Secondary experimental confirmation results of model predicted anti-SARS-CoV-2 compounds.

Sample ID	Sample Name	Structure	CPE AC50 (uM)	CPE Efficacy (%)	Cell Viabili
MLS000699212-03		CC1=CC=CC(\C	0.501187	95.328	14.12538
NCGC00100647-01		CC1=CC(=CC=C	0.794328	92.738	11.22019
MLS000703078-02		C1CN(CCO1)C2	1.778279	118.473	inactive
NCGC00024633-08	AMI-193	FC1=CC=C(OCC	2.511886	80.432	inactive
NCGC00273535-01		ClC1=CC(=CC=(	3.162278	87.546	inactive
NCGC00160483-02	Ftormetazine	CN1CCN(CC1)(	3.548134	63.682	11.22019
NCGC00100453-02		COC1=CC=C(CN	3.981072	44.168	11.22019
NCGC00602255-01	Prenylamine	CC(CC1=CC=CC	3.981072	72.644	11.22019
NCGC00073791-02	BEPP monohydroch	OC(COC1=CC=(	3.981072	33.036	14.12538
NCGC00104248-01		CCN(CC)C1=CC	3.981072	88.434	10
NCGC00165907-04	Triparanol	CCN(CC)CCOC1	3.981072	70.775	8.912509
NCGC00102295-02		CCN(CC)CCN1(	3.981072	105.087	12.58925
NCGC00015759-05	Octoclothepine mal	O=C(O)/C=C\C(	4.466836	42.12	12.58925
NCGC00024655-02	Metaphit	S=C=NC1=CC=(	4.466836	40.731	inactive
NCGC00015587-04	L-703,606 oxalate sa	IC1=C(CNC2C3	4.466836	101.544	12.58925
NCGC00347348-01		C[C@@H]1C[C	5.011872	81.89	inactive
NCGC00164483-03	Amindocate	CN(C)CCOC(=O	5.011872	23.936	inactive
NCGC00108974-01		CCN(CC)CCOC(	7.943282	115.266	inactive
MLS000541553-02		CN(C)C1=NC(=I	7.943282	80.288	3.162278
NCGC00183805-01		CN1CCN(CC1)(	7.943282	46.329	11.22019
NCGC00015490-03	Hexahydro-sila-difer	O[Si](CCCN1CC	10	101.37	inactive
NCGC00179625-05	Thioproperazine din	CN(C)[S+]([O-])(	10	90.577	inactive
NCGC00168047-01		CN(C)CCCN1C2	10	87.669	inactive
NCGC00595011-01		CCOC1=CC=C(N	10	116.452	inactive
NCGC00108226-01		CCC1=C(NC2=N	10	87.989	inactive
NCGC00092383-04	AMN082	C(CNC(C1=CC=	10	81.521	inactive
NCGC00379305-01		CC(NC1=C2C=C(	10	49.227	14.12538
NCGC00015591-05	L-741,626	OC1(CCN(CC1)	10	67.961	inactive
NCGC00104278-01		CCN(CC)C1=NC	10	45.41	12.58925
NCGC00098573-01		CC[N]1C2=C(C=	10	73.16	inactive
NCGC00674557-01		CC(C)NCC(O)CN	10	72.758	12.58925
NCGC00025187-05	Rimcazole	C[C@@H]1CN(	11.220185	96.025	inactive
NCGC00390051-01		C[C@H](NC1=C(	11.220185	95.197	inactive
NCGC00605328-01		CC1=C(C)C2=C(	11.220185	65.729	inactive
NCGC00060290-02		CCN1CCN(CCC	11.220185	69.658	14.12538
NCGC00162169-02	S-(-)-Eticlopride hyd	CCN1CC[C@@	11.220185	38.082	inactive
NCGC00108774-01		CCCN(CCC)CCN	11.220185	97.657	inactive
NCGC00118583-01		CN1CCN(CC1)(	11.220185	92.638	inactive
NCGC00059062-04		C1CCN(C1)C2=	11.220185	37.215	inactive
MLS000711217-02		Cl.ClC1=CC=C(	11.220185	95.319	inactive
NCGC00162079-02	Chlorprothixene hy	CN(C)CC\C=C/1	11.220185	81.693	inactive
NCGC00106614-01		BrC1=CC(=CC=(	12.589254	25.629	inactive
NCGC00610088-01		COC1=C(OC)C=	12.589254	28.849	inactive
NCGC00127260-01		CN(C)CCN(CC1	12.589254	92.099	inactive
NCGC00015799-04	SKF-525A hydrochlo	CCCC(C(=O)OC(	12.589254	95.895	inactive

NCGC00126980-01		CN(C)CCN(CC1	12.589254	92.087	inactive
NCGC00015957-06	Zolantidine dimalea	O=C(O)/C=C\C(	12.589254	94.354	inactive
NCGC00107855-01		CCCC/1=N/C2=	12.589254	108.807	inactive
NCGC00106835-01		FC1=CC=C(C=C	12.589254	71.313	inactive
NCGC00123932-01		CCN1CCC(CC1	12.589254	106.977	inactive
NCGC00015180-04	CGS 12066B	CN1CCN(CC1)(	12.589254	99.389	inactive
NCGC00117714-01		CC1=CC=C(CN2	12.589254	91.358	inactive
NCGC00108198-02		COC1=CC(=C(N	12.589254	99.412	inactive
NCGC00117690-01		CC1=CC=C(CN2	12.589254	81.323	inactive
NCGC00052917-03	Importazole	CC(NC1=NC(=N	12.589254	109.817	inactive
NCGC00183145-01		COC1=CC=C(C=	12.589254	103.865	inactive
NCGC00024872-03	3alpha-Bis-(4-fluoro	CN1C2CCC1CC	12.589254	101.169	inactive
NCGC00160412-04	Indocate	CN(C)CCOC(=O	12.589254	110.393	inactive
NCGC00167817-03	Bucindolol	CC(C)(CC1=CN(	12.589254	71.359	inactive
NCGC00686309-02		OC(COC(C1=CC	12.589254	115.824	inactive
NCGC00102299-02		CCCCN1C(=N)N	12.589254	85.298	inactive
NCGC00024625-03	BD 1008 dihydrobro	CN(CCN1CCCC	12.589254	85.984	inactive
MLS001072189-02		CCCN1N=CC(Cl	12.589254	96.201	inactive
NCGC00015484-05	GBR-12935	C(CN1CCN(CC(	12.589254	71.884	14.12538
NCGC00118549-01		CN1CCN(CC1)(	12.589254	77.158	inactive
NCGC00111284-01		ClC1=CC=C(CN	12.589254	97.547	inactive
NCGC00099280-01		CCN(CC)CCN\1	12.589254	63.47	inactive
NCGC00598531-01		CC1=CC=C(OC(	12.589254	99.61	inactive
NCGC00108148-01		CN(C)CCNC(=O	12.589254	102.944	inactive
NCGC00127044-01		COC1=CC=CC(=	12.589254	97.12	inactive
NCGC00099905-01		CCOC1=C(CN(C	12.589254	46.731	inactive
NCGC00160480-01	Pecazine	CN1CCCC(C1)C	12.589254	106.561	inactive
NCGC00167818-02	UCL 2077	C(NC(C1=CC=C	14.125375	33.967	12.58925
NCGC00486018-01	Alimemazine D6	CC(CN(C([2H])(	14.125375	31.845	inactive
NCGC00108931-01		CN1C(=O)\C=C(	14.125375	33	inactive
NCGC00103768-01		FC1=CC=C(C=C	14.125375	31.276	inactive
NCGC00141157-01		CC1=NOC(\C=C	14.125375	102.736	inactive
NCGC00015171-05	BP 897	COC1=C(C=CC=	14.125375	36.082	inactive
NCGC00610713-01		FC1=CC=C(C=C	14.125375	37.629	inactive
NCGC00117963-01		C[N]1N=NN=C1	14.125375	67.415	inactive
NCGC00598560-01		CC1=CC=C(C=C	14.125375	34.993	inactive
NCGC00167765-03	LP 44	CSC1=C(C=CC=	14.125375	102.39	inactive
NCGC00480833-01	MDL-72222	CN1[C@@H]2(	14.125375	113.489	inactive
NCGC00164077-02	4-Aminoazobenzene	Nc2ccc(/N=N/(	25.118864	65.192	inactive
NCGC00255599-01	Oxycarboxin	CC=1OCCS(=O)	28.183829	68.511	31.62278
NCGC00163815-04	Oryzalin	O=S(N)(=O)c1c(	inactive	0	inactive
NCGC00186032-01	LP 12 hydrochloride	O=C(CCCCCN1(	inactive	0	14.12538
NCGC00117931-01		C[N]1N=NN=C1	inactive	0	inactive
NCGC00632056-01		CC1=CC=C(OC2	inactive	0	14.12538
NCGC00600997-01		CCN1CCN(CC1	inactive	0	inactive
NCGC00015983-04	Trifluperidol hydroc	Cl.FC(F)(F)c1cc	inactive	0	inactive
NCGC00166070-02	Decominol hydroch	Cl.OC(COCCCC	inactive	0	14.12538
NCGC00014998-03	TMB-8	CCN(CC)CCCC(	inactive	0	11.22019

NCGC00160646-01	Pipofezine	CN1CCN(CC1)c	inactive	0 inactive

Cell Viabili	SI
-54.809	28.18384
-42.969	14.12538
0	56.23415
0	39.81072
0	31.62277
-30.457	3.162278
-43.869	2.818383
-34.45	2.818383
-36.751	3.548134
-75.212	2.511886
-111.783	2.238721
-46.395	3.162277
-100.735	2.818383
0	22.38721
-107.971	2.818383
0	19.95262
0	19.95262
0	12.58925
-60.287	0.398107
-63.366	1.412538
0	10
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-56.099	1.412538
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-59.401	1.258925
0	10
-34.744	1.258925
0	8.912509
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-33.037	1.258925
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-71.405	0.891251
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0	7.079458
0	7.079458
0	3.981072
-33.843	1.122018
0	N/A
-104.988	N/A
0	N/A
-68.395	N/A
0	N/A
0	N/A
-49.584	N/A
-94.945	N/A

0 N/A

Mechanistic assay results of experimental confirmed anti-SARS-CoV-2 compounds.

Sample ID	Sample Name	Structure	3CLpro AC50 (uM)	3CLpro Efficacy (%)
MLS000699212-03		CC1=CC=CC(\C	inactive	inactive
NCGC00100647-01		CC1=CC(=CC=C	inactive	inactive
MLS000703078-02		C1CN(CCO1)C2	inactive	inactive
NCGC00024633-08	AMI-193	FC1=CC=C(OCC	inactive	inactive
NCGC00273535-01		ClC1=CC(=CC=(	inactive	inactive
NCGC00160483-02	Ftormetazine	CN1CCN(CC1)(	inactive	inactive
NCGC00100453-02		COC1=CC=C(CN	inactive	inactive
NCGC00602255-01	Prenylamine	CC(CC1=CC=CC	inactive	inactive
NCGC00073791-02	BEPP monohydrochlo	OC(COC1=CC=(	inactive	inactive
NCGC00104248-01		CCN(CC)C1=CC	inactive	inactive
NCGC00165907-04	Triparanol	CCN(CC)CCOC1	inactive	inactive
NCGC00102295-02		CCN(CC)CCN1(	inactive	inactive
NCGC00015759-05	Octoclothepine malea	O=C(O)/C=C\C(	inactive	inactive
NCGC00024655-02	Metaphit	S=C=NC1=CC=(	inactive	inactive
NCGC00015587-04	L-703,606 oxalate salt	IC1=C(CNC2C3	8.627517433	-28.1159853
NCGC00347348-01		C[C@@H]1C[C	inactive	inactive
NCGC00164483-03	Amindocate	CN(C)CCOC(=O	inactive	inactive
NCGC00108974-01		CCN(CC)CCOC(	inactive	inactive
MLS000541553-02		CN(C)C1=NC(=I	inactive	inactive
NCGC00183805-01		CN1CCN(CC1)(	inactive	inactive
NCGC00015490-03	Hexahydro-sila-difenic	O[Si](CCCN1CC	inactive	inactive
NCGC00179625-05	Thioproperazine dime	CN(C)[S+]([O-])(	inactive	inactive
NCGC00168047-01		CN(C)CCCN1C2	inactive	inactive
NCGC00595011-01		CCOC1=CC=C(N	inactive	inactive
NCGC00108226-01		CCC1=C(NC2=N	inactive	inactive
NCGC00092383-04	AMN082	C(CNC(C1=CC=	inactive	inactive
NCGC00379305-01		CC(NC1=C2C=C	inactive	inactive
NCGC00015591-05	L-741,626	OC1(CCN(CC1)	inactive	inactive
NCGC00104278-01		CCN(CC)C1=NC	inactive	inactive
NCGC00098573-01		CC[N]1C2=C(C=	inactive	inactive
NCGC00674557-01		CC(C)NCC(O)CN	inactive	inactive
NCGC00025187-05	Rimcazole	C[C@@H]1CN(	inactive	inactive
NCGC00390051-01		C[C@H](NC1=C	inactive	inactive
NCGC00605328-01		CC1=C(C)C2=C(	inactive	inactive
NCGC00060290-02		CCN1CCN(CCC	inactive	inactive
NCGC00162169-02	S-(-)-Eticlopride hydro	CCN1CC[C@@	inactive	inactive
NCGC00108774-01		CCCN(CCC)CCN	inactive	inactive
NCGC00118583-01		CN1CCN(CC1)(	inactive	inactive
NCGC00059062-04		C1CCN(C1)C2=	inactive	inactive
MLS000711217-02		Cl.ClC1=CC=C(C	inactive	inactive
NCGC00162079-02	Chlorprothixene hydr	CN(C)CC\C=C/1	inactive	inactive
NCGC00106614-01		BrC1=CC(=CC=C	inactive	inactive
NCGC00610088-01		COC1=C(OC)C=	inactive	inactive
NCGC00127260-01		CN(C)CCN(CC1	inactive	inactive
NCGC00015799-04	SKF-525A hydrochlori	CCCC(C(=O)OC(	inactive	inactive

NCGC00126980-01		CN(C)CCN(CC1	inactive	inactive	
NCGC00015957-06	Zolantidine dimaleate	O=C(O)/C=C\C(	inactive	inactive	
NCGC00107855-01		CCCC/1=N/C2=	inactive	inactive	
NCGC00106835-01		FC1=CC=C(C=C	inactive	inactive	
NCGC00123932-01		CCN1CCC(CC1)	inactive	inactive	
NCGC00015180-04	CGS 12066B	CN1CCN(CC1)C	inactive	inactive	
NCGC00117714-01		CC1=CC=C(CN2	inactive	inactive	
NCGC00108198-02		COC1=CC(=C(N	inactive	inactive	
NCGC00117690-01		CC1=CC=C(CN2	inactive	inactive	
NCGC00052917-03	Importazole	CC(NC1=NC(=N	inactive	inactive	
NCGC00183145-01		COC1=CC=C(C=	inactive	inactive	
NCGC00024872-03	3alpha-Bis-(4-fluorophl	CN1C2CCC1CC	inactive	inactive	
NCGC00160412-04	Indocate	CN(C)CCOC(=O	inactive	inactive	
NCGC00167817-03	Bucindolol	CC(C)(CC1=CN(	inactive	inactive	
NCGC00686309-02		OC(COC(C1=CC	inactive	inactive	
NCGC00102299-02		CCCCN1C(=N)N	inactive	inactive	
NCGC00024625-03	BD 1008 dihydrobron	CN(CCN1CCCC	inactive	inactive	
MLS001072189-02		CCCN1N=CC(Cl	inactive	inactive	
NCGC00015484-05	GBR-12935	C(CN1CCN(CC(	inactive	inactive	
NCGC00118549-01		CN1CCN(CC1)C	inactive	inactive	
NCGC00111284-01		ClC1=CC=C(CN	inactive	inactive	
NCGC00099280-01		CCN(CC)CCN\1	inactive	inactive	
NCGC00598531-01		CC1=CC=C(OC(	inactive	inactive	
NCGC00108148-01		CN(C)CCNC(=O	inactive	inactive	
NCGC00127044-01		COC1=CC=CC(=	inactive	inactive	
NCGC00099905-01		CCOC1=C(CN(C	inactive	inactive	
NCGC00160480-01	Pecazine	CN1CCCC(C1)C	inactive	inactive	
NCGC00167818-02	UCL 2077	C(NC(C1=CC=C	inactive	inactive	
NCGC00486018-01	Alimemazine D6	CC(CN(C([2H])(	inactive	inactive	
NCGC00108931-01		CN1C(=O)\C=C(	inactive	inactive	
NCGC00103768-01		FC1=CC=C(C=C	inactive	inactive	
NCGC00141157-01		CC1=NOC(\C=C	inactive	inactive	
NCGC00015171-05	BP 897	COC1=C(C=CC=	inactive	inactive	
NCGC00610713-01		FC1=CC=C(C=C	inactive	inactive	
NCGC00117963-01		C[N]1N=NN=C1	inactive	inactive	
NCGC00598560-01		CC1=CC=C(C=C	inactive	inactive	
NCGC00167765-03	LP 44	CSC1=C(C=CC=	inactive	inactive	
NCGC00480833-01	MDL-72222	CN1[C@@H]2(	inactive	inactive	
NCGC00164077-02	4-Aminoazobenzene	Nc2ccc(/N=N/c	55.86268942		-27.39989937
NCGC00255599-01	Oxycarboxin	CC=1OCCS(=O)	inactive	inactive	

3CLpro Counter AC50 (uM)	3CLpro Counter Efficacy (%)	PP AC50 (uM)	PP Efficacy (%)
inactive	inactive	0.591727619	-129.1456723
inactive	inactive	2.575644059	-88.62753821
inactive	inactive	3.524697417	-83.0582113
inactive	inactive	24.31564787	-89.5752053
inactive	inactive	30.61158701	-57.23711834
inactive	inactive	7.689283006	-86.63514486
inactive	inactive	12.77396884	-108.5878335
inactive	inactive	18.23416354	-95.54888406
inactive	inactive	14.48391093	-89.90583491
inactive	inactive	12.90879921	-90.11073966
inactive	inactive	22.95545184	-103.2854983
inactive	inactive	10.25382369	-119.104277
inactive	inactive	17.21416041	-68.30721098
inactive	inactive	12.90879921	-86.01706975
inactive	inactive	9.13872998	-108.9918706
inactive	inactive	11.5049794	-112.1449351
inactive	inactive	20.45906799	-73.96785998
inactive	inactive	21.67134398	-111.3629656
inactive	inactive	9.680233774	-125.7575335
inactive	inactive	2.575644059	-108.2504849
inactive	inactive	24.31564787	-85.76434756
inactive	inactive	21.67134398	-141.4457884
inactive	inactive	27.28260564	-96.40459306
inactive	inactive	24.31564787	-97.00172756
inactive	inactive	19.31460565	-157.4797692
inactive	inactive	20.45906799	-86.01680338
inactive	inactive	6.853080692	-131.21785
inactive	inactive	19.31460565	-127.0665432
inactive	inactive	24.31564787	-94.97603623
inactive	inactive	13.67369365	-72.3603803
inactive	inactive	30.61158701	-97.42365579
inactive	inactive	24.31564787	-61.67451101
inactive	inactive	20.45906799	-73.09661811
inactive	inactive	6.853080692	-107.2470305
inactive	inactive	21.67134398	-67.81102835
inactive	inactive	2.889920166	-86.85612231
inactive	inactive	10.86140094	-143.7933675
inactive	inactive	19.31460565	-85.15937856
inactive	inactive	10.86140094	-105.942115
inactive	inactive	9.13872998	-120.2702119
inactive	inactive	0.544359549	-103.8162342
inactive	inactive	12.90879921	-67.10604386
inactive	inactive	17.21416041	-94.67205927
inactive	inactive	19.31460565	-61.22758816
inactive	inactive	22.95545184	-121.8387122

inactive	inactive	19.31460565	-118.7952782
inactive	inactive	17.21416041	-61.68557235
inactive	inactive	19.31460565	-114.9221638
inactive	inactive	28.89920165	-70.37816927
inactive	inactive	24.31564787	-83.84157119
inactive	inactive	21.67134398	-53.41337222
inactive	inactive	inactive	inactive
inactive	inactive	21.67134398	-88.17791949
inactive	inactive	3.061158701	-136.0894367
inactive	inactive	9.680233774	-97.77025801
inactive	inactive	21.67134398	-99.89974748
inactive	inactive	12.18669229	-107.0321117
inactive	inactive	27.28260564	-92.630142
inactive	inactive	27.28260564	-60.45951112
inactive	inactive	13.67369365	-83.83218164
inactive	inactive	12.18669229	-102.5553356
inactive	inactive	8.144901668	-97.82690637
inactive	inactive	15.34213661	-74.562439
inactive	inactive	30.61158701	-106.6486186
inactive	inactive	18.23416353	-117.8028412
inactive	inactive	19.31460565	-91.08870494
inactive	inactive	9.138729979	-130.9098251
inactive	inactive	inactive	inactive
inactive	inactive	34.34676554	-58.35858937
inactive	inactive	27.28260564	-89.82142962
inactive	inactive	1.086140094	-85.78644042
inactive	inactive	41.89110732	-88.96184232
inactive	inactive	24.31564787	-81.70811588
inactive	inactive	17.21416041	-87.80243006
inactive	inactive	0.45802148	-52.84256155
inactive	inactive	27.28260564	-88.10611939
inactive	inactive	18.23416354	-73.3087829
inactive	inactive	22.95545184	-78.39597545
inactive	inactive	27.28260564	-58.65899866
inactive	inactive	24.31564787	-77.31599785
inactive	inactive	21.67134398	-104.2419915
inactive	inactive	16.25121536	-88.1795839
inactive	inactive	24.31564787	-57.77121772
inactive	inactive	inactive	inactive
inactive	inactive	inactive	inactive

PP Cell Viability AC50 (uM)	PP Cell Viability Efficacy (%)
44.37331147	-40.9376154
19.31460565	-69.07044474
inactive	inactive
inactive	inactive
43.24001595	-71.0319613
inactive	inactive
32.08675901	-52.37372994
34.34676554	-52.71727489
15.34213661	-63.61155029
9.680233774	-69.7161351
43.24001595	-125.0234792
43.24001595	-59.27749801
43.24001595	-43.87450648
inactive	inactive
43.24001595	-88.68548768
inactive	inactive
inactive	inactive
inactive	inactive
32.42543757	-84.51975689
24.31564787	-90.9478281
inactive	inactive
inactive	inactive
inactive	inactive
9.680233774	-80.51011986
30.61158701	-75.48809856
7.689283006	-55.65218747
34.34676554	-47.48952292
inactive	inactive
27.28260563	-44.71696462
38.53770478	-38.97586027
inactive	inactive
inactive	inactive
inactive	inactive
12.18669229	-112.4066796
21.67134398	-58.43221016
inactive	inactive
inactive	inactive
inactive	inactive
inactive	inactive
15.34213661	-65.91500326
32.42543757	-39.76563216
inactive	inactive
16.25121536	-89.69562144
inactive	inactive
43.24001595	-53.45635873

inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
	48.51609586		-46.57583266
	34.34676554		-34.29733309
inactive		inactive	
	15.34213661		-27.29898173
inactive		inactive	
inactive		inactive	
inactive		inactive	
	48.51609586		-54.64648685
inactive		inactive	
inactive		inactive	
	30.61158701		-44.43608457
inactive		inactive	
	43.24001595		-98.81152504
	43.24001595		-77.79952136
	0.034346766		-21.72146605
inactive		inactive	
	24.31564787		-34.57534639
	21.67134398		-67.62952432
inactive		inactive	
inactive		inactive	
	22.95545184		-79.28587894
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
	48.51609586		-47.42659008
	21.67134398		-72.09505211
	40.82120735		-60.27081984
inactive		inactive	
inactive		inactive	
inactive		inactive	

GFP-LC3 (% of positive cells) AC50 (uM)	GFP-LC3 (% of positive cells) Efficacy (%)
21.47975174	71.38648446
17.27666569	42.621177
inactive	inactive
inactive	inactive
34.47147997	96.58843732
20.14311333	71.03311665
20.7125357	172.2882588
20.93115833	76.15799058
33.17365034	160.6522536
29.56604699	33.39379465
24.40393893	141.2443867
22.60094488	138.6516554
28.45290384	61.32194813
inactive	inactive
10.49042934	86.7751703
17.27666569	122.0980268
23.48514591	60.05041415
24.87672829	29.81894528
15.3978445	29.91273218
inactive	0
31.92468319	68.70813638
19.38473773	155.5991412
27.91214823	71.08975421
33.17365034	98.83181363
20.93115833	47.30086591
inactive	inactive
26.35076712	76.08417062
23.48514591	123.4322464
inactive	inactive
21.75003346	128.9448007
26.35076712	94.69844888
22.17140743	77.66263543
20.14311333	31.88090882
inactive	inactive
16.62621004	51.08121872
inactive	0
22.60094488	50.88530163
20.93115833	72.55156251
inactive	inactive
20.93115833	74.7276276
inactive	0
inactive	inactive
inactive	inactive
inactive	inactive
29.56604699	42.54234763

	20.93115833		40.96543098
inactive			0
	29.56604699		132.8791707
inactive			0
	22.60094488		45.95046956
	20.93115833		69.24086159
inactive			0
	18.6549145		62.30896691
inactive			0
inactive		inactive	
	31.31794541		98.54170437
	30.72273886		45.94016267
inactive		inactive	
	23.48514591		57.07153102
	23.48514591		55.56736548
inactive		inactive	
	35.1393127		97.69611984
	17.61137493		73.40466717
	23.48514591		84.24320418
	27.91214823		47.03068766
	20.93115833		60.51997839
inactive		inactive	
inactive		inactive	
inactive		inactive	
	29.56604699		54.40330816
inactive		inactive	
	48.08717428		131.6080714
inactive		inactive	
	22.60094488		40.12478129
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
	26.35076712		39.96040494
inactive		inactive	
	27.38166983		80.09965424
inactive		inactive	
inactive		inactive	
inactive		inactive	

GFP-LC3 (Relative Spot Intensity) AC50 (uM)	GFP-LC3 (Relative Spot Intensity) Efficacy (%)
49.96845532	37.75856693
inactive	inactive
inactive	inactive
inactive	inactive
34.47147997	97.12194011
31.92468319	77.24625229
18.46006687	122.8293871
29.56604699	68.34561031
33.17365034	376.0263599
inactive	inactive
33.17365034	321.1323566
23.48514591	339.6123175
35.1393127	58.00438638
inactive	inactive
14.8181253	100.5617042
17.61137493	225.2093524
35.1393127	37.71633339
inactive	inactive
inactive	inactive
inactive	0
inactive	inactive
26.35076712	383.9058051
29.56604699	54.83170296
33.17365034	95.24669615
26.35076712	34.25600794
inactive	inactive
33.17365034	72.36853452
31.31794541	131.2423619
inactive	inactive
27.91214823	299.3882036
31.92468319	41.74179807
28.45290384	40.40670797
inactive	inactive
inactive	inactive
inactive	0
inactive	inactive
inactive	0
30.72273886	61.36505172
inactive	inactive
33.17365034	71.93450272
inactive	inactive
inactive	inactive
inactive	inactive
inactive	inactive
inactive	inactive

inactive		inactive	
inactive		inactive	
	33.17365034		217.0147683
inactive		inactive	
inactive			0
	29.56604699		59.895075
inactive		inactive	
	27.91214823		37.16585122
inactive		inactive	
inactive		inactive	
	33.17365034		96.28907084
inactive			0
inactive		inactive	
	37.22144788		38.73906766
inactive			0
inactive		inactive	
	35.1393127		38.17279965
	26.35076712		118.7588638
	33.17365034		55.48829663
inactive			0
	34.47147997		34.1102211
inactive		inactive	
inactive		inactive	
inactive		inactive	
	37.22144788		32.57437423
inactive		inactive	
	67.92493908		240.0027401
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
	33.17365034		60.46932938
inactive		inactive	
inactive		inactive	
inactive		inactive	

GFP-LC3 (Total Spot Area) AC50 (uM)	GFP-LC3 (Total Spot Area) Efficacy (%)
42.85773919	80.67845706
13.98921236	28.90209493
inactive	0
inactive	inactive
33.17365034	63.50042729
26.35076712	62.84549767
24.61689482	189.4148204
20.93115833	58.33601199
33.17365034	190.7579048
inactive	inactive
33.17365034	231.4894199
26.35076712	170.655599
33.17365034	63.60030492
inactive	inactive
13.20666808	104.4381663
18.6549145	211.0361015
30.72273886	43.9530809
inactive	inactive
inactive	inactive
inactive	0
35.1393127	33.42025803
25.35867724	293.1945499
29.56604699	44.69880506
31.92468319	94.98807163
26.35076712	36.81022908
inactive	inactive
33.17365034	58.35083391
29.56604699	93.67820357
inactive	inactive
24.40393893	152.8145523
30.72273886	51.42389936
26.35076712	62.18082087
inactive	inactive
inactive	inactive
33.17365034	43.19148673
inactive	inactive
26.35076712	39.27603124
25.35867724	38.45127828
inactive	inactive
34.47147997	51.12901493
inactive	inactive
inactive	inactive
inactive	inactive
inactive	inactive
inactive	inactive

inactive			0
inactive			0
	34.47147997		158.1491311
inactive		inactive	
inactive			0
	29.56604699		45.26472683
inactive		inactive	
	22.17140743		38.32262863
inactive			0
inactive		inactive	
	35.1393127		106.1502904
	35.1393127		33.67973482
inactive		inactive	
	29.56604699		32.78916392
	29.56604699		24.79238628
inactive		inactive	
	35.1393127		69.24123933
	23.48514591		100.0801898
	31.31794541		45.58439373
inactive			0
	28.45290384		37.73562964
inactive		inactive	
inactive		inactive	
inactive		inactive	
	33.17365034		34.33026331
inactive		inactive	
	62.90655819		190.6764937
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
inactive		inactive	
	29.56604699		79.53040009
inactive		inactive	
inactive		inactive	
inactive		inactive	

Secondary experimental confirmation results of model predicted ZIKV NS1 inibitors.

Sample ID	Name	Structure	NS-1 IC50 (uM)	NS-1 Efficacy (%)
NCGC00378623-01	Dolastatin 10	CC[C@H](C)[C@@H]([	0.001662621	-123.7609559
NCGC00025125-18	Colchicine	CC(=O)N[C@H]2CCc3c	0.01250822	-80.44964471
NCGC00387651-01	T-2 Toxin	CC(C)CC(=O)O[C@H]1(	0.014260232	-169.7078916
NCGC00357393-02	Narciclasine	O[C@H]1\C=C\2[C@@	0.017952569	-123.9408855
NCGC00246789-03		CC1CC(C)(CC(C(O)CC2(	0.018654914	-173.5699728
NCGC00179895-03	Diacetoxyscirpenol	CC(=O)OC[C@]12CC\C	0.041763151	-166.5446006
MLS002702975-01		COC1=C(OC)C(OC)=C2(	0.043396752	-72.08167992
NCGC00022001-13	Podofilox	COc1cc(cc(OC)c1OC)[(	0.04869226	-130.7486731
MLS002702890-01		COC1=C(OC)C2=C(CCC	0.050596898	-81.2048446
NCGC00390533-01	7-Epi-docetaxel	CC(=O)O[C@@]12CO[(	0.050597213	-144.8149481
NCGC00071621-03		COC1=CC=CC=C1C2=N	0.079194665	-115.9823972
NCGC00024379-16	Emetine	COc4cc5CCN[C@H](C[	0.284529038	-158.5526636
NCGC00107023-01		CC1=C([NH]C2=C1C(=C	0.319246832	-111.2326565
NCGC00107055-01		COC1=CC(=CC(=C1OC)	0.319246832	-131.373377
NCGC00161928-01		COC1=CC(=CC(OC)=C1	0.351393127	-99.583209
NCGC00112054-01		CCCNC(=O)C1=CC\2=C	0.468590266	-142.555562
NCGC00018238-09	Oxibendazole	O=C(OC)Nc1nc2cc(ccc	0.468590266	-108.8408382
NCGC00131231-01		CC(C)(C)C1=CC=C(C=C1	0.50597213	-177.4482846
NCGC00161926-01	beta-PELTATIN	[H][C@]12COC(=O)[C@	0.525766926	-162.8258892
NCGC00016806-14	Mebendazole	COC(=O)NC1=NC2=C([N	0.567710067	-121.2735182
NCGC00130596-01		CC(C)C/1=N/N\2C(=O)/	0.589920193	-125.3535929
NCGC00263862-02	FLOXURIDINE	OC[C@H]1OC(C[C@H]	0.636981172	-153.3276354
NCGC00119573-01		CCC1=CC=C(C=C1)[N]2	0.661901343	-178.1237003
NCGC00131197-01		CC1=CC=CC=C1C(=O)N	0.687796449	-154.7522269
NCGC00165745-01	Borrelidin	[H]C1(CCC[C@H]1C(O)	0.801911785	-146.0308237
NCGC00386770-01	Suprafenacine	CC1=CC=C(C=C1)/C=N/	0.833284421	-115.3008695
NCGC00255694-01	Fenbendazole	O=C(OC)Nc1nc2cc(ccc	0.923342	-137.4792344
NCGC00137609-01		CC1=CC(=CC=C1)OCC(=	0.934954682	-98.95892744
NCGC00126601-01		COC1=CC(=C(CCNC2=N	0.971538307	-139.1856329
NCGC00104735-01		CCOC(=O)C1=C(NC(=O)	1.09008391	-117.9238478
NCGC00131403-01		COC1=CC=C(CN2CCC3	1.132730503	-129.316064
NCGC00098841-01		CC(=C)CN\1C(=O)C2=C	1.223094263	-124.7861732
NCGC00112060-01		CC1=CC=C(C)C\2=C1S(	1.320666807	-145.59745
NCGC00118008-01		COC1=CC=CC(=C1)CN(	1.320666807	-133.6513183
NCGC00100750-01		CC1=CC=CC(=C1)NC(=(	1.398921235	-120.1673267
NCGC00017007-05	Methiazole	COC(=O)NC1=NC2=C([N	1.408302415	-102.4945465
NCGC00132685-01		FC1=CC=CC=C1CN2\C=	1.426023215	-156.91981
NCGC00107639-01		CCC/1=N/C2=C(SC3=C	1.481812529	-104.2261321
NCGC00108968-01		COC1=CC(=C(OC)C=C1	1.539784449	-105.5376902
NCGC00131179-01		COC1=CC(=CC(=C1)OC	1.539784449	-185.5049438
NCGC00115110-01		COC1=CC=CC=C1N2C(	1.539784449	-137.7581833
NCGC00109656-01		CC1=CC(=C(C)C=C1)CN	1.600024364	-127.4828157
NCGC00105676-01		CCCC1=CC(=NO1)C(=O	1.727666567	-144.2052628
NCGC00131199-01		ClC1=CC=CC=C1C(=O)N	1.795256864	-134.840151
NCGC00139416-01		CCCC/1=N/C2=C(SC3=	1.865491448	-121.7074214

NCGC00112548-01		COC1=CC(=C(OC)C=C1	1.865491448	-142.6195377
NCGC00112058-01		CC1=CC=C(C)C\2=C1S(	1.938473772	-151.5801759
NCGC00100746-01		COC1=CC(=CC=C1)NC(	1.938473772	-137.5829331
NCGC00104897-01		CCCCC(CC)CNC(=O)C1=	2.014311331	-138.9099153
NCGC00104879-01		COCCN1C(=O)NC2=CC	2.014311331	-123.1009422
NCGC00112544-01		COC1=CC(=C(CCNC(=O	2.175003345	-120.2468603
NCGC00131207-01		FC(F)(F)C1=CC=CC(=C1	2.175003345	-180.4848162
NCGC00118646-01		CCC(CC)C(=O)NC1=CC=	2.260094487	-141.261246
NCGC00131111-02		CN(C1=CC=C(C)C=C1)[S	2.260094487	-104.2458148
NCGC00131201-01		CC(C)OC1=CC=C(C=C1)	2.440393891	-156.8968294
NCGC00117664-01		FC1=CC=C(NC2=NC3=I	2.440393891	-151.496651
NCGC00141977-01		CCC1=NC2=CC(=CC=C2	2.535867722	-133.7493762
NCGC00108525-01		CCOC(=O)C1=CC=C(C=(	2.535867722	-136.3408408
NCGC00103947-01		COC1=CC(=C(C)C=C1N	2.535867722	-124.1896277
NCGC00138165-01		FC1=CC=CC=C1C(=O)N	2.535867722	-127.9025113
NCGC00119579-01		COC1=CC=CC(=C1OC)(	2.738166982	-181.2228729
NCGC00108970-01		COC1=C(NC2=C3CCCC	2.845290382	-110.0633641
NCGC00102074-01		COC1=CC(=C(OC)C=C1	2.845290382	-146.7300199
NCGC00072088-02		O=C(NC1=CC=CN=C1)(	2.845290382	-142.6032945
NCGC00108397-01		C[N]1C=C(CN(C2CCCC(	2.956604697	-143.6730953
NCGC00131233-01		CCCCOC1=CC=C(C=C1)	2.956604697	-132.6197915
NCGC00107109-01		CC1=C([NH]C2=C1C(=(	3.072273884	-153.5928677
NCGC00142060-01		CCCC1=C(C(=O)OCC)C2	3.317365032	-121.0091927
NCGC00113159-01		COC(=O)C1=CC2=C(C=(	3.317365032	-119.5013425
NCGC00107103-01		CC(C)OC1=CC=CC(=C1)	3.722144786	-123.8572952
NCGC00138127-01		CN1C(=O)C2=C(SC3=C(	3.722144786	-152.4847369
NCGC00114471-01		CC[N]1C(=CC2=C1C3=(	3.867763665	-144.9916556
NCGC00137837-01		COC1=CC=C(OCC(=O)N	3.867763665	-131.1708977
NCGC00182341-01		[O-][S+](=O)(N1CCN(CC	4.019054486	-33.71364791
NCGC00102779-01		CCOC1=CC=C(C=C1)N2	4.01907949	-127.836475
NCGC00132979-01		COC1=CC=C(CN2CCC/:	4.01907949	-122.8164819
NCGC00138157-01		CC(=O)NC1=CC=C(C=C:	4.176315139	-133.5362617
NCGC00100556-01		CCOC1=CC=C(C=C1)[S-	4.339702209	-165.5406669
NCGC00126217-01		COC1=CC=C(C=C1)C2N	4.509481357	-154.4172168
NCGC00105670-01		CC(C)C1=CC(=NO1)C(=	4.685902657	-142.6976273
MLS000830213-01		COC1=CC=C(C=C1)C2=	4.869195671	-83.11827179
NCGC00108581-01		CCOC(=O)C1=CC=C(C=(	4.869225964	-123.3721798
NCGC00164807-01		CCN1C2=C(S\C1=N/C(=	5.059689824	-80.63625292
NCGC00389858-01	DIGITONIN	C[C@@H]1CC[C@@]2	5.123388247	-155.9856398
MLS000100790-01		CC1=CC(=CC=C1)N2N=	5.463327401	-77.06403875
NCGC00255429-01	Nonoxynol	CCCCCCCCCc1ccc(OC(	5.46807648	-130.4130555
NCGC00169957-03		CCC(C)C1NC(=O)C2CC(	5.53362838	-189.3506146
NCGC00109606-01		[O-][S+]1(=O)C2=C(C=C	5.899201932	-133.7940625
NCGC00134651-01		ClC1=CC=C(C=C1)C2N(	6.129992302	-125.0640176
NCGC00121687-01		CCOC1=CC=C(C=C1)C2	6.248751622	-126.3098178
NCGC00138099-01		COC1=CC=C(C=C1OC)(	6.248751622	-128.3061623
NCGC00356796-01		CCOC(=O)C1=CC=C(NC	6.369811724	-163.9438553
NCGC00104681-01		COC1=CC=CC(=C1OC)(	6.369811724	-185.1861977

NCGC00131586-01		CCCCOC1=CC=C(CNC(=	7.426655222	-130.4886612
NCGC00184875-01		CC1=CC=C(CNCC2=C[N	8.332792371	-101.9547019
NCGC00246910-02		OCC1OC(C(O)C1O)[N]2	8.332844212	-146.0509681
NCGC00125691-01		COC1=CC=C(C[N]2C3=	8.332844212	-191.6668462
NCGC00129956-01		CC(C)C/1=N/N\2C(=O),	9.349604983	-181.146835
NCGC00102585-01		COC1=CC=C(C=C1)C2=	9.715322627	-88.02203959
NCGC00239676-01		CC1=CN=C(SCC2=CC=C	9.71538307	-179.0531209
NCGC00141038-01		COC1=CC=C(C=C1)C(=C	9.71538307	-144.6245406
NCGC00108419-01		CC[N]1C=C(CN(C2CCC	10.49042933	-184.753585
NCGC00125689-01		COC1=CC=C(C[N]2C3=	10.49042933	-166.1007499
MLS000564956-01		ClC1=CC=CC(Cl)=C1CN	10.90077128	-65.70047881
NCGC00108313-01		CCOC(=O)C1=CC=C(C=C	11.11202635	-77.69631941
MLS000579506-01		CC1=C(C2=C(S1)N=CN=	11.32723456	-80.99576574
NCGC00113062-01		CC1=CC=C(NC(=O)C2=C	11.32730503	-128.2572464
NCGC00166344-01		CCNC1=NC(=NC(=N1)C	12.23086654	-85.38387868
NCGC00187882-01		C[S+]([O-])(=O)C1=CC=C	12.23086654	-126.9894587
NCGC00106742-02		CC(C)C1=CC=C(NC2=C(	12.23094263	-145.0616882
NCGC00114058-01		CC1=CC(=CC(=C1)NC(=	12.46789863	-109.6206199
MLS000624892-01		COC1=C(OCC2=C(Cl)C=	12.70936622	-96.9582229
NCGC00107199-01		CC1=CC2=C(C=CC=C2)	12.70944529	-157.6625989
NCGC00138993-01		COC1=CC=C(OC)C(=C1	12.70944529	-126.2639584
NCGC00119990-01		CCN1C(=O)C2=CC=CC=	13.2065859	-104.8827046
NCGC00187802-01		OC1=C2N=CC=CC2=CC	13.2065859	-89.82070742
NCGC00239467-01		CSC1=C(C=CC=C1)C(=C	13.20666807	-167.3258365
NCGC00139155-01		CC1=C(Cl)C=C(C=C1)[N	13.72325797	-95.31872525
NCGC00108493-01		CCOC(=O)C1=CC=C(C=C	13.72334335	-134.0122437
NCGC00108521-01		CCOC(=O)C1=CC=C(C=C	13.72334335	-160.8382455
NCGC00092346-01	GW 583340 dihydroc	C[S+]([O-])(=O)CCNCC1	14.26014344	-57.91807118
NCGC00119375-01		CN1CCN(CC1)C2=CC=C	14.81812529	-83.38670019
NCGC00239870-01		COCC(C)NCC1=CC2=C(	15.39774869	-103.8508397
NCGC00100011-01		CCOC1=C(NC(=O)N2C3	15.39784449	-149.4218168
NCGC00167507-09	Lapatinib	C[S+]([O-])(=O)CCNCC1	15.69605676	-88.49041584
NCGC00354561-04		CCC1=C(N2\C(=C(/C=C	16.6261066	-109.9226859
NCGC00126562-01		CC1=CC=C(Cl)C=C1N2(	16.62621003	-71.33493284
NCGC00099020-01		CC1=CC=C2N=C3CCCC	16.62621003	-145.8565702
NCGC00116349-01		COC(=O)C1=C(OC2=CC	16.62621003	-136.3194129
NCGC00139449-01		COC1=CC=C(C=C1OC)N	16.62621003	-117.5021542
NCGC00165957-20	Amlodipine besylate	CCOC(=O)C/1=C(COCC	16.62621003	-88.13208559
NCGC00091182-01	Triglycidyl isocyanura	O=C4N(CC1CO1)C(=O)	16.62621003	-149.5240579
NCGC00108317-01		CCOC(=O)C1=CC=C(C=C	17.27666567	-173.866854
NCGC00185692-01		CC1=C(C2=C(C=CC=C2	18.65479842	-64.54495119
NCGC00118620-01		COC1=CC=C(C=C1)C(=C	18.65491448	-158.7556101
NCGC00099684-01		FC1=CC=C(C=C1)C2=N	18.65491448	-174.9156532
NCGC00240223-01		COC1=CC=CC=C1N2C(	19.76016472	-90.13719703
NCGC00127015-01		CC(C)(C)OC(=O)N1CCC	19.76028766	-172.3868358
NCGC00107641-01		CCC/1=N/C2=C(SC3=C	19.76028766	-102.1976023
NCGC00111226-01		COC1=C(CNC2=NC=NC	20.142988	-80.02678174
NCGC00014374-03		O[C@@H]1CC2=C(O)C	20.93102809	-51.27436981

NCGC00015619-13	Loratadine	Clc3cc4CCc1cccnc1C(	20.93115831	-149.0691478
NCGC00108391-01		C[N]1C=C(CN(C2CCCC(	20.93115831	-119.6808203
NCGC00164437-02	2,2-Bis(4-hydroxyphe	OC1=CC=C(C=C1)C(C2=	21.4796181	-30.66542526
NCGC00011767-02		CC1=CC=CC(=C1)CNC2	22.17126948	-75.56485962
NCGC00167513-14	Vandetanib	COC1=CC2=C(NC3=CC	22.17140742	-148.5525376
NCGC00106584-01		CC1=CC=C(NC(=O)NCC	22.60080426	-67.70271511
NCGC00100979-01		CC1CCC2=C(C1)SC(=C2	22.60094487	-141.5199719
NCGC00182086-01		C1OC2=CC=C(\C=C/C3	23.48499979	-73.58064035
NCGC00163320-01	N6-METHYLADENOSIN	CNC1=C2N=CN([C@@	23.48499979	-94.29593471
NCGC00240089-01		OC1=C2OCCN(CC3=CC	23.48499979	-94.73112901
NCGC00379019-02	Calcifediol-D6	C[C@H](CCCC(C([2H])(	23.4851459	-81.12092973
NCGC00108621-01		CCOC(=O)C1=CC=C(C=(	28.45290382	-114.2610521
NCGC00138676-01		COC1=CC=C(C=C1CSC2	28.45290382	-146.8997366
NCGC00104723-01		CCCC[N]1C(=NC2=C1C	29.56604697	-163.1650487
NCGC00138698-01		ClC1=CC=CC=C1CSC2=	30.72254771	-65.86643976
NCGC00098192-01		COC1=CC2=C(C=C1)N=	31.92468317	-90.21293662
NCGC00090749-12	Diethylstilbestrol	Oc1ccc(cc1)C(CC)=C(C	33.17365032	-156.2382706
NCGC00254528-01	4,4',4"-Ethane-1,1,1-t	CC(c1ccc(O)cc1)(c2cc(	34.0429005	-94.62209675
NCGC00255488-01	4,6-Di-tert-butyl-m-cr	CC(C)(C)c1cc(c(C)cc1C	48.08687508	-106.1390135
NCGC00108810-01		COC1=CC(=C(OC)C=C1	inactive	0
NCGC00103968-01		FC1=CC2=C(NC(=O)CN	inactive	-56.08529442
NCGC00139105-01		ClC1=CC=C(CCNC2=NC	inactive	0
NCGC00187697-01		COC1=CC=C(C=C1)C2=	inactive	-39.76590134
NCGC00164910-01		FC1=CC=C(C=C1)C2=N	inactive	-26.6211889
NCGC00167965-01	Lutein	CC2(C)C[C@H](O)CC(C	inactive	0
MLS002391605-01		COC1=CC(=CC(OC)=C1	inactive	0
NCGC00187905-01		C[S+]([O-])(=O)C1=CC=C	inactive	0
NCGC00256909-01	Benzyl 3-methylbutyl	CC(C)CCOCc1ccccc1	inactive	0
NCGC00255814-01	Styrene glycol	OC(CO)c1ccccc1	inactive	0

Cell Viability IC50 (uM)	Cell Viability Efficacy (%)	SI
inactive	0	60146
inactive	0	7994.743
inactive	0	7012.509
inactive	0	5570.234
0.070112146	-37.23885238	3.758374
inactive	0	2394.455
inactive	0	2304.32
inactive	0	2053.715
inactive	0	1976.406
inactive	0	1976.393
2.067105254	-78.60615294	26.10157
0.372214479	-34.34227491	1.308177
0.742665522	-38.32698871	2.326305
0.307227388	-32.38286121	0.962351
inactive	0	284.5815
0.417631514	-42.21797846	0.891251
0.372214479	-32.28980048	0.794328
4.685902657	-68.08511616	9.261187
inactive	0	190.1983
1.320666807	-42.78229485	2.326305
1.372334335	-59.88717951	2.326305
inactive	0	156.9905
2.487672828	-56.11065674	3.758374
1.17704553	-47.3615285	1.711328
0.417631514	-39.34028649	0.520795
1.223094263	-50.36255271	1.467799
2.410067784	-38.26630065	2.610157
13.2065859	-41.41688174	14.12538
0.61299923	-57.02066048	0.630957
1.481812529	-35.42702596	1.359356
1.372334335	-72.9760468	1.211528
0.636981172	-37.34222548	0.520795
1.17704553	-32.30104301	0.891251
0.882659627	-35.50622942	0.668344
0.132066681	-30.95392737	0.094406
2.147975174	-52.41586345	1.525223
5.899201932	-58.92494994	4.13682
1.481812529	-38.85828232	1
1.662621003	-39.66193143	1.079775
1.372334335	-38.18887701	0.891251
1.223094263	-33.37853771	0.794328
1.320666807	-36.87170502	0.825404
1.17704553	-34.56343	0.681292
4.685902657	-55.26668442	2.610157
1.481812529	-36.18319745	0.794328

	1.865491448	-45.87538073	1
inactive		0	51.58698
	2.014311331	-39.54249827	1.039122
	1.398921235	-32.30036997	0.694491
inactive		0	49.64476
	1.246789863	-39.76516953	0.573236
	1.426023215	-39.56196088	0.655642
	2.175003345	-44.54396336	0.962351
	2.093115831	-37.98926055	0.926119
	6.877964488	-88.668866	2.818383
	1.481812529	-62.80488179	0.607202
	1.727666567	-37.95965103	0.681292
	25.35867722	-40.65016881	10
	10.49042933	-69.66103367	4.13682
	2.63507671	-38.13793248	1.039122
	1.398921235	-32.1990887	0.510897
	3.131794539	-56.6258126	1.100694
	2.34851459	-39.35940096	0.825404
inactive		0	35.1458
	12.23094263	-98.2277467	4.13682
	1.17704553	-53.05779427	0.398107
	3.867763665	-35.05905411	1.258925
	2.63507671	-40.32378356	0.794328
inactive		0	30.14441
	3.94269573	-42.45400805	1.059254
	4.869225964	-52.2991014	1.308177
	1.426023215	-36.44558181	0.368695
	2.956604697	-30.9192058	0.764422
inactive		0	24.88147
inactive		0	24.88132
	3.192468317	-51.74530164	0.794328
	4.176315139	-42.80762354	1
	3.447147995	-59.10516354	0.794328
	2.63507671	-34.83000394	0.584341
	3.447147995	-35.41143658	0.735642
inactive		0	20.53727
inactive		0	20.53715
	7.14700184	-66.33895416	1.412538
	8.120023155	-44.64695986	1.584893
	14.26014344	-52.87589002	2.610157
	4.343447537	-59.92234643	0.794328
inactive		0	18.07133
	4.176315139	-42.69705499	0.707946
	13.98921235	-52.21636221	2.282093
	30.72273884	-49.52108871	4.91662
	4.339702209	-41.70621262	0.694491
	7.011214636	-42.2668587	1.100694
	4.685902657	-39.30345109	0.735642

	8.997598212	-58.87961061	1.211528
	7.426609018	-53.87687782	0.891251
inactive		0	12.0007
	11.7704553	-35.75064299	1.412538
	4.423777369	-30.46323891	0.473151
	10.49036407	-59.16374006	1.079775
	12.70944529	-88.92495782	1.308177
	11.7704553	-37.56043394	1.211528
	20.93115831	-80.74756773	1.995262
inactive		0	9.532498
	11.77038208	-39.56839069	1.079775
inactive		0	8.999259
	8.332792371	-39.89835545	0.735642
	6.369811724	-64.81235188	0.562341
	10.09540843	-44.74951598	0.825404
	24.40378709	-59.3633296	1.995262
	6.877964488	-65.1665593	0.562341
	14.26023215	-60.14630884	1.143756
	27.91197456	-34.76330426	2.196174
	4.01907949	-36.02244275	0.316228
	11.7704553	-40.7674938	0.926119
	20.142988	-85.00351517	1.525223
	16.6261066	-51.96283957	1.258925
	14.26023215	-85.64542202	1.079775
	15.69605676	-33.80042776	1.143756
	18.65491448	-55.34581527	1.359356
	23.4851459	-47.79119987	1.711328
inactive		0	7.012552
	14.81812529	-60.88923475	1
inactive		0	6.494456
	9.349604983	-39.99945327	0.607202
inactive		0	6.371027
inactive		0	6.014637
	8.826596273	-49.77746299	0.530884
	10.49042933	-69.28206152	0.630957
	4.339702209	-36.87735749	0.261016
inactive		0	6.0146
inactive		0	6.0146
inactive		0	6.0146
	26.3507671	-43.74191582	1.525223
inactive		0	5.360551
	10.9008391	-59.47299251	0.584341
	24.87672828	-45.30276772	1.333521
	18.65479842	-65.72754967	0.944061
	18.65491448	-57.95328782	0.944061
inactive		0	5.060655
inactive		0	4.964507
inactive		0	4.777596

inactive		0	4.777566
	16.00024364	-43.61390223	0.764422
inactive		0	4.655576
	18.65479842	-58.84574944	0.841395
inactive		0	4.510314
inactive		0	4.424621
inactive		0	4.424594
	6.618972254	-54.76932375	0.281838
inactive		35.41495403	4.258037
	20.142988	-47.09482001	0.857696
	18.65491448	-40.83196514	0.794328
inactive		0	3.51458
inactive		0	3.51458
	9.349604983	-50.63874556	0.316228
	24.87657351	-41.29558713	0.809717
	19.76028766	-44.31502113	0.618966
	16.62621003	-57.48709022	0.501187
inactive		0	2.93747
	3.537473719	-41.44284991	0.073564
	25.35867722	-82.90440082	N/A
inactive		0	N/A
inactive		0	N/A
inactive		0	N/A
inactive		0	N/A
inactive		0	N/A
inactive		0	N/A
inactive		0	N/A
inactive		0	N/A
inactive		0	N/A

Secondary experimental confirmation results of model predicted anti-EBOV compounds.

Sample ID	Name	Structure	EBOV IC50 (uM)
NCGC00182117-01		CCC(=O)NC(C1=CC=C(C	0.398107
NCGC00125691-01		COC1=CC=C(C[N]2C3=	2.511886
NCGC00133073-02		ClC1=CC=CC(=C1)NC(=	2.511886
NCGC00181913-02	Difeterol	OC(C(C)N(C)CCOC(c1c	3.162278
NCGC00131197-01		CC1=CC=CC=C1C(=O)N	3.162278
NCGC00108517-02		CCOC(=O)C1=CC=C(C=	3.162278
NCGC00246387-06	Arbidol	CCOC(=O)C1=C(CSC2=	5.011872
NCGC00131135-01		CCOC1=CC=CC=C1CN[	0.251189
NCGC00131075-01		COC1=CC=CC=C1CN[S-	1.258925
NCGC00095996-03	Acivicin	N[C@H]([C@@H]1C\C	3.981072
NCGC00118167-01		CCOC(=O)N1CCN(CC1)	3.981072
NCGC00115464-01		CCCC\1=C\C(=O)N\C(=	5.011872
NCGC00127044-01		COC1=CC=CC(=C1)CNC	5.011872
NCGC00128675-01		CC1=NOC(=C1)C2=CC=	6.309573
NCGC00135673-01		CCOC1=CC=C(C=C1)C(=	6.309573
NCGC00160678-01	Fenoverine	O=C(CN3CCN(Cc1ccc2	10
NCGC00356798-01		CCOC1=CC=CC=C1N2C	12.589254
NCGC00104607-01		ClC1=CC=CC(=C1)N2C	12.589254
NCGC00115319-01		C[N]1C(=NC2=C1C=CC	12.589254
NCGC00024762-07	Tesmilifene hydrochlc	CCN(CC)CCOC1=CC=C(	12.589254
NCGC00185768-05	Benidipine hydrochlo	COC(=O)C\1=C(C)\N\C(	15.848932
NCGC00167817-03	Bucindolol	CC(C)(CC1=CNC2=C1C	15.848932
NCGC00167493-14	Manidipine	COC(=O)C\1=C(C)\N\C(	15.848932
NCGC00115545-01		COC1=CC=C(C=C1)C2=	15.848932
NCGC00103037-01		COC1=C(OCC2=C(Cl)C=	15.848932
NCGC00108569-01		CCOC(=O)C/1=C(CN(CC	15.848932
NCGC00485224-01	Î±-Zearalenol	C[C@H]1CCC[C@H](O	25.118864

EBOV Efficacy (%)	Cell Viability IC50 (uM)	Cell Viability Efficacy (%)	SI
-91.748	12.589254	-132	31.62279
-115.801	19.952623	-104.1	7.943284
-128.957	25.118864	-32.5	10
-102.46	25.118864	-106.1	7.943281
-93.194	31.622777	-22.5	9.999999
-109.743	25.118864	-26	7.943281
-144.135	>30	0	5.985787
-100.35	0.794328	-68.1	3.162272
-131.169	3.162278	-76.9	2.511888
-102.902	7.943282	-66.3	1.995262
-117.145	15.848932	-77.3	3.981071
-104.35	12.589254	-71.4	2.511887
-125.88	19.952623	-114.86	3.981072
-133.332	19.952623	-92.4	3.162278
-111.91	25.118864	-79.7	3.981072
-118.836	25.118864	-54.5	2.511886
-148.868	19.952623	-61.5	1.584893
-106.362	>30	0	2.382985
-91.846	>30	0	2.382985
-134.226	19.952623	-26.5	1.584893
-100.748	19.952623	-132.7	1.258925
-116.128	25.118864	-37.5	1.584893
-126.206	19.952623	-114.86	1.258925
-94.3	>30	0	1.892872
-122.398	19.952623	-26.5	1.258925
-89.387	>30	0	1.892872
-131.16	>30	0	1.194322