_699754_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S699754 2 GI50 AVG	42
0.92	0.27	15	0.92	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_358304_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S358304 2 GI50 AVG	44
0.91	0.2	16	0.91	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_720793_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S720793 2 GI50 AVG	43
0.91	0.1	17	0.91	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_699391_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S699391 2 GI50 AVG	43
0.89	0.13	18	0.89	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_699400_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S699400 2 GI50 AVG	42
0.88	0.28	19	0.88	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_705638_-4.3_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S705638 2 GI50 AVG	43
0.86	0.26	20	0.86	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_691343_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S691343 2 GI50 AVG	40
0.86	0.08	21	0.86	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_617576_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S617576 2 GI50 AVG	43
0.86	0.2	22	0.86	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_722460_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S722460 2 GI50 AVG	43
0.84	0.1	23	0.84	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_617584_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S617584 2 GI50 AVG	46
0.82	0.01	24	0.82	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_699755_-4.0_2_GI50_AV	NSC S34521 2 GI50 AVG	NSC S699755 2 GI50 AVG	41
0.81	0.45	25	0.81	NSC_S_34521_-4.0_2_GI50_AV	NSC_S_92339_-4.0_2_GI50_AVG	NSC S34521 2 GI50 AVG	NSC S92339 2 GI50 AVGD	45

Suppl. Table 7- List of compounds correlated to Hycanthone. Highlighted rows indicate drugs that are approved or in clinical development

pearson(	spearma	rank	correlati	seed ide	target id	seed des	target de	count co	seed mo	seed gen	seed pro	seed pro	seed miF	Seed SM	seed nsc	seed log	seed enc	seed tar	target m	target pr	target ge	target pr	target m	Target Sl	target ns	target lo	target er	target target
1	1	1	1	NSC_S_7	NSC_S_7	NSC S75	NSC S75	60						CCN(CC)	758434	-4	GI50							CCN(CC)	758434	-4	GI50	
0.64	0.65	2	0.64	NSC_S_7	NSC_S_7	NSC S75	NSC S73	59						CCN(CC)	758434	-4	GI50							COc1ccc	736379	-4	GI50	
0.63	0.63	3	0.63	NSC_S_7	NSC_S_7	NSC S75	NSC S75	59						CCN(CC)	758434	-4	GI50							CCCCCC	758691	-4	GI50	
0.61	0.56	4	0.61	NSC_S_7	NSC_S_4	NSC S75	NSC S40	57						CCN(CC)	758434	-4	GI50							CN1CCc	402303	-4	GI50	
0.6	0.54	5	0.6	NSC_S_7	NSC_S_7	NSC S75	NSC S75	60						CCN(CC)	758434	-4	GI50							CC(C)CO	758390	-4	GI50	
0.59	0.52	6	0.59	NSC_S_7	NSC_S_3	NSC S75	NSC S38	44						CCN(CC)	758434	-4	GI50							COc1ccc	383229	-4	GI50	
0.58	0.61	7	0.58	NSC_S_7	NSC_S_7	NSC S75	NSC S75	60						CCN(CC)	758434	-4	GI50							Nc1c2cc	757794	-4	GI50	
0.56	0.44	8	0.56	NSC_S_7	NSC_S_7	NSC S75	NSC S71	59						CCN(CC)	758434	-4	GI50							O=C(C=P	717572	-4	GI50	
0.56	0.51	9	0.56	NSC_S_7	NSC_S_7	NSC S75	NSC S75	60						CCN(CC)	758434	-4	GI50							Oc1cccc	756457	-4.6	GI50	
0.56	0.52	10	0.56	NSC_S_7	NSC_S_7	NSC S75	NSC S76	59						CCN(CC)	758434	-4	GI50							CCN(CC)	764805	-4.3	GI50	
0.55	0.53	11	0.55	NSC_S_7	NSC_S_7	NSC S75	NSC S75	59						CCN(CC)	758434	-4	GI50							COc1cc(	752365	-4	GI50	
0.55	0.41	12	0.55	NSC_S_7	NSC_S_7	NSC S75	NSC S76	52						CCN(CC)	758434	-4	GI50							CC(C)(C)	764134	-4	GI50	Braf
0.55	0.53	13	0.55	NSC_S_7	NSC_S_7	NSC S75	NSC S70	52						CCN(CC)	758434	-4	GI50							Clc1ccc(	707477	-4	GI50	
0.55	0.5	14	0.55	NSC_S_7	NSC_S_7	NSC S75	NSC S75	60						CCN(CC)	758434	-4	GI50							CC(NCC	757826	-4	GI50	
0.54	0.52	15	0.54	NSC_S_7	NSC_S_6	NSC S75	NSC S64	47						CCN(CC)	758434	-4	GI50							CC(=C)C	646147	-4	GI50	
0.53	0.55	16	0.53	NSC_S_7	NSC_S_7	NSC S75	NSC S75	60						CCN(CC)	758434	-4	GI50							Nc1cccc	756642	-4	GI50	HDAC
0.52	0.55	17	0.52	NSC_S_7	NSC_S_3	NSC S75	NSC S32	60						CCN(CC)	758434	-4	GI50							COc1cc2	329226	-4	GI50	
0.52	0.55	18	0.52	NSC_S_7	NSC_S_3	NSC S75	NSC S32	58						CCN(CC)	758434	-4	GI50							[O-][N+]	329124	-4	GI50	
0.52	0.52	19	0.52	NSC_S_7	NSC_S_1	NSC S75	NSC S16	56						CCN(CC)	758434	-4	GI50							COc1ccc	165715	-4	GI50	N-(4-methoxyphenyl)-9-acridinamine
0.52	0.46	20	0.52	NSC_S_7	NSC_S_9	NSC S75	NSC S93	58						CCN(CC)	758434	-4	GI50							CCCC(CC	93819	-1.7	GI50	Valproic acid
0.52	0.42	21	0.52	NSC_S_7	NSC_S_7	NSC S75	NSC S70	53						CCN(CC)	758434	-4	GI50							CN([C@	707469	-4	GI50	
0.52	0.46	22	0.52	NSC_S_7	NSC_S_1	NSC S75	NSC S17	59						CCN(CC)	758434	-4	GI50							CN(C)CC	178827	-4	GI50	
0.52	0.6	23	0.52	NSC_S_7	NSC_S_7	NSC S75	NSC S75	57						CCN(CC)	758434	-4	GI50							CS(=O)c1	755772	-4	GI50	p38 MAPK
0.51	0.39	24	0.51	NSC_S_7	NSC_S_7	NSC S75	NSC S75	57						CCN(CC)	758434	-4	GI50							CCCN(CC	757912	-4	GI50	
0.51	0.52	25	0.51	NSC_S_7	NSC_S_7	NSC S75	NSC S75	60						CCN(CC)	758434	-4	GI50							CN(C)CC	756281	-4.6	GI50	
0.51	0.42	26	0.51	NSC_S_7	NSC_S_7	NSC S75	NSC S75	60						CCN(CC)	758434	-4	GI50							Fc1ccc(c	756429	-4.6	GI50	
0.51	0.48	27	0.51	NSC_S_7	NSC_S_7	NSC S75	NSC S76	60						CCN(CC)	758434	-4	GI50							CC1(C)C	761584	-4.5	GI50	
0.51	0.5	28	0.51	NSC_S_7	NSC_S_6	NSC S75	NSC S63	47						CCN(CC)	758434	-4	GI50							CCN(CC)	639618	-4	GI50	
0.51	0.44	29	0.51	NSC_S_7	NSC_S_7	NSC S75	NSC S76	55						CCN(CC)	758434	-4	GI50							NCCOCC	764392	-4	GI50	
0.5	0.53	30	0.5	NSC_S_7	NSC_S_7	NSC S75	NSC S73	56						CCN(CC)	758434	-4	GI50							COc1ccc	736596	-4	GI50	
0.5	0.47	31	0.5	NSC_S_7	NSC_S_7	NSC S75	NSC S75	59						CCN(CC)	758434	-4	GI50							OCCN1c	756084	-4.3	GI50	
0.5	0.47	32	0.5	NSC_S_7	NSC_S_7	NSC S75	NSC S75	60						CCN(CC)	758434	-4	GI50							CCCCc1n	758249	-4	GI50	HDAC
0.5	0.48	33	0.5	NSC_S_7	NSC_S_6	NSC S75	NSC S65	47						CCN(CC)	758434	-4	GI50							O=C(N(C	656464	-4	GI50	
0.5	0.47	34	0.5	NSC_S_7	NSC_S_6	NSC S75	NSC S68	55						CCN(CC)	758434	-4	GI50							O=C(N(C	681744	-4	GI50	
0.5	0.42	35	0.5	NSC_S_7	NSC_S_6	NSC S75	NSC S64	48						CCN(CC)	758434	-4	GI50							CC(C)OP	648099	-4	GI50	
0.5	0.43	36	0.5	NSC_S_7	NSC_S_3	NSC S75	NSC S37	55						CCN(CC)	758434	-4	GI50							COc1ccc	375387	-4	GI50	
-0.54	-0.5	2	-0.54	NSC_S_7	NSC_S_6	NSC S75	NSC S64	59						CCN(CC)	758434	-4	GI50							Clc1ccc2	642947	-4	GI50	
-0.56	-0.56	1	-0.56	NSC_S_7	NSC_S_6	NSC S75	NSC S62	41						CCN(CC)	758434	-4	GI50							Cc1cc(O	627786	-4	GI50	