Recent advances in the design of inhibitors targeting the viral entry and replication of the SARS-CoV-2 virus, driven by *in silico* approaches

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Supporting Information

Table S1. Pharmacological and physicochemical profiles for SARS-CoV-2 Spike ACE2 inhibitors

No.	Name[1]	IC_{50}	EC50	CC50	Type of Assay	Metabolic profiling (CL_{int}) (μl/min/mg)	Approval status	Reference
1	ErB	0.43 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Control (+)	[1]
2	SY (FD&C#6)	>500 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Control (-)	[1]
3	NBIBk	>500 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
4	CgRd	0.99 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
5	DV1	1.47 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
6	EvBI	2.25 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
7	ChBk	2.57 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
8	CSc3B	4.25 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
9	MeBlu	3.26 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
10	Suramin	>500 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
11	Chloroquine	>500 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
12	DRI-C21041	1.81 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
13	DRI-C23041	0.52 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Experimental	[1]
14	DRI-C24041	3.35 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
15	DRI-C61041	7.67 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
16	DRI-C71041	9.95 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
17	DRI-C2204745	4.04 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
18	DRI-C91005	0.16 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
19	DRI-C2105041	>500 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]

No.	Name[1]	IC_{50}	EC50	CC50	Type of Assay	Metabolic profiling (CL_{int}) (μl/min/mg)	Approval status	Reference
20	DRI-C2105045	120.80 µM	ND*	ND*	SARS-CoV-2-RBD-hACE2	ND*	Hit	[1]
21	CgRd	3.92 µM	ND*	ND*	SARS-CoV-2-S1S2-hACE2	ND*	Hit	[1]
22	DV1	2.63 µM	ND*	ND*	SARS-CoV-2-S1S2-hACE2	ND*	Hit	[1]
23	EvBI	1.27 µM	ND*	ND*	SARS-CoV-2-S1S2-hACE2	ND*	Hit	[1]
24	CSc3B	9.94 µM	ND*	ND*	SARS-CoV-2-S1S2-hACE2	ND*	Hit	[1]
25	DRI-C23041	3.38 µM	ND*	ND*	SARS-CoV-2-S1S2-hACE2	ND*	Experimental	[1]
26	DRI-C61041	6.81 µM	ND*	ND*	SARS-CoV-2-S1S2-hACE2	ND*	Hit	[1]
27	DRI-C71041	8.60 µM	ND*	ND*	SARS-CoV-2-S1S2-hACE2	ND*	Hit	[1]
28	DRI-C2204745	4.42 µM	ND*	ND*	SARS-CoV-2-S1S2-hACE2	ND*	Hit	[1]
29	DRI-C91005	0.24 µM	ND*	ND*	SARS-CoV-2-S1S2-hACE2	ND*	Hit	[1]
30	Chloroqunine	>200 µM	ND*	ND*	SARS-CoV-2-S1 – hACE2	ND*	Hit	[1]
31	CgRd	0.31 µM	ND*	ND*	SARS-CoV-2-S1 – hACE2	ND*	Hit	[1]
32	DVI	0.31 µM	ND*	ND*	SARS-CoV-2-S1 – hACE2	ND*	Hit	[1]
33	EvBI	0.19 µM	ND*	ND*	SARS-CoV-2-S1 – hACE2	ND*	Hit	[1]
34	CSC3B	2.88 µM	ND*	ND*	SARS-CoV-2-S1 – hACE2	ND*	Hit	[1]
35	MeBlu	2.65 µM	ND*	ND*	SARS-CoV-2-S1 – hACE2	ND*	Hit	[1]
36	DRI-C23041	1.88 µM	ND*	ND*	SARS-CoV-2-S1 – hACE2	ND*	Experimental	[1]
37	DRI-C24041	3.16 µM	ND*	ND*	SARS-CoV-2-S1 – hACE2	ND*	Hit	[1]
38	DRI-C91005	0.18 µM	ND*	ND*	SARS-CoV-2-S1 – hACE2	ND*	Hit	[1]
39	Ligand_003	2.371 µM	ND*	ND*	Theoretical obtained, experimental (Spike-ACE2)	ND*	Experimental	[2]
40	Ligand_013	0.586 µM, 0.586 µM	ND*	ND*	Theoretical obtained, experimental (Spike-ACE2)	ND*	Hit	[2]
41	Ligand_033	0.663 µM	ND*	ND*	Theoretical obtained (Spike-ACE2)	ND*	Hit	[2]
42	Ligand_044	1.047 µM	ND*	ND*	Theoretical obtained (Spike-ACE2)	ND*	Hit	[2]
43	Ligand_080	0.459 µM	ND*	ND*	Theoretical obtained (Spike-ACE2)	ND*	Hit	[2]
44	Hydroxychloroquine	7.268 µM	ND*	ND*	Theoretical obtained (Spike-ACE2)	ND*	Hit	[2]

No.	Name[1]	IC_{50}	EC50	CC50	Type of Assay	Metabolic profiling (CL_{int}) (μl/min/mg)	Approval status	Reference
45	Heparin sodium	5.5 µg/mL	ND*	ND*	Plaque reduction assay (RBD-ACE2)	ND*	Hit	[3]
46	Aurintricarboxylic acid (ATA)	0.6 µg/mL	ND*	ND*	Plaque reduction assay (RBD-ACE2)	ND*	Experimental	[3]
47	Ellagic acid	2.5 µg/mL	ND*	ND*	Plaque reduction assay (RBD-ACE2)	ND*	Experimental	[3]
48	Compound 1	0.193 ± 0.01* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
39	Compound 2	0.32 ± 0.08* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
50	Compound 3	0.45 ± 0.005* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
51	Compound 4	0.77 ± 0.01* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
52	Compound 5	0.91 ± 0.27* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
53	Compound 6	1.75 ± 0.39* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
54	Compound 7	1.81 ± 0.23* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
55	Compound 8	1.86 ± 0.008* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
56	Compound 9	1.91 ± 0.04* µM	ND*	99.7 ± 1.5 µM	Cell-based assay (Vero E6) RBD	ND*	Experimental	[4]
57	Compound 10	2.35 ± 0.02* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
58	Compound 11	2.82 ± 0.08* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
59	Compound 12	3.3 ± 1.09* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
60	Compound 13	3.31 ± 0.14* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
61	Compound 14	4.17 ± 0.01* µM	ND*	96.8 ± 1.5 µM	Cell-based assay (Vero E6) RBD	ND*	Experimental	[4]
62	Compound 15	4.33 ± 0.80* µM	ND*	≥ 100 µM	Cell-based assay (Vero E6) RBD	ND*	Experimental	[4]
63	Compound 16	4.9 ± 0.24* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
64	Compound 17	5.42 ± 1.53* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
65	Compound 18	4.96 ± 1.45* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Hit	[4]
66	Etravirine (positive control)	4.15 ± 0.16* µM	ND*	ND*	Cell-based assay (Vero E6) RBD	ND*	Control	[4]

No.	Name[1]	IC_{50}	EC50	CC50	Type of Assay	Metabolic profiling (CL_{int}) (μl/min/mg)	Approval status	Reference
67	SB27012	3.7 69 µM	ND*	3.13 µM	ELISA-based RBD-ACE2 binding assay, enzymatic assay	ND*	Hit	[5]
68	SB27041	2.2 72 µM	ND*	ND*	ELISA-based RBD-ACE2 binding assay	ND*	Experimental	[5]
69	SB27047	2.6 69 µM	ND*	ND*	ELISA-based RBD-ACE2 binding assay	ND*	Experimental	[5]
		2.6 µM	ND*	ND*	Vero monkey kidney epithelial cells (ACE2)	ND*		
70	SB27051	8.1 53 µM	ND*	ND*	ELISA-based RBD-ACE2 binding assay	ND*	Hit	[5]
71	SB27052	7.0 49 µM	ND*	ND*	ELISA-based RBD-ACE2 binding assay	ND*	Hit	[5]
72	SB27053	7.8 48 µM	ND*	ND*	ELISA-based RBD-ACE2 binding assay	ND*	Hit	[5]
73	Analogue - I (11) Ac-PPSCN-NH2	ND*	ND*	ND*	Cell-based assay (Vero E6 cells, S-RBD/ACE2)	ND*	Hit	[6]
74	Analogue - II (12) Ac-PHPCN-NH2	ND*	ND*	ND*	Cell-based assay (Vero E6, Spike RBD/ACE2)	ND*	Hit	[6]
75	Analogue - III (13) Ac-PHSPN-NH2	0.6 µM	ND*	ND*	Cell-based assay (Vero E6, Spike RBD/ACE2)	ND*	Experimental	[6]
76	ATN-161 Ac-PHSCN-NH2	3.16 µM	ND*	ND*	Cell-based assay (Vero E6, Spike RBD/ACE2)	ND*	Hit	[6]
77	AB-00011778	0.25 µM	ND*	>30 µM	A549-ACE2	ND*	Experimental	[6]
		0.25 µM	ND*	>30 µM	A549-ACE2			185
78	AB-00047476	2.5 µM	ND*	>30 µM	A549-ACE2	ND*	Experimental	[6]
79	H69C2	85.75 µM	ND*	>250	Vero E6-spike	ND*	Experimental	[7]
80	Clofazimine	>100 µM	0.31 µM	ND*	Vero E6-spike RBD		Phase 2 (NCT044695)	[8]
81	ALD-R491	13.5 nM	0.036 µM	>10 µM	HEK-GFP-spike	ND*	Experimental	[9]
82	Sertraline	1.638 ± 0.622 µM	ND*	ND*	Cell-based assay (Vero E6-spike)	ND*	Experimental	[10]
83	Aminobenztropine	0.21 µM	ND*	>200 µM	293T-spike	ND*	Experimental	[11]
84	15f	ND*	1.45 µM	323 µM	Huh-7	ND*	Experimental	[12]
85	MU-UNMC-1	<0.21 µM	ND*	>100 µM	INCN1T (S-RBD)	ND*	Experimental	[13]
86	MU-UNMC-2	0.45 µM	ND*	>100 µM	INCN1T (S-RBD)	ND*	Experimental	[13]
87	MU-UNMC-7	>5 .0 µM	ND*	ND*	INCN1T (S-RBD)	ND*	Hit	[13]
88	MU-UNMC-6	1.91 µM	ND*	ND*	INCN1T (S-RBD)	ND*	Hit	[13]

No.	Name[1]	IC_{50}	EC50	CC50	Type of Assay	Metabolic profiling (CL_{int}) (μl/min/mg)	Approval status	Reference
89	MU-UNMC-8	>5.0 μM	ND*	ND*	INCN1T (S-RBD)	ND*	Hit	[13]
90	P2119	ND*	22 ± 5.6 ng/mL	ND*	spike	ND*	Experimental	[14]
91	P2165	ND*	37 ± 4.7 ng/mL	ND*	spike	ND*	Experimental	[14]
92	6-Thioguanine	ND*	0.55 μM	>40 μM	Calu-3 spike	ND*	Experimental	[15]
93	6-Thioguanosine	ND*	0.49 μM	>40 μM	Calu-3 spike	ND*	Hit	[15]
94	6-mercaptopurine	ND*	0.26 μM	>40 μM	Calu-3 spike	ND*	Hit	[15]
95	Glycyrrhetinic acid	ND*	3.17 μM	>100 μM	Vero-E6 spike-RBD	ND*	Experimental	[15]
96	HCC1	ND*	125.6 μM	391.5 μM	293T-ACE2 spike	ND*	Hit	[16]
97	HCC4	ND*	128.2 μM	515.7 μM	293T-ACE2 spike	ND*	Hit	[16]
98	HCC11	ND*	26.7 μM	>74.1 μM	293T-ACE2 spike	ND*	Hit	[16]
99	HCC1+4+11	ND*	13.3 μM	121.5 μM	293T-ACE2 spike	ND*	experimental	[16]
100	Dichlorcyclizine	ND*	2.9 ± 1.6 μM	>100 μM	Vero-E6-ACE2 spike	ND*	Experimental	[17]
101	Fluoxazolevir	ND*	3.9 ± 1.0 μM	>100 μM	Vero-E6-ACE2 spike	ND*	Experimental	[17]
102	(-)-hopeaphenol	0.11 μM	13.5 μM	>100 μM	Vero-E6-ACE2 spike	ND*	Experimental	[18]
103	Bifonazole	38.84 μM, 40.00 μM	ND*	ND*	VerohACE2-TMPRSS2 cells, Vero E6 ACE2	ND*	Hit	[19]
104	NMT5	ND*	5.28 μM	48.66 μM	HeLa-ACE2	ND*	Experimental	[20]
105	NMT1	ND*	53.88 μM	144.95 μM	HeLa-ACE2	ND*	Hit	[20]
106	NMT3	ND*	87.68 μM	>200 μM	HeLa-ACE2	ND*	Hit	[20]
107	NMT4	ND*	70.02 μM	>200 μM	HeLa-ACE2	ND*	Hit	[20]
108	NMT6	ND*	3.32 μM	17.65 μM	HeLa-ACE2	ND*	Hit	[20]
109	NMT8	ND*	3.75 μM	16.35 μM	HeLa-ACE2	ND*	Hit	[20]
110	Bruceine A	ND*	54 ± 5 nM	>40 μM	Vero E6, ACE2	ND*	Experimental	[21]
111	Gamabufotalin	ND*	2.7 ± 0.2 nM	>40 μM	Vero E6, ACE2	ND*	Experimental	[21]
112	Anisomycin	ND*	0.016 ± 0.001 μM	>40 μM	Vero E6, ACE2	ND*	Experimental	[21]
113	Homoharringtonine	ND*	0.054 ± 0.005 μM	>40 μM	Vero E6, ACE2	ND*	Hit	[21]
114	Bruceine D	ND*	0.22 ± 0.02 μM	>40 μM	Vero E,6 ACE2	ND*	Hit	[21]
115	Remdesivir	ND*	0.43 ± 0.05 μM	>40 μM	Vero E6, ACE2	ND*	Hit	[21]
116	Mitoxantrone	ND*	0.44 ± 0.05 μM	>40 μM	Vero E6, ACE2	ND*	Hit	[21]
117	Digoxin	ND*	0.16 ± 0.02 μM	>40 μM	Vero E6, ACE2	ND*	Hit	[21]
118	Cinobufotalin	ND*	0.14 ± 0.01 μM	>40 μM	Vero E6, ACE2	ND*	Hit	[21]
119	Brexpiprazole	ND*	0.67 ± 0.13 μM	24.5 ± 0.8 μM	Vero E6, ACE2	ND*	Hit	[21]

No.	Name[1]	IC_{50}	EC50	CC50	Type of Assay	Metabolic profiling (CL_{int}) (μl/min/mg)	Approval status	Reference
120	6048589 (CKP-25)	3.5 ± 0.5 µM	ND*	ND*	Vero E6, Spike RBD/ACE2	<8.6	Experimental	[21]
121	5979349 (CKP-22)	55 µM	ND*	ND*	Vero E6, Spike RBD/ACE2	ND*	Hit	[22]
122	5465527	9.6 µM	ND*	ND*	Vero E6, Spike RBD/ACE2	ND*	Hit	[22]
123	6052953	11 µM	ND*	ND*	Vero E6, Spike RBD/ACE2	ND*	Hit	[22]
124	6659989	8.4 µM	ND*	ND*	Vero E6, Spike RBD/ACE2	ND*	Hit	[22]
125	5315079	5.5 µM	ND*	ND*	Vero E6, Spike RBD/ACE2	ND*	Hit	[22]
126	5260662	62 µM	ND*	ND*	Vero E6, Spike RBD/ACE2	ND*	Hit	[22]

Table S2. Pharmacological and physicochemical profiles of inhibitors targeting SARS-CoV-2 TMPRSS2.

No.	Name[1]	IC_{50}	EC50	K_i (nM)	Type of TMPRSS Assay	Approval status	Design strategy	Reference
1	N-0130	3.1 ± 1.5 nM	30.1 ± 30.1 nM	0.13 ± 0.03	Vero E6	Hit	Retention of peptidomimetic chemotype	[23]
2	N-0438	5.2 ± 5.4 nM	35.7 ± 24.5 nM	1.11 ± 0.09	Vero E6	Hit	Retention of peptidomimetic chemotype	[23]
3	N-0386	3.9 ± 4.4 nM	2.3 ± 1.7 nM	0.51 ± 0.09	Vero E6	Hit	Retention of peptidomimetic chemotype	[23]
4	N-0385	1.9 ±1.4 nM	2.8 ± 1.4 nM	2.6 ± 0.4	Vero E6	Experimental	Retention of peptidomimetic chemotype	[23]
5	N-0385(OH)	>10000 nM	>1000 nM	ND*	Vero E6	Hit	Retention of peptidomimetic chemotype	[23]
6	Camostat mesylate	17.5 ± 18.8 nM	10.6 ± 8.4 nM	5.6 ± 1.0	Vero E6)	Hit	Retention of peptidomimetic chemotype	[23]
7	Camostat	1.5 nM	83 Nm	ND*	Calu-3 Cells	Hit	Repurposed	[24]
8	Nafamostat	0.14 nM	ND*	ND*	Enzymatic assay	Hit	Repurposed	[24]
9	Ac-SKLR-kbt-V (1)	74 nM	307 nM	ND*	Calu-3 Cells	Hit	Retention of peptidomimetic chemotype	[24]
10	Cyclo(DLK)R-kbt (2)	2.6 nM	104 nM	ND*	Calu-3 Cells	Hit	Retention of peptidomimetic chemotype	[24]

11	Cyclo(DMK)R-kbt (19)	19 nM	119 nM	ND*	Calu-3 Cells	Hit	Retention of peptidomimetic chemotype	[24]
12	Cyclo(aGLY)R-kbt (21)	197 nM	565 nM	ND*	Calu-3 Cells	Hit	Retention of peptidomimetic chemotype	[24]
13	Cyclo(DQK)R-kbt (20)	ND*	138 nM	ND*	Calu-3 Cells	Hit	Retention of peptidomimetic chemotype	[24]
14	Ac-WFR-kbt (8)	9.4 nM	ND*	ND*	Enzymatic assay	Hit	Retention of peptidomimetic chemotype	[24]
15	Ac-SKFR-kt (9)	7.9 nM	ND*	ND*	Enzymatic assay	Hit	Retention of peptidomimetic chemotype	[24]
16	Ac-KQFR-kt (10)	29 nM	ND*	ND*	Enzymatic assay	Hit	Retention of peptidomimetic chemotype	[24]
17	Ac-SQLR-kt (11)	16 nM	ND*	ND*	Enzymatic assay	Hit	Retention of peptidomimetic chemotype	[24]
18	Ac-LLR-kt (18)	54 nM	349 nM	ND*	Calu-3 Cells	Hit	Retention of peptidomimetic chemotype	[24]
19	Ac-SKLR-kbt (3)	39 nM	ND*	ND*	Enzymatic assay	Hit	Retention of peptidomimetic chemotype	[24]
20	Ac-FLFR-kbt (12)	3.0 nM	ND*	ND*	Enzymatic assay	Hit	Retention of peptidomimetic chemotype	[24]
21	Ac-dWFR-kbt (13)	1.1 nM	32 nM	ND*	Calu-3 Cells	Hit	Retention of peptidomimetic chemotype	[24]
22	dWFR-kbt (14)	39 nM	ND*	ND*	Enzymatic assay	Hit	Retention of peptidomimetic chemotype	[24]
23	dWFR-kbt-CO2H (15)	42 nM	ND*	ND*	Enzymatic assay	Hit	Retention of peptidomimetic chemotype	[24]
24	Ac-WLFR-kbt (16)	6.3 nM	150 nM	ND*	Calu-3 Cells	Hit	Retention of peptidomimetic chemotype	[24]
25	Ac-KQLR-kbt (17)	ND	78 nM	ND*	Calu-3 Cells	Hit	Retention of peptidomimetic chemotype	[24]
26	MM3122 (4)	340 pM	430 pM	ND*	Calu-3 Cells	Lead	Retention of peptidomimetic chemotype	[24]
27	MM3144 (6)	310 pM	530 pM	ND*	Calu-3 Cells	Experimental	Retention of peptidomimetic chemotype	[24]
28	MM3116 (7)	250 pM	3.6 nM	ND*	Calu-3 Cells	Experimental	Retention of peptidomimetic chemotype	[24]
29	MM3123 (5)	280 pM	860 pM	ND*	Calu-3 Cells	Experimental	Retention of peptidomimetic chemotype	[24]
30	N-0385	ND*	ND*	0.28 ± 0.03	Inhibition assay	Lead	Retention of peptidomimetic chemotype	[25]
31	1	ND*	ND*	0.33 ± 0.09	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
32	2	ND*	ND*	0.38 ± 0.11	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
33	3	ND*	ND*	0.41 ± 0.13	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
34	4	ND*	ND*	0.36 ± 0.10	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]

35	5	ND*	ND*	0.60 ± 0.16	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
36	6	ND*	ND*	0.29 ± 0.06	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
37	7	ND*	ND*	0.37 ± 0.04	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
38	8	ND*	ND*	0.39 ± 0.05	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
39	9	ND*	ND*	0.13 ± 0.03	Inhibition assay	Experimental	Retention of peptidomimetic chemotype	[25]
40	10	ND*	ND*	0.14 ± 0.02	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
41	11	ND*	ND*	0.70 ± 0.07	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
42	12	ND*	ND*	0.39 ± 0.05	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
43	13	ND*	ND*	0.15 ± 0.00 03	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
44	14	ND*	ND*	0.16 ± 0.01	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
45	15	ND*	ND*	0.85 ± 0.05	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
46	16	ND*	ND*	0.53 ± 0.03	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
47	17	ND*	ND*	0.44 ± 0.12	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
48	18	ND*	ND*	1.55 ± 0.17	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
49	19	ND*	ND*	0.34 ± 0.07	Inhibition assay	Hit	Retention of peptidomimetic chemotype	[25]
50	Nafamostat mesylate	ND*	5 nM	ND*	Cell-based assay (Calu-3)	Experimental	Non-peptidomimetic	[26]
51		0.8 nM	ND*	ND*				
52	Camostat mesylate	ND*	87 nM	ND*	Cell-based assay (Calu-3)	Experimental	Non-peptidomimetic	[26]
53		6.7 nM	ND*	ND*				[27]
54	Gabeexate mesylate	ND*	1.2 M	ND*	Cell-based assay (Calu-3)	Hit	Non-peptidomimetic	[26]
55	1	ND*	ND*	86.7 nM	Cell-based assay (Caco-2)	Hit	Retention of peptidomimetic chemotype	[28]
56	2	32 nM	ND*	3.8 nM	Cell-based assay (Caco-2)	Experimental	Retention of peptidomimetic chemotype	[28]
57	3	ND*	ND*	9.1 nM	Cell-based assay (Caco-2)	Hit	Retention of peptidomimetic chemotype	[28]
58	4	ND*	ND*	8.5 nM	Cell-based assay (Caco-2)	Hit	Retention of peptidomimetic chemotype	[28]
59	5	12.7 nM	ND*	2.5 nM	Cell-based assay (Caco-2)	Experimental	Retention of peptidomimetic chemotype	[28]

60	6	ND*	ND*	71.5 nM	Cell-based assay (Caco-2)	Hit	Retention of peptidomimetic chemotype	[28]
61	7	ND*	ND*	57.7 nM	Cell-based assay (Caco-2)	Hit	Retention of peptidomimetic chemotype	[28]
62	8	ND*	ND*	215.9 nM	Cell-based assay (Caco-2)	Hit	Retention of peptidomimetic chemotype	[28]
63	CM	ND*	ND*	0.4 nM	Cell-based assay (Caco-2)	Hit	Retention of peptidomimetic chemotype	[28]
64	FOY-251	ND*	ND*	9.7 nM	Cell-based assay (Caco-2)	Hit	Retention of peptidomimetic chemotype	[28]
65	Halofuginone	30 nM, 0.069 μM	ND*	CC50 ~5.54 μM	Caco-2 cells, TMPRSS2-HiBiT-BEAS-2B cells	Experimental	Repurposed	[29]
66	Homoharringtonine	30 nM, 0.061 μM	ND*	CC50>10 μM	Caco-2 cells, TMPRSS2-HiBiT-BEAS-2B cells	Experimental	Repurposed	[29]
67	Avoralstat	2.7 ± 0.19 nM	2.8 ± 0.7 μM	ND*	Calu-3 2B4 Cells	Experimental	Repurposed	**[30]**
68	SBTI	121 ± 4 nM	ND*	ND*	Calu-3 2B4 Cells	Hit	Repurposed	**[30]**
69	Antipain	748 ± 63 nM	ND*	ND*	Calu-3 2B4 Cells	Hit	Repurposed	**[30]**
70	PC1-2748	1.41 ± 0.04 μM	ND*	ND*	Calu-3 2B4 Cells	hit	Repurposed	**[30]**
71	Benzimidine	120 ± 20 μM	ND*	ND*	Biochemical assay	Hit	Repurposed	[27]
72	6-amidino-2-napthol	1.6 ± 0.5 μM	ND*	ND*	Biochemical assay	Hit	Repurposed	[27]
73	Sunflowertrypsin inhibitor-1	0.4 ± 0.2 μM	ND*	ND*	Biochemical assay	Hit	cyclic peptide	[27]
74	Otamixaban	18.7 μM	ND*	ND*	Calu-3	Hit	Repurposed	[31]
75	Compound 7	14.33 ± 0.23 μM	11.77 ± 0.04 μM	110.90 μM	Vero E6	Experimental	Repurposed	[32]
76	Tafenoquine	31.8 μM	9.48 ± 0.48 μM	9.74 ± 1.31 μM	Vero E6	Hit	Repurposed	[32]
77	Compound 3	ND*	ND*	15.74 ± 3.84 μM	Vero E6	Hit	TFQ derivative	[32]
78	Compound 8	ND*	ND*	5.36 ± 0.61 μM	Vero E6	Hit	TFQ derivative	[32]
79	Compound 13	ND*	ND*	4.70 ± 0.65 μM	Vero E6	Hit	TFQ derivative	[32]
80	Compound 14	ND*	ND*	13.37 ± 1.70 μM	Vero E6	Hit	TFQ derivative	[32]

Table S3. Pharmacological and physicochemical profiles of inhibitors targeting SARS-CoV-2 Cathepsin L.

No.	**Name[1]**	**IC_{50} (catsL)**	**IC_{50} (Mpro)**	**IC_{50} (PLpro)**	**EC_{50}**	**CC_{50}**	**Type of Assay**	**Approval status**	**Design strategy**	**Reference**
1	MPI1	0.079 ± 0.029 nM	100 ± 23 nM	ND*	ND*	ND*	Inhibition assay	Hit	Peptidomimetic	[33]
2	MPI2	0.19 ± 0.03 nM	103 ± 14 nM	ND*	ND*	ND*	Inhibition assay	Hit	Peptidomimetic	[33]
3	MPI3	0.30 ± 0.07 nM	8.5 ± 1.5 nM	ND*	ND*	ND*	Inhibition assay	Hit	Peptidomimetic	[33]

4	MPI4	0.33 ± 0.04 nM	15 ± 5 nM	ND*	ND*	ND*	Inhibition assay	Hit	Peptidomimetic	[33]
5	MPI5	2.3 ± 1.9 nM	33 ± 2 nM	ND*	ND*	ND*	Inhibition assay	Hit	Peptidomimetic	[33]
6	MPI6	0.45 ± 0.08 nM	60 ± 4 nM	ND*	ND*	ND*	Inhibition assay	Hit	Peptidomimetic	[33]
7	MPI7	0.61 ± 0.15 nM	47 ± 3 nM	ND*	ND*	ND*	Inhibition assay	Hit	Peptidomimetic	[33]
8	MPI8	1.2 ± 1.0 nM	105 ± 22 nM	ND*	ND*	ND*	Inhibition assay	Experimental	Peptidomimetic	[33]
9	MPI9	0.56 ± 0.06 nM	56 ± 14 nM	ND*	ND*	ND*	Inhibition assay	Hit	Peptidomimetic	[33]
10	11a	0.14 ± 0.04 nM	31 ± 3 nM	ND*	ND*	ND*	Inhibition assay	Hit	Peptidomimetic	[33]
11	GC376	0.23 ± 0.05 nM	31 ± 4 nM	ND*	ND*	ND*	Inhibition assay	Hit	Peptidomimetic	[33]
12	Disulfiram	2.2 ± 1.4	1.5 ± 0.1 µM	3.8 ± 0.1 µM	0.5 ± 0.2 µM	0.9 ± 0.3 µM	Cell-based assay and enzymatic assay	Hit	Repurposed	[34]
13	RI173	1.7 ± 0.6	0.6 ± 0.1 µM	0.2 ± 0.1 µM	0.1 ± 0.00 µM	0.3 ± 0.1 µM	Cell-based assay and enzymatic assay	Experimental	Thiuram disulfide derivatives	[34]
14	RI175	1.9 ± 0.6	0.3 ± 0.1 µM	0.6 ± 0.1 µM	>60 µM	>60 µM	Cell-based assay and enzymatic assay	Hit	Thiuram disulfide derivatives	[34]
15	RI172	0.2 ± 0.0	0.6 ± 0.1 µM	0.7 ± 0.0 µM	<0.08 µM	<0.08 µM	Cell-based assay and enzymatic assay	Hit	Thiuram disulfide derivatives	[34]
16	RI174	16.9 ± 6.9	2.0 ± 0.3 µM	0.6 ± 0.0 µM	<0.08 µM	<0.08 µM	Cell-based assay and enzymatic assay	Hit	Thiuram disulfide derivatives	[34]
17	RI171	4.5 ± 0.7	3.2 ± 0.1 µM	1.9 ± 0.1 µM	1.9 ± 0.2 µM	1.7 ± 0.4 µM	Cell-based assay and enzymatic assay	Hit	Thiuram disulfide derivatives	[34]
18	RI177	>50	3.8 ± 0.6 µM	>50 µM	>60 µM	>60 µM	Cell-based assay and enzymatic assay	Hit	Thiuram disulfide derivatives	[34]
19	RI176	>50	>50 µM	>50 µM	ND*	ND*	Cell-based assay and enzymatic assay	Hit	Thiuram disulfide derivatives	[34]
20	Calpain inhibitor II	0.41 ± 0.16 nM	970 ± 268 nM	ND*	ND*	ND*	FRET-Based enzymatic assay	Experimental	analogs of GC-376	[35]
21	Calpain inhibitor I	ND*	8.60 ± 1.46 µM	ND*	ND*	ND*	FRET-Based enzymatic assay	Hit	analogs of GC-377	[35]
22	Calpain inhibitor XII	1.62 ± 0.33 nM	453 ± 71 nM	ND*	ND*	ND*	FRET-Based enzymatic assay	Experimental	analogs of GC-378	[35]
23	UAWJ257	ND*	64.5 ± 15.4 µM	ND*	ND*	ND*	FRET-Based enzymatic assay	Hit	analogs of GC-379	[35]
24	E-64d	ND*	ND*	ND*	0.27 µM	ND*	Vero E6	Experimental	ND*	[36]
25	Z-FY-CHO	5 µM	ND*	ND*	0.62 µM	ND*	Vero E6	Experimental	ND*	[36]
26	MOL-28170	ND*	ND*	ND*	1.56 µM	ND*	Vero E6	Experimental	ND*	[36]
27	Cathepsin inhibitor 1	ND*	ND*	ND*	0.14 µM	ND*	Vero E6	Experimental	ND*	[36]
28	Oxocarbate	ND*	ND*	ND*	10.89 µM	ND*	Vero E6	hit	ND*	[36]
29	SM141	60 ± 1 nM	900 ± 100 nM	ND*	8.2 ± 0.9 nM	ND*	A549-hACE2	Experimental	Peptidomimetic	[37]

30	SM142	145 ± 14 nM	1800 ± 100 nM	ND*	14.7 ± 2.2 nM	ND*	A549-hACE2	Experimental	Peptidomimetic	[37]
31	Obatoclax	<1 μM	ND*	ND*	ND*	>100 μM	Cau-3, Caco-2 cells	Experimental	Repurposed	[38]
32	K777	ND*	ND*	ND*	74 nM	ND*	Vero E6	Experimental	Irreversible covalent inhibitor	[39]
		ND*	ND*	ND*	0.035 μM	ND*	Vero E6	Experimental	Irreversible covalent inhibitor	[36]

Table S4. Pharmacological and physicochemical profiles of inhibitors targeting SARS-CoV-2 Mpro.

Name	**IC_{50} (nM)**	**K_i (nM)**	**Type of Mpro Assay**	**EC_{50} μM**	**Type of Viral assay**	**CC_{50}**	**Metabolic profiling (CL_{int}) (μl/min/mg)**	**Metabolite ID**	**Log D**	**Approval status**	**Design strategy**	**References**
Ebselen	9.35 ± 0.18 μM	ND*	Enzymatic Assay	4.67 μM	Vero E6	ND*	ND*	ND*	ND*	Experimental	Repurposed	[40]
Ebselen	0.67 ±0.09 μM	ND*	Enzymatic Assay	4.67 μM	ND*	ND*	ND*	ND*	ND*	Experimental	Repurposed	[40]
Disulfiram	1.55 ± 0.30 μM	ND*	Enzymatic Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[40]
Tideglusib	1.82 ± 0.06 μM	ND*	Enzymatic Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[40]
Carmofur	15.75 ± 8.22 μM	ND*	Enzymatic Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[40]
Shikonin	21.39 ± 7.06 μM	ND*	Enzymatic Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[40]
PX-12	ND*	ND*	Enzymatic Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Irreversible inhibitor	[40]
Atovaquone	ND*	ND*	Cell based and enzymatic assay	1.20 μM	Vero E6	>100	ND*	ND*	ND*	Hit	Repurposed	[41]
Mebendazole	19.94 μM	ND*	Cell based and enzymatic assay	1.30 μM	Vero E6	>100	ND*	ND*	ND*	Experimental	Repurposed	[41]
Dronedarone	18.03 μM	ND*	Cell based and enzymatic assay	1.50 μM	Vero E6	22.70	ND*	ND*	ND*	Experimental	Repurposed	[41]

Ouabain	ND*	ND*	Cell based and enzymatic assay	0.03 μM	Vero E6	>100	ND*	ND*	ND*	Hit	Repurposed	[41]
Digoxin	ND*	ND*	Cell based and enzymatic assay	0.07 μM	Vero E6	>100	ND*	ND*	ND*	Hit	Repurposed	[41]
Entacapone	9.04 μM	ND*	Cell based and enzymatic assay	ND*	Vero E6	>100	ND*	ND*	ND*	Experimental	Repurposed	[41]
Nirmatrelvir, 1	ND*	3.11 nM	FRET assay	81.4 nM	Vero E6	ND*	25	CYP3A4	1.9	FDA approved	Retention of peptidomimetic chemotype	[42]
Nirmatrelvir	28.1 nM	ND*	Enzymatic Fluorescence Assay	148 nM	HeLa-ACE2	>40 μM	32.8	CYP3A4	1.5	FDA approved	Retention of peptidomimetic chemotype	[43]
Nirmatrelvir	2.57 nM	ND*	Biochemical assay	pIC50 = 8.59	CPE – Reduction	pEC50 = 7.00	ND*	CYP3A4	ND*	FDA approved	Retention of peptidomimetic chemotype	[44]
Nirmatrelvir	ND*	0.003 ± 0.0004 μM	Enzymatic assay	<0.01 μM	Huh-7-ACE2	>100 μM	ND*	ND*	ND*	FDA approved	Retention of peptidomimetic chemotype	[45]
2	ND*	5.49 nM	FRET assay	2740 nM	Vero E6	ND*	24.3	ND*	0.8	Hit	Retention of peptidomimetic chemotype	[42]
3	ND*	1.12 nM	FRET assay	118 nM	Vero E6	ND*	8.1	ND*	1.2	Hit	Retention of peptidomimetic chemotype	[42]
4	ND*	0.71 nM	FRET assay	80.9 nM	Vero E6	ND*	9.42	ND*	1.7	Hit	Retention of peptidomimetic chemotype	[42]
5	ND*	0.63 nM	FRET assay	141 nM	Vero E6	ND*	7.12	ND*	1.0	Hit	Retention of peptidomimetic chemotype	[42]

6	ND*	2.83 nM	FRET assay	193 nM	Vero E6	ND*	7.12	ND*	1.2	Hit	Retention of peptidomimetic chemotype	[42]
7	ND*	3.88 nM	FRET assay	450 nM	Vero E6	ND*	7.12	ND*	0.6	Hit	Retention of peptidomimetic chemotype	[42]
8	ND*	4.46 nM	FRET assay	65.5 nM	Vero E6	ND*	13.0	ND*	1.4	Hit	Retention of peptidomimetic chemotype	[42]
PF-07817883, 9	18 nM	2.48 nM	FRET assay	180 nM	Vero E6	ND*	4.7	CYP3A4/5	0.9	Phase II	Retention of peptidomimetic chemotype	[42]
PF-07817883, Ibuzatrelvir	19	5 nM	FRET assay	ND*	ND*	ND*	4.7	ND*	ND*	Phase II	Retention of peptidomimetic chemotype	[46]
10	ND*	0.17 nM	FRET assay	46.2	Vero E6	ND*	9.5	ND*	1.2	Hit	Retention of peptidomimetic chemotype	[42]
11	ND*	13.27 nM	FRET assay	488	Vero E6	ND*	7.12	ND*	0.9	Hit	Retention of peptidomimetic chemotype	[42]
12	ND*	1.13 nM	FRET assay	78.9	Vero E6	ND*	7.12	ND*	0.7	Hit	Retention of peptidomimetic chemotype	[42]
1	0.74 μM	ND*	Enzymatic Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
5	20 μM	ND*	Enzymatic Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]

8	20 μM	ND*	Enzymatic Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
13	0.6 μM	ND*	Enzymatic Fluorescence Assay	2.60 μM	Vero	12.1 μM	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
14	0.95 μM	ND*	Enzymatic Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
15	3.2 μM	ND*	Enzymatic Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
16	3.6 μM	ND*	Enzymatic Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
17	3.6 μM	ND*	Enzymatic Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
18	3.6 μM	ND*	Enzymatic Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
19	2.2 μM	ND*	Enzymatic Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
22	1.61 μM	ND*	Enzymatic Fluoresce	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design	[47]

			nce Assay								Targeting Cys44 in the S2 Pocket	
24	2.4 μM	ND*	Enzymatic Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
25	6.6 μM	ND*	Enzymatic Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
26	0.49 μM	ND*	Enzymatic Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
30	0.76 μM	ND*	Enzymatic Fluorescence Assay	4.88 μM	Vero	> 300 µM	ND*	ND*	ND*	Experimental	Inhibitor Design Targeting Cys44 in the S2 Pocket	[47]
PF-00835231	101 nM	ND*	Enzymatic Florescence Assay	630 nM	HeLa-ACE2	ND*	13.9	ND*	1.2	Lead	hydroxymethyl ketone warhead	[43]
CMX990	23.4 nM	ND*	Enzymatic Florescence Assay	9.6 nM	HeLa-ACE2	>40 µM	7.5	No CYP450	2.3	Phase I	trifluoromethoxymethyl ketone warhead	[43]
1	ND*	ND*	Enzymatic Florescence Assay	72 nM	HeLa-ACE2	ND*	147.7	ND*	4.4	Hit	Interconversion of warheads	[43]
2	14.8 nM	ND*	Enzymatic Florescence Assay	54 nM	HeLa-ACE2	ND*	1109.4	ND*	3.3	Hit	Interconversion of warheads	[43]
3	76.3 nM	ND*	Enzymatic Florescence Assay	17 nM	HeLa-ACE2	ND*	29.6	ND*	2.8	Hit	Interconversion of warheads	[43]
4	16.1 nM	ND*	Enzymatic Florescence Assay	23 nM	HeLa-ACE2	ND*	53.7	ND*	2.4	Hit	Interconversion of warheads	[43]

5	81.1 nM	ND*	Enzymatic Florescence Assay	145 nM	HeLa-ACE2	ND*	45.3	ND*	1.6	Hit	Interconversion of warheads	[43]
6	28.8 nM	ND*	Enzymatic Florescence Assay	99 nM	HeLa-ACE2	ND*	34.2	ND*	2.0	Hit	Interconversion of warheads	[43]
7	24.0 nM	ND*	Enzymatic Florescence Assay	117 nM	HeLa-ACE2	ND*	62.2	ND*	2.6	Hit	Interconversion of warheads	[43]
8	34.7 nM	ND*	Enzymatic Florescence Assay	61 nM	HeLa-ACE2	ND*	26.2	ND*	3.0	Hit	Interconversion of warheads	[43]
9	36.5 nM	ND*	Enzymatic Florescence Assay	108 nM	HeLa-ACE2	ND*	16.3	ND*	2.0	Hit	Interconversion of warheads	[43]
10	35.4 nM	ND*	Enzymatic Florescence Assay	346 nM	HeLa-ACE2	ND*	12.8	ND*	1.3	Hit	Interconversion of warheads	[43]
11	34.5 nM	ND*	Enzymatic Florescence Assay	62 nM	HeLa-ACE2	ND*	8.4	ND*	2.0	Hit	Interconversion of warheads	[43]
12	33.7 nM	ND*	Enzymatic Florescence Assay	24 nM	HeLa-ACE2	ND*	17.4	ND*	1.0	Hit	Interconversion of warheads	[43]
13	34.8 nM	ND*	Enzymatic Florescence Assay	14 nM	HeLa-ACE2	ND*	19.2	ND*	3.6	Hit	Interconversion of warheads	[43]
14	60.1 nM	ND*	Enzymatic Florescence Assay	138 nM	HeLa-ACE2	ND*	12.2	ND*	2.0	Hit	Interconversion of warheads	[43]
15	160 nM	ND*	Enzymatic Florescence Assay	245 nM	HeLa-ACE2	ND*	13.0	ND*	0.3	Hit	Interconversion of warheads	[43]
16	22.0 nM	ND*	Enzymatic Florescence Assay	50 nM	HeLa-ACE2	ND*	14.9	ND*	2.6	Hit	Interconversion of warheads	[43]
1	2,45 E-09	ND*	SARS-CoV-2 Mpro biochemical assay	pEC50 = 6.89	Vero E6	ND*	185.8	ND*	1.65	Lead	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
2	4,27 E-06	ND*	SARS-CoV-2 Mpro biochemical assay	pEC50 = 4.66	Vero E6	ND*	ND*	ND*	ND*	Hit	Peptidomimetic with tetrafluorophe	[43]

											noxymethyl ketone warhead	
3	1,15 E-08	ND*	SARS-CoV-2 Mpro biochemical assay	pEC 50 = 7.15	Vero E6	ND*	206.3	ND*	2.23	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
4	3,80 E-06	ND*	SARS-CoV-2 Mpro biochemical assay	pEC 50 = 5.65	Vero E6	ND*	9.31	ND*	>3.5	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
5	4,17 E-08	ND*	SARS-CoV-2 Mpro biochemical assay	pEC 50 = 5.93	Vero E6	ND*	181.7	ND*	1.50	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
6	6,03 E-09	ND*	SARS-CoV-2 Mpro biochemical assay	pEC 50 = 5.72	Vero E6	ND*	155.5	ND*	3.08	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
7	2,75 E-09	ND*	SARS-CoV-2 Mpro biochemical assay	pEC 50 = 7.30	Vero E6	ND*	121.2	ND*	2.82	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
8	5,62 E-09	ND*	SARS-CoV-2 Mpro biochemical assay	pEC 50 = 6.80	Vero E6	ND*	64.5	ND*	3.26	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
9	5,50 E-09	ND*	SARS-CoV-2 Mpro biochemical assay	pEC 50 = 5.92	Vero E6	ND*	133.6	ND*	2.60	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]

10	7,08 E-09	ND*	SARS-CoV-2 Mpro biochemical assay	pEC50 = 6.92	Vero E6	ND*	47.6	ND*	3.15	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
11	6,76 E-09	ND*	SARS-CoV-2 Mpro biochemical assay	pEC50 = 6.12	Vero E6	ND*	124.3	ND*	2.03	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
12	1,78 E-07	ND*	SARS-CoV-2 Mpro biochemical assay	pEC50 = 6.19	Vero E6	ND*	76.8	ND*	2.88	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
13	2,95 E-07	ND*	SARS-CoV-2 Mpro biochemical assay	pEC50 = 5.78	Vero E6	ND*	78.8	ND*	2.70	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
14	3,63 E-09	ND*	SARS-CoV-2 Mpro biochemical assay	pEC50 = 7.40	Vero E6	ND*	112.1	ND*	2.52	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
15	5,89 E-09	ND*	SARS-CoV-2 Mpro biochemical assay	pEC50 = 7.40	Vero E6	ND*	240.3	ND*	2.99	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
16	6,76 E-09	ND*	SARS-CoV-2 Mpro biochemical assay	pEC50 = 7.40	Vero E6	ND*	153.7	ND*	2.95	Hit	Peptidomimetic with tetrafluorophenoxymethyl ketone warhead	[43]
1	4.1 μM	ND*	Mpro Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Algorithmic de novo design	[48]

2	16 μM	ND*	Mpro Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Algorithmic de novo design	[48]
3	58 μM	ND*	Mpro Fluorescence Assay	13 μM	Vero-E6 (Viral replication)	> 100 μM	ND*	ND*	ND*	Hit	Algorithmic de novo design	[48]
JOR-UNI-2fc98d0b-12	3.06 μM	ND*	Mpro Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Algorithmic de novo design	[48]
TRY-UNI-2eddb1ff-7	3.61 μM	ND*	Mpro Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Algorithmic de novo design	[48]
AGN-NEW-891393a6-1	6.68 μM	ND*	Mpro Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Algorithmic de novo design	[48]
TRY-UNI-7149760b-6	24.0 μM	ND*	Mpro Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	AI/FEP & Crowdsourcing	[49]
MAT-POS-b3e365b9-1	140 nM	ND*	Mpro Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	AI/FEP & Crowdsourcing	[49]
APL-POS-C59291d4-6	3.1 μM	ND*	Mpro Fluorescence Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	AI/FEP & Crowdsourcing	[49]
MAT-POS-f24609ef-1	ND*	ND*	Mpro Fluorescence Assay	0.102 μM	ND*	ND*	ND*	ND*	ND*	Hit	AI/FEP & Crowdsourcing	[49]
ADA-UCB-6c2cb422-1	720 nM	ND*	Mpro Fluorescence Assay	4.2 μM	Vero-E6	>50 μM	ND*	ND*	ND*	Hit	AI/FEP & Crowdsourcing	[49]
VLA-UCB-1dbca3b4-15	360 nM	ND*	Mpro Fluorescence Assay	ND*	ND*	>50 μM	ND*	ND*	ND*	Hit	AI/FEP & Crowdsourcing	[50]
PET-UNK-29afea89-2	80 nM	ND*	Mpro Fluorescence Assay	550 nM	Vero-E6	>50 μM	ND*	ND*	ND*	Hit	AI/FEP & Crowdsourcing	[50]
MAT-POS-3ccb8ef6-1	0.28 μM	ND*	Mpro Fluorescence Assay	1.9 μM	Vero-E6	>50 μM	ND*	ND*	ND*	Hit	AI/FEP & Crowdsourcing	[49]
MAT-POS-e194df51-1	0.14 μM	ND*	Mpro Fluorescence Assay	1,65 μM	Vero-E6	>50 μM	ND*	ND*	ND*	Hit	AI/FEP & Crowdsourcing	[49]
MAT-POS-e194df51-1	0.037 μM	ND*	Mpro Fluorescence Assay	0.064 μM	Vero-E6	>50 μM	152	Cyp450 2C9/2	2.5	Lead	AI/FEP & Crowd	[49]

								D6/3A4			sourcing	
112	21.3 nM	ND*	Mpro FRET-based enzymatic assay	ND*	ND*	ND*	1100	ND*	4.1	Hit-Lead	AI-generated Diazepane Scaffold	[51]
119	15.7 nM	ND*	Mpro FRET-based enzymatic assay	ND*	ND*	ND*	2011	ND*	4.0	Lead	AI-generated Diazepane Scaffold	[51]
121	51.2 nM	ND*	Mpro FRET-based enzymatic assay	ND*	ND*	ND*	451	ND*	3.9	Hit-Lead	AI-generated Diazepane Scaffold	[51]
123	74.4 nM	ND*	Mpro FRET-based enzymatic assay	ND*	ND*	ND*	633	ND*	4.2	Hit-Lead	AI-generated Diazepane Scaffold	[51]
2c	ND*	2.95 μM	Mpro FRET-based enzymatic assay	10.3 μM	Huh-7-ACE2	>100 µM	ND*	ND*	ND*	Hit	γ-lactam glutamine derivatives harbouring a methyl vinyl ketone	[52]
2f	ND*	1.61 μM	Mpro FRET-based enzymatic assay	ND*	Huh-7-ACE2	12.6 μM	ND*	ND*	ND*	Hit	γ-lactam glutamine derivatives harbouring a methyl vinyl ketone	[52]
3f	ND*	3.66 μM	Mpro FRET-based enzymatic assay	ND*	Huh-7-ACE2	22.6 μM	ND*	ND*	ND*	Hit	γ-lactam glutamine derivatives harbouring a methyl vinyl ketone	[52]
4b	ND*	5.58 μM	Mpro FRET-based enzymatic assay	7.63 µM	Huh-7-ACE2	> 100 μM	ND*	ND*	ND*	Hit	γ-lactam glutamine derivatives harbouring a methyl vinyl ketone	[52]

4d	ND*	5.54 μM	Mpro FRET-based enzymatic assay	3.50 µM	Huh-7-ACE2	> 100 μM	ND*	ND*	ND*	Hit	γ-lactam glutamine derivatives harbouring a methyl vinyl ketone	[52]
4e	ND*	10.72 μM	Mpro FRET-based enzymatic assay	ND*	Huh-7-ACE2	> 100 μM	ND*	ND*	ND*	Hit	γ-lactam glutamine derivatives harbouring a methyl vinyl ketone	[52]
4f	ND*	3.14 μM	Mpro FRET-based enzymatic assay	ND*	Huh-7-ACE2	46.9 μM	ND*	ND*	ND*	Hit	γ-lactam glutamine derivatives harbouring a methyl vinyl ketone	[52]
SPR39	ND*	1.5 ± 0.3 µM	Enzymatic assay	ND*	Huh-7-ACE2 cells	100 µM	ND*	ND*	ND*	Experimental	Peptide-based vinyl methyl ketones	[45]
SPR35	ND*	1.77 ± 0.16 µM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Peptide-based Michael acceptors	[45]
SPR36	ND*	33 ± 2% µM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Peptide-based Michael acceptors	[45]
SPR37	ND*	0.386 ± 0.055 µM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Peptide-based Michael acceptors	[45]
SPR38	ND*	0.260 ± 0.066	Enzymatic assay	18.5 ± 6.5 μM	Huh-7-ACE2	60.9 ± 11.5 µM	ND*	ND*	ND*	Hit	Peptide-based Michael acceptors	[45]
SPR39	ND*	0.252 ± 0.028 µM	Enzymatic assay	1.5 ± 0.3 μM	Huh-7-ACE3	100 µM	ND*	ND*	ND*	Hit	Peptide-based Michael acceptors	[45]
SPR40	ND*	0.416 ± 0.058 µM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Peptide-based Michael acceptors	[45]

SPR41	ND*	0.184 ± 0.025	Enzymatic assay	1.8 ± 0.1 μM	Huh-7-ACE2	14.5 ± 3.4 µM	ND*	ND*	ND*	Hit	Peptide-based Michael acceptors	[45]
SPR42	ND*	29 ± 4% µM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Peptide-based Michael acceptors	[45]
SPR43	ND*	50 ± 5% µM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Peptide-based Michael acceptors	[45]
SPR44	ND*	47 ± 2% µM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Peptide-based Michael acceptors	[45]
11a	ND*	0.008 ± 0.0009 µM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Peptide-based vinyl methyl ketones	[45]
1	0.021 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Novel dithiocarbamates	[53]
1A	35.000 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Novel dithiocarbamates	[53]
1B	0.178 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Novel dithiocarbamates	[53]
1C	0.023 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Novel dithiocarbamates	[53]
1D	>100 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Novel dithiocarbamates	[53]
1x	0.027 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Novel dithiocarbamates	[53]
1	21.4 µM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Acrylamide fragment	[54]
2	10 µM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	Acrylamide fragment	[53]
3	56.6 µM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Acrylamide fragment	[53]
4	20.2 µM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Acrylamide fragment	[53]
5	17 µM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	Acrylamide fragment	[53]

6	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Acrylamide fragment	[53]
7	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Acrylamide fragment	[53]
Schaftoside	1.73 ± 0.22 μM	ND*	Enzymatic assay	11.83 ± 3.23 μM	Vero E6	>200 μM	ND*	ND*	ND*	experimental	Plant based	[55]
vicenin-2	1.43 ± 0.20 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Plant based	[55]
licoisoflavanone	1.52 ± 0.14 μM	ND*	Enzymatic assay	20.26 ± 1.98 μM	Vero E6	84.45 ± 5.26 μM	ND*	ND*	ND*	Hit	Plant based	[55]
GC376	1.01 ± 0.41 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Control	Clinical candidate	[55]
GD-3	1.60 ± 0.2 μM	ND*	Enzymatic assay	183.0 ± 20.6 nM	Vero E6	>100 μM	ND*	ND*	ND*	Experimental	Nonpeptidic Piperazine Derivatives	[56]
GD-8	0.18 ± 0.01 μM	ND*	Enzymatic assay	2.64 ± 0.62 μM	Vero E6	12.5 ± 2.1 μM	ND*	ND*	ND*	Hit	Nonpeptidic Piperazine Derivatives	[56]
GD-12	0.31 ± 0.02 μM	ND*	Enzymatic assay	4.24 ± 0.72 μM	Vero E6	6.50 ± 1.65 μM	ND*	ND*	ND*	Hit	Nonpeptidic Piperazine Derivatives	[56]
GD-24	2.8 ± 0.1 μM	ND*	Enzymatic assay	1.37 ± 0.43 μM	Vero E6	11.9 ± 2.8 μM	ND*	ND*	ND*	Hit	Nonpeptidic Piperazine Derivatives	[56]
Pimozide	42 ± 2 μM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Ebastine	57 ± 12 μM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Rupintrivir	68 ± 7 μM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Bepridil	72 ± 3 μM	ND*	FRET-based assay	0.86 μM	Vero E6	ND*	ND*	ND*	ND*	Experimental	Repurposed	[57]
Sertaconazole	76 ± 2 μM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Rimonabant	85 ± 3 μM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Oxiconazole	99 ± 6 μM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Itraconazole	111 ± 35 μM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]

Tipranavir	180 ± 20 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Nelfinavir	234 ± 15 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Zopiclone	349 ± 77 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Trihexyphenidyl	370 ± 53 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Saquinavir	411 ± 6 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Isavuconazole	438 ± 11 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Lopinavir	486 ± 2 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Clemastine	497 ± 148 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Metixene	635 ± 43 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Duloxetine	3,047 ± 634 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[57]
Boceprevir	5.24 ± 0.20 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	FDA-approved	Compounds with electrophilic moieties	[30]
Narlaprevir	2.30 ± 0.38 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	In clinical trials	Compounds with electrophilic moieties	[30]
Telaprevir	14.15 ± 1.94 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	FDA-approved	Compounds with electrophilic moieties	[30]
Bardoxolone methyl	5.81 ± 0.79 µM	ND*	Enzymatic assay	0.29 µM	Vero	6.94 µM	Vero E6	ND*	ND*	Phase 2 (NCT04494646)	Compounds with electrophilic moieties	[30]
Bardoxolone	27.99 ± 2.34 µM	ND*	Enzymatic assay	0.43 µM	Vero	24.36 µM	Vero E6	ND*	ND*	Experimental	Compounds with electrophilic moieties	[30]
Tideglusib	1.91 ± 0.16 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	In clinical trials	Compounds with electrophilic moieties	[30]

Domatinostat tosylate	7.31 ± 0.86	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	In clinical trials	Compounds with electrophilic moieties	[30]
WP1066	16.61 ± 1.92	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Veterinary	Compounds with electrophilic moieties	[30]
Ceftiofur hydrochloride	29.55 ± 1.80	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Preclinical	Compounds with electrophilic moieties	[30]
Z-DEVD-FMK	0.31 ± 0.03	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Preclinical	Compounds with electrophilic moieties	[30]
MG132	1.64 ± 0.18	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Preclinical	Compounds with electrophilic moieties	[30]
Bay 11-7085	2.95 ± 0.10	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Preclinical	Compounds with electrophilic moieties	[30]
0600-5807	4.80 ± 0.12	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Preclinical	Compounds with electrophilic moieties	[30]
6H05	9.18 ± 0.52	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Preclinical	Compounds with electrophilic moieties	[30]
NSC129010	27.35 ± 1.71	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Preclinical	Compounds with electrophilic moieties	[30]
9a	1.66 ± 0.02 μM	ND*	Enzymatic assay	15.7 ± 8.3 μM	Vero E6	ND*	ND*	ND*	ND*	Experimental	α-ketoamides	[58]
9b	0.144 ± 0.02 μM	ND*	Enzymatic assay	>100 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	α-ketoamides	[58]
9c	0.10 ± 0.002 μM	ND*	Enzymatic assay	>100 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	α-ketoamides	[58]

9d	0.21 ± 0.02 μM	ND*	Enzymatic assay	>100 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	α-ketoamides	[58]
9e	2.63 ± 0.11 μM	ND*	Enzymatic assay	>100 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	α-ketoamides	[58]
9f	1.93 ± 0.16 μM	ND*	Enzymatic assay	>100 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	α-ketoamides	[58]
9g	1.71 ± 0.14 μM	ND*	Enzymatic assay	>100 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	α-ketoamides	[58]
9h	>30 μM	ND*	Enzymatic assay	>100 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	α-ketoamides	[58]
9i	0.026 ± 0.002 μM	ND*	Enzymatic assay	>100 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	α-ketoamides	[58]
9j	0.03 ± 0.003 μM	ND*	Enzymatic assay	>100 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	α-ketoamides	[58]
GC376	0.0005 ± 0.00003 μM	ND*	Enzymatic assay	4.32 ± 1.33 μM	Vero E6	ND*	ND*	ND*	ND*	Control	Control	[58]
AG7404	47 ± 1.05 μM	ND*	Biochemical assay	6.8 μM	A549-ACE2	250 μM	ND*	ND*	ND*	Experimental	orally bioavailable enterovirus	[59]
Rupintrivir	101 ± 1.40 μM	ND*	Biochemical assay	8.46 μM	A549-ACE2	>250 μM	ND*	ND*	ND*	Hit	orally bioavailable enterovirus	[59]
Remdesivir	ND*	ND*	Biochemical assay	0.145 μM	A549-ACE2	>250 μM	ND*	ND*	ND*	FDA-approved	orally bioavailable enterovirus	[59]
Compound 1	ND*	ND*	ND*	ND*	DENV 2proHeLa	>100	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 2	ND*	ND*	ND*	ND*	DENV 2proHeLa	>100	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 3	ND*	ND*	ND*	ND*	DENV 2proHeLa	>100 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 4	10.0 ± 0.5 μM	ND*	Enzymatic assay	ND*	DENV 2proHeLa	>100 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 5	37.2 ± 12.4 μM	ND*	Enzymatic assay	19.2 ± 5.3 μM	DENV 2proHeLa	>200 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 6	ND*	ND*	ND*	ND*	DENV 2proHeLa	>50 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]

Compound 7	ND*	ND*	ND*	ND*	DENV 2proHeLa	>200 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 8	13.9 ± 0.7 μM	ND*	Enzymatic assay	ND*	DENV 2proHeLa	>200 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 9	ND*	ND*	ND*	6.4 ± 1.8 μM	DENV 2proHeLa	>100 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 10	ND*	ND*	ND*	ND*	DENV 2proHeLa	>100 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 11	ND*	ND*	ND*	9.2 ± 2.0 μM	DENV 2proHeLa	>50 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 12	ND*	ND*	ND*	>50	DENV 2proHeLa	>50 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 13	ND*	ND*	ND*	22.5 ± 2.5 μM	DENV 2proHeLa	>200 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 14	ND*	ND*	ND*	4.0 ± 0.7	DENV 2proHeLa	>50 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 15	ND*	ND*	ND*	3.5 ± 0.4	DENV 2proHeLa	>50 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 16	ND*	ND*	ND*	6.4 ± 1.5	DENV 2proHeLa	>50 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 17	ND*	ND*	ND*	6.1 ± 1.7	DENV 2proHeLa	>50 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 18	6.1 ± 0.5 μM	ND*	Enzymatic assay	2.4 ± 0.1 μM	DENV 2proHeLa	55.2 ± 8.5 μM	ND*	ND*	ND*	Experimental	benzoxaborole based inhibitors	[60]
Compound 19	ND*	ND*	ND*	8.8 ± 1.6 μM	DENV 2proHeLa	>50 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 20	ND*	ND*	ND*	14.5 ± 3.1 μM	DENV 2proHeLa	>50 μM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 21	ND*	ND*	ND*	3.1 ± 0.8 μM	DENV 2proHeLa	>50 μM	ND*	ND*	ND*	Hit	benzoxaborole based	[60]

											inhibitors	
Compound 22	56.9 ± 6.2 µM	ND*	Enzymatic assay	5.2 ± 0.4 µM	DENV 2proHeLa	144.1 ± 5.0 µM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 23	52.3 ± 4.6 µM	ND*	Enzymatic assay	13.1 ± 2.2 µM	DENV 2proHeLa	>200 µM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 24	ND*	ND*	ND*	17.1 ± 4.7 µM	DENV 2proHeLa	>50 µM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 25	ND*	ND*	ND*	21.6 ± 5.0 µM	DENV 2proHeLa	>100 µM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Tavaborole	ND*	ND*	ND*	ND*	DENV 2proHeLa	>50 µM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 26	ND*	ND*	ND*	12.5 ± 1.9 µM	DENV 2proHeLa	>50 µM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
Compound 27	ND*	ND*	ND*	14.0 ± 2.9 µM	DENV 2proHeLa	>50 µM	ND*	ND*	ND*	Hit	benzoxaborole based inhibitors	[60]
MB-53	ND*	ND*	ND*	19.6 ± 1.8 µM	DENV 2proHeLa	>50 µM	ND*	ND*	ND*	Control	benzoxaborole based inhibitors	[60]
NK-189	ND*	ND*	ND*	0.6 ± 0.1 µM	DENV 2proHeLa	>50 µM	ND*	ND*	ND*	Control	benzoxaborole based inhibitors	[60]
boceprevir	17.2 ± 1.5 µM	ND*	Enzymatic assay	ND*	DENV 2proHeLa	>50 µM	ND*	ND*	ND*	Control	benzoxaborole based inhibitors	[60]
MAC-5576	1.7 ± 0.0 µM	ND*	Enzymatic assay	ND*	DENV 2proHeLa	>50 µM	ND*	ND*	ND*	Control	benzoxaborole based inhibitors	[60]
JMX0207	ND*	ND*	ND*	1.222 µM	A549-hACE2	13.17 µM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0281	ND*	ND*	ND*	2.078 µM	A549-hACE2	8.32 µM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0285	ND*	ND*	ND*	3.031 µM	A549-hACE2	6.13 µM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0286	4.8 µM	ND*	FRET-based enzymatic assay	2.251 µM	A549-hACE2	3.53.1 µM	ND*	ND*	ND*	Experimental	Niclosamide derivatives	[61]

JMX0308	ND*	ND*	ND*	0.8065 μM	A549-hACE2	1.80 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0310	ND*	ND*	ND*	2.414 μM	A549-hACE2	10.06 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0312	ND*	ND*	ND*	1.129 μM	A549-hACE2	1.97 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0317	ND*	ND*	ND*	4.025 μM	A549-hACE2	11.70 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0321	ND*	ND*	ND*	1.186 μM	A549-hACE2	3.76 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0325	ND*	ND*	ND*	0.1228 μM	A549-hACE2	1.81 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0330	ND*	ND*	ND*	0.4981 μM	A549-hACE2	10.15 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0510–2	ND*	ND*	ND*	4.88 μM	A549-hACE2	11.50 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0670	ND*	ND*	ND*	3.202 μM	A549-hACE2	9.17 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0671	ND*	ND*	ND*	1.563 μM	A549-hACE2	8.03 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0672	ND*	ND*	ND*	1.921 μM	A549-hACE2	8.34 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0673	ND*	ND*	FRET-based enzymatic assay	1.743 μM	A549-hACE2	5.20 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0674	ND*	ND*	ND*	9.752 μM	A549-hACE2	>10 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0679	ND*	ND*	ND*	2.514 μM	A549-hACE2	7.14 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0680	ND*	ND*	ND*	4.566 μM	A549-hACE2	10.10 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0681	ND*	ND*	ND*	9.753 μM	A549-hACE2	>10 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0682	ND*	ND*	ND*	1.568 μM	A549-hACE2	6.48 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0887	ND*	ND*	ND*	0.9203 μM	A549-hACE2	4.18 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]

JMX0895	ND*	ND*	ND*	0.665 μM	A549-hACE2	4.57 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0929	ND*	ND*	ND*	2.425 μM	A549-hACE2	5.06 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0936	ND*	ND*	ND*	2.214 μM	A549-hACE2	3.74 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0940	ND*	ND*	ND*	1.216 μM	A549-hACE2	7.72 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0941	3.9 μM	ND*	FRET-based enzymatic assay	1.7 μM	A549-hACE2	3.0 μM	ND*	ND*	ND*	Experimental	Niclosamide derivatives	[61]
JMX0942	ND*	ND*	ND*	2.891 μM	A549-hACE2	7.20 μM	ND*	ND*	ND*	Hit	Niclosamide derivatives	[61]
JMX0301	4.5 μM	ND*	FRET-based enzymatic assay	No dose response curve	A549-hACE2	342.4 μM	ND*	ND*	ND*	Experimental	Niclosamide derivatives	[61]
Boceprevir	4.9 μM	ND*	FRET-based enzymatic assay	15.6 μM	A549-hACE2	>200 μM	ND*	ND*	ND*	Control	Clinical trial	[61]
10a	3.889±0.051 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tripeptidomimetic inhibitors	[61]
10b	0.374±0.006 μM	ND*	Enzymatic assay	1.06 μM	VeroE6	>100	ND*	ND*	ND*	Experimental	Tripeptidomimetic inhibitors	[61]
10c	0.373±0.011 μM	ND*	Enzymatic assay	1.11 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tripeptidomimetic inhibitors	[61]
10d	0.277±0.008 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tripeptidomimetic inhibitors	[61]
10e	12.32±0.59 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tripeptidomimetic inhibitors	[61]
10f	6.928±0.340 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tripeptidomimetic inhibitors	[61]
10g	0.321±0.006 μM	ND*	Enzymatic assay	1.51 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tripeptidomimetic inhibitors	[61]
10h	3.436±0.034 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tripeptidomimetic inhibitors	[61]

10i	0.298±0.014 μM	ND*	Enzymatic assay	1.13 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tripeptidomimetic inhibitors	[61]
10j	2.044±0.120 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tripeptidomimetic inhibitors	[61]
10k	1.338±0.137 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tripeptidomimetic inhibitors	[61]
10l	3.275±0.033 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tripeptidomimetic inhibitors	[61]
Positive control	0.858±0.017 μM	ND*	Enzymatic assay	0.36 μM	VeroE6	>100	ND*	ND*	ND*	Control	Control	[61]
14a	0.543±0.008 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
14b	0.357±0.021 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
14c	0.281±0.033 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
14d	1.497±0.101 μM	ND*	Enzymatic assay	1.67 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17a	0.196±0.004 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17b	0.230±0.002 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17c	0.295±0.020 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17d	0.249±0.010 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17e	0.592±0.017 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17f	0.307±0.014 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]

17g	0.173±0.014 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17h	0.255±0.010 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17i	0.271±0.001 μM	ND*	Enzymatic assay	1.36 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17j	0.295±0.012 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17k	0.221±0.001 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17l	0.199±0.001 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17m	0.257±0.024 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17n	0.404±0.003 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17o	1.409±0.124 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17p	0.234±0.007 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17q	0.173±0.013 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17r	0.172±0.018 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17s	0.153±0.010 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17t	0.640±0.009 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17u	0.565±0.006 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic	[61]

											inhibitors	
17v	0.197±0.008 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17w	0.148±0.004 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17x	0.209±0.002 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17y	1.426±0.026 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
17z	0.285±0.006 μM	ND*	Enzymatic assay	>3.00 μM	VeroE6	>100	ND*	ND*	ND*	Hit	Tetrapeptidomimetic inhibitors	[61]
Positive control	0.858±0.017 μM	ND*	Enzymatic assay	0.36 μM	VeroE6	>100	ND*	ND*	ND*	Control	Control	[61]
SAA	2.49 ± 0.57 μM	ND*	Fluorescence-Based TSA	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[62]
EGCG	11.58 ± 1.62 μM	ND*	Fluorescence-Based TSA	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[62]
Oridonin	2.16 ± 0.22 μM	ND*	Fluorescence-Based TSA	4.95 μM	Vero E6	24.94 μM	ND*	ND*	ND*	Experimental	Repurposed	[62]
GC376	ND*	ND*	ND*	1.87 μM	Vero E6	ND*	ND*	ND*	ND*	Control	Repurposed	[62]
MPI3	8.5 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI4	15 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI5	33 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI6	60 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]

MPI7	47 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI8	105 nM	ND*	Enzymatic assay	0.030 µM	Vero E6	109.2 µM	ND*	ND*	ND*	Experimental	Aldehyde-based tripeptidyl inhibitors	[63]
MPI11	19 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI12	11 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI13	4.8 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI14	5.2 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI15	ND*	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI16	150 nM	ND*	Enzymatic assay	1.2 µM	Vero E6	>200 µM	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI17	60 nM	ND*	Enzymatic assay	1.2 µM	Vero E6	>200 µM	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI18	36 nM	ND*	Enzymatic assay	>5	Vero E6	>200 µM	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI19	13 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl	[63]

											inhibitors	
MPI20	16 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI21	77 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI22	49 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI23	350 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI24	8.4 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI25	650 nM	ND*	Enzymatic assay	2.2 μM	Vero E6	130.0 μM	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI26	530 nM	ND*	Enzymatic assay	1.9 μM	Vero E6	182.9 μM	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI27	160 nM	ND*	Enzymatic assay	>5 μM	Vero E6	114.0 μM	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
MPI28	52 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aldehyde-based tripeptidyl inhibitors	[63]
Nirmatrelvir	66 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Control	Aldehyde-based tripeptidyl inhibitors	[63]
GC376	30 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Control	Aldehyde-based	[63]

											tripeptidyl inhibitors	
Boceprevir	4200 ± 600 nM/800 ± 1500 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Refference	Nirmatelvir-based main protease inhibitors	[64]
MPI29	9.3 ± 0.8 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI30	40 ± 4 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI31	360 ± 50 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI32	620 ± 170 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI33	75 ± 9 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI34	370 ± 30 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI35	720 ± 80 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI36	102 ± 2 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease	[64]

											inhibitors	
MPI37	23 ± 1 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI38	17 ± 2 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI39	26 ± 1 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI40	180 ± 20 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI41	150 ± 20 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI42	22 ± 4 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
MPI43	45 ± 5 nM	ND*	Enzymatic assay	0.61 µM	Vero E6	34.2 µM	ND*	ND*	ND*	Experimental	Boceprevir-based main protease inhibitors	[64]
MPI44	59 ± 7 nM	ND*	Enzymatic assay	2.94 µM	Vero E6	143.7 µM	ND*	ND*	ND*	Experimental	Boceprevir-based main protease inhibitors	[64]
MPI46	120 ± 10 nM	ND*	Enzymatic assay	1.08 µM	Vero E6	163.4 µM	ND*	ND*	ND*	Experimental	Boceprevir-based main protease inhibitors	[64]

MPI47	720 ± 90 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir-based main protease inhibitors	[64]
PF-07321332	66 ± 12 nM	ND*	Enzymatic assay	1.3 µM	Vero E6	ND*	ND*	ND*	ND*	Control	Boceprevir-based main protease inhibitors	[64]
Leupeptin	127.2 µM	ND*	Enzymatic assay	42.34 µM	Vero	ND*		ND*	ND*	Hit	Plant-based	[65]
Tideglusib	0.30 ± 0.02 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogs of F8	[66]
F8	21.28 ± 0.89 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogs of F8	[66]
F8–S22	25.02 ± 1.11 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogs of F8	[66]
F8–S24	17.50 ± 1.65 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogs of F8	[66]
F8–S40	10.88 ± 0.16 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogs of F8	[66]
F8–S43	10.76 ± 0.48 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogs of F8	[66]
F8–S43	10.76 ± 0.48 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogs of F8–S43	[66]
F8–S43–S2	8.08 ± 0.38 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogs of F8–S43	[66]
F8–S43–S3	9.69 ± 0.45 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogs of F8–S43	[66]
F8-A1 (F8–S40)	10.88 ± 0.16 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8-A1 to F8-A9	[66]
F8-A2	17.53 ± 3.98 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8-A1 to F8-A9	[66]
F8-A2	17.53 ± 3.98 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B1	4.00 ± 0.25 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1	[66]

											to F8–B22	
F8–B2	5.39 ± 0.14 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B3	4.05 ± 0.26 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B4	8.14 ± 1.14 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B5	4.69 ± 0.34 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B6	1.57 ± 0.08 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	Analogues of F8–B1 to F8–B22	[66]
F8–B7	32.53 ± 2.33 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B8	40.59 ± 1.06 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B9	25.39 ± 2.05 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B10	10.0 ± 0.50 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B12	9.09 ± 1.05 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B13	4.14 ± 0.16 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B14	5.81 ± 0.07 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B16	7.09 ± 0.51 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B17	8.76 ± 0.75 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B20	10.40 ± 2	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of	[66]

	.20 µM										F8–B1 to F8–B22	
F8–B21	10.30 ± 0.70 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8–B22	1.55 ± 0.08 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of F8–B1 to F8–B22	[66]
F8-A2	17.53 ± 3.98 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	F8–C1 to F8–C4.	[66]
F8–C1	24.56 ± 0.70 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	F8–C1 to F8–C4.	[66]
F8–C2	5.78 ± 0.30 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	F8–C1 to F8–C4.	[66]
F8–C3	5.44 ± 0.16 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	F8–C1 to F8–C4.	[66]
X77(rac)	2.8 ± 0.6 µM	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Control	Reffernce	[67]
MLI(rac)	6.7 ± 1.3	ND*	Hydrolysis assay	14.1 ± 0.5 µM	ND*	ND*	ND*	ND*	ND*	Control	Reffernce	[67]
1	26 ± 5 %	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Enamine compounds	[67]
2	55 ± 2 %	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Enamine compounds	[67]
3	63 ± 3 %	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Enamine compounds	[67]
4	101 ± 1 %	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Enamine compounds	[67]
5	20 ± 1.4 µM	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Enamine compounds	[67]
6	44 ± 4 %	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Enamine compounds	[67]
7	54 ± 2 %	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Enamine compounds	[67]
8	61 ± 3 %	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Enamine compounds	[67]
9	67 ± 1 %	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Enamine compounds	[67]
10	18 µM	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	S1 optimization	[67]

11	7.5 μM	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	S1 optimization	[67]
12	1.3 μM	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	S1 optimization	[67]
16	0.46 μM	ND*	Hydrolysis assay	ND*	Vero E6	>20 μM	ND*	ND*	ND*	Hit	S1 optimization	[67]
16a	ND*	ND*	ND*	0.95 ± 0.10 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Derivative of compound 16	[67]
16b	ND*	ND*	ND*	16 ± 1 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Derivative of compound 17	[67]
13	79 μm	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	S2 optimization	[67]
14	8.3 μM	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	S2 optimization	[67]
15	6.9 μM	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	S2 optimization	[67]
17	0.33 μM	ND*	Hydrolysis assay	ND*	Vero E6	>20 μM	ND*	ND*	ND*	Hit	S2 optimization	[67]
17a	ND*	ND*	ND*	1.5 ± 0.1 μM	Huh7	ND*	ND*	ND*	ND*	Hit	Derivative of compound 17	[67]
17b	ND*	ND*	ND*	1.4 ± 0.1 μM	Huh7	ND*	ND*	ND*	ND*	Hit	Derivative of compound 18	[67]
21	2.1 μM	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Merge (8 +5)	[67]
18	0.39 μM	ND*	Hydrolysis assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Merge (8 +5)	[67]
19	0.077 μM	ND*	Hydrolysis assay	0.11 ± 0.03 μM	Vero E6	>20 μM	ND*	ND*	ND*	Experimental	Merge (8 +5)	[67]
GC376	ND*	ND*	ND*	4.4 ± 0.3 μM	Vero E6	ND*	ND*	ND*	ND*	Control	Clinical candidate	[67]
PF-07321332	ND*	ND*	ND*	0.08 ± 0.03 μM	Vero E6/Huh7	>100 μM	ND*	ND*	ND*	Control	FDA approved	[67]
Y180	8.1 nM	ND*	Enzyme kinetics assay	11.4 nM	VeroE6-TMPRSS2	>81 μM	ND*	ND*	ND*	Experimental	α-ketoamide-containing	[68]
F01	54 μM	ND*	Enzymatic assay	150 μM	Vero-81	>400 μM	ND*	ND*	ND*	Experimental	Fragment-based	[69]
2a	0.18 ± 0.03 μM	ND*	Biochemical assay	0.035 ± 0.001 μM	Vero E6	> 100 μM	ND*	ND*	ND*	Experimental	Aldehyde warhead	[70]
3a	0.17 ± 0.02 μM	ND*	Biochemical assay	0.032 ± 0.001 μM	Vero E6	> 100 μM	ND*	ND*	ND*	Experimental	Aldehyde warhead	[70]
2b	0.29 ±	ND*	Biochemical assay	ND*	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Aldehyde	[70]

	0.05 µM										warhead	
3b	0.29 ± 0.01 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2c	0.31 ± 0.06 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
3c	0.26 ± 0.05 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2d	0.28 ± 0.08 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	
3d	0.30 ± 0.03 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2e	0.26 ± 0.05 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
3e	0.28 ± 0.03 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2f	0.14 ± 0.02 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
3f	0.10 ± 0.01 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2g	1.90 ± 0.14 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
3g	1.71 ± 0.16 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2h	0.39 ± 0.02 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
3h	0.37 ± 0.03 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2i	0.27 ± 0.02 µM	ND*	Biochemical assay	ND*	Vero E6	21 ± 1 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
3i	0.30 ± 0.02 µM	ND*	Biochemical assay	ND*	Vero E6	21 ± 3 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2j	0.31 ± 0.03 µM	ND*	Biochemical assay	ND*	Vero E6	20 ± 3 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
3j	0.31 ± 0.06 µM	ND*	Biochemical assay	ND*	Vero E6	23 ± 1 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2k	0.18 ± 0.04 µM	ND*	Biochemical assay	ND*	Vero E6	> 100 µM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]

3k	0.15 ± 0.04 μM	ND*	Biochemical assay	ND*	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2l	0.29 ± 0.04 μM	ND*	Biochemical assay	ND*	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
3l	0.27 ± 0.04 μM	ND*	Biochemical assay	ND*	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2m	0.27 ± 0.02 μM	ND*	Biochemical assay	ND*	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
3m	0.25 ± 0.04 μM	ND*	Biochemical assay	ND*	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2n	0.82 ± 0.19 μM	ND*	Biochemical assay	ND*	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
3n	1.03 ± 0.24 μM	ND*	Biochemical assay	ND*	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
2o	0.74 ± 0.26 μM	ND*	Biochemical assay	ND*	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
3o	0.78 ± 0.18 μM	ND*	Biochemical assay	ND*	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Aldehyde warhead	[70]
MG132	3.91 ± 1.12 μM	ND*	Hydrolytic activity	ND*	Vero E6	ND*	ND*	ND*	ND*	Hit	Proteasome inhibitor	[71]
Z-VAD(Ome)-FMK	0.59 ± 0.44 μM	ND*	Hydrolytic activity	1.88 ± 0.52 μM	Vero E6	>300 μM	ND*	ND*	ND*	Experimental	Caspase inhibitors	[71]
Z-DEVD-FMK	2.8 ± 0.32 μM	ND*	Hydrolytic activity	0.87 ± 0.10 μM	Vero E6	>300 μM	ND*	ND*	ND*	Hit	Caspase inhibitors	[71]
Z-IETD-FMK	1.61 ± 0.05 μM	ND*	Hydrolytic activity	0.64 ± 0.08 μM	Vero E6	>300 μM	ND*	ND*	ND*	Hit	Caspase inhibitors	[71]
1	100–250 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
2	9.99 ± 2.50 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
3	6.38 ± 1.21 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
4	4.02 ± 1.36 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
5	0.14 ± 0.02 μM	ND*	FRET assay	2.5 ± 0.7 μM	MTT assay	22 ± 7.2 μM	ND*	ND*	ND*	Lead	Cyanophenyl analogues	[72]

6	0.47 ± 0.02 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
7	0.28 ± 0.05 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
8	0.51 ± 0.02 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
9	1 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
10	1.20 ± 0.03 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
11	0.120 ± 0.016 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
12	0.25 ± 0.09 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
13	0.19 ± 0.03 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
14	0.128 ± 0.015 μM	ND*	FRET assay	ND*	ND*	12.3 ± 7.0 μM	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
15	0.110 ± 0.013 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
16	0.100 ± 0.007 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
17	0.110 ± 0.035 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
18	0.024 ± 0.007 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
19	0.037 ± 0.007 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
20	0.036 ± 0.003 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
21	0.018 ± 0.002 μM	ND*	FRET assay	ND*	ND*	1.7 ± 0.9 μM		ND*	ND*	Hit	Cyanophenyl analogues	[72]
22	0.036 ± 0.004 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
23	0.020 ± 0.005 μM	ND*	FRET assay	ND*	ND*	1.15 ± 0.5 μM	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
24	0.037 ± 0	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl	[72]

	.004 μM										analogues	
25	0.025 ± 0.003 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
26	0.170 ± 0.022 μM	ND*	FRET assay	2.0 ± 0.7 μM	MTT assay	>100 μM	ND*	ND*	ND*	Experimental	Cyanophenyl analogues	[72]
27	0.120 ± 0.006 μM	ND*	FRET assay	1.1 ±0.5 μM	MTT assay	22 ± 8 μM	ND*	ND*	ND*	Hit	Cyanophenyl analogues	[72]
Remdesivir	ND*	ND*	ND*	1.1 ± 0.2 μM	MTT assay	72 ± 28 μM	ND*	ND*	ND*	Control	FDA approved	[72]
Perampanel	100–250 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Lead		[73]
2	9.99 ± 2.50 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Perampanel analogs	[73]
3	6.38 ± 1.21 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Perampanel analogs	[73]
4	4.02 ± 1.36 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Perampanel analogs	[73]
5	0.14 ± 0.02 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Perampanel analogs	[73]
6	0.47 ± 0.02 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Perampanel analogs	[73]
11	0.120 ± 0.016 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Perampanel analogs	[73]
14	0.128 ± 0.015 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Perampanel analogs	[73]
15	0.110 ± 0.013 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Perampanel analogs	[73]
16	0.100 ± 0.035 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Perampanel analogs	[73]
19	0.037 ± 0.007 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Perampanel analogs	[73]
21	0.018 ± 0.002 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Perampanel analogs	[73]
23	0.020 ± 0.00	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Perampanel analogs	[73]

	5 μM											
25	0.025 ± 0.003 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Peramp anel analogs	[73]
26	0.170 ± 0.022 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Peramp anel analogs	[73]
29	0.25 – 0.50 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Peramp anel analogs	[73]
31	0.037 ± 0.004 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Peramp anel analogs	[73]
50	0.25 – 0.50 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Peramp anel analogs	[73]
11a	53 ± 5 nM	ND*	FRET assay	0.53 ± 0.01 μM	Vero E6	>100 μM	ND*	ND*	ND*	Experimental	ND*	[74]
11b	40 ± 2 nM	ND*	FRET assay	0.72 ± 0.09 μM	Vero E6	>100 μM	ND*	ND*	ND*	Experimental	ND*	[74]
MI-01	453.0 ± 3.2 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-02	52.1 ± 1.4 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-03	16.5 ± 1.4 nM	ND*	FRET assay	2.23 ± 0.62 μM	Vero E6	>500 μM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-04	18.5 ± 0.5 nM	ND*	FRET assay	1.64 ± 0.88 μM	Vero E6	>500 μM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-05	13.2 ± 0.4 nM	ND*	FRET assay	5.57 ± 1.00 μM	Vero E6	>500 μM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-06	14.5 ± 0.4 nM	ND*	FRET assay	1.73 ± 1.01 μM	Vero E6	>500 μM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-07	43.3 ± 0.8 nM	ND*	FRET assay	16.95 ± 0.90 μM	Vero E6	>500 μM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-08	37.2 ± 0.7 nM	ND*	FRET assay	4.68 ± 0.83 μM	Vero E6	>500 μM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]

MI-09	15.2 ± 0.4 nM	ND*	FRET assay	0.86 ± 0.07 μM	Vero E6	>500 μM	22.67 ± 2.97 mL/min/kg	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-10	50.8 ± 0.5 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-11	13.3 ± 0.2 nM	ND*	FRET assay	1.18 ± 0.10 μM	Vero E6	>500 μM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-12	19.0 ± 0.6 nM	ND*	FRET assay	0.53 ± 0.07 μM	Vero E6	>500 μM	31.17 ± 4.65	ND*	ND*	Experimental	Boceprevir or telaprevir based	[75]
MI-13	12.4 ± 0.2 nM	ND*	FRET assay	2.08 ± 0.81 μM	Vero E6	>500 μM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-14	13.0 ± 0.3 nM	ND*	FRET assay	0.66 ± 0.06 μM	Vero E6	>500 μM	18.05 ± 2.57	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-15	748.5 ± 2.3 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-16	153.1 ± 1.0 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
11b	27.4 ± 0.5 nM	ND*	FRET assay	0.89 ± 0.04 μM	Vero E6	>500 μM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-17	298.8 ± 2.3 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-18	525.9 ± 8.3 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-19	195.6 ± 0.8 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-20	375.0 ± 1.0 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-21	7.6 ± 0.2 nM	ND*	FRET assay	2.97 ± 0.81 μM	Vero E6	>500 μM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-22	17.4 ± 0.4 nM	ND*	FRET assay	30.49 ± 1.24 μM	Vero E6	>500 μM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir	[75]

											vir based	
MI-23	7.6 ± 0.1 nM	ND*	FRET assay	5.63 ± 1.09 µM	Vero E6	>500 µM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-24	378.2 ± 2.3 nM	ND*	FRET assay	24.72 ± 17.17 µM	Vero E6	>500 µM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-25	36.2 ± 0.7 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-26	69.1 ± 1.6 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-27	93.5 ± 1.2 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-28	9.2 ± 0.2 nM	ND*	FRET assay	0.67 ± 0.06 µM	Vero E6	>500 µM	14.25 ± 0.54	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-29	34.7 ± 0.4 nM	ND*	FRET assay	1.65 ± 0.23 µM	Vero E6	>500 µM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-30	17.2 ± 0.6 nM	ND*	FRET assay	0.54 ± 0.13 µM	Vero E6	>500 µM	17.10 ± 1.12	ND*	ND*	Experimental	Boceprevir or telaprevir based	[75]
MI-31	30.0 ± 0.4 nM	ND*	FRET assay	0.83 ± 0.28 µM	Vero E6	>500 µM	8.94 ± 1.63	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
MI-32	19.7 ± 0.7 nM	ND*	FRET assay	1.50 ± 0.28 µM	Vero E6	>500 µM	ND*	ND*	ND*	Hit	Boceprevir or telaprevir based	[75]
GC376	37.4 ± 1.9 nM	ND*	FRET assay	1.46 ± 0.14 µM	Vero E6	>100 µM	ND*	ND*	ND*	Control		[75]
1(ML300)	4.99 ± 0.62 µm	ND*	FRET assay	19.90 ± 6.32 µM	Vero E6	ND*	ND*	ND*	ND*	Lead		[76]
7(17a)	31.8 ± 4.65 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
8(17b)	0.95 ± 0.06 µM	ND*	FRET assay	12.07 ± 0.31 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
9	18.87 ± 1.34 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]

10	0.44 ± 0.06 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
11	15.94 ± 1.01 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
12	1.61 ± 0.44 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
13	8.77 ± 0.20 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
14	2.09 ± 0.27 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
15	1.40 ± 0.21 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
16	5.07 ± 0.60 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
17	0.92 ± 0.21 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
18	20.39 ± 0.42 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
19	0.106 ± 0.025 µM	ND*	FRET assay	5.76 ± 1.96 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
20	9.55 ± 0.99 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
21	0.063 ± 0.014 µM	ND*	FRET assay	1.74 ± 0.19 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
35	0.746 ± 0.098 µM	ND*	FRET assay	8.77 ± 1.14 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
36	0.270 ± 0.067 µM	ND*	FRET assay	1.98 ± 0.24 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
37	0.328 ± 0.027 µM	ND*	FRET assay	2.93 ± 0.28 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
38	0.197 ±0.050 µM	ND*	FRET assay	2.30 ± 0.33 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
39	0.333 ± 0.09	ND*	FRET assay	3.81 ± 0.18 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]

	3 µM											
40	0.171 ±0.029 µM	ND*	FRET assay	1.91 ± 0.30 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
41	0.068 ± 0.023 µM	ND*	FRET assay	0.497 ± 0.009 µM	Vero E6	ND*	ND*	ND*	ND*	Experimental	ML300 derivatives	[76]
22	4.62 ± 0.44 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
23	2.51 ± 0.44 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
24	0.83 ± 0.03 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
25	1.16 ± 0.19 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
26	23.0 ± 1.38 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
27	1.59 ± 0.44 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
28	0.39 ± 0.11 µM	ND*	FRET assay	7.61 ± 1.43 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
29	8.53 ± 1.82 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
30	>200 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
31	0.119 ± 0.05 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
32	0.176 ± 0.025 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
33	0.312 ± 0.073 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
34	0.540 ± 0.070 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
42	1.27 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]
43	3.44 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	ML300 derivatives	[76]

Remdesivir	ND*	ND*	ND*	0.34 ± 0.01 μM	Vero E6	ND*	ND*	ND*	ND*	Control	FDA approved	[76]
GC376	0.11 ± 0.06 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Control		[77]
X77	4.1 ± 1.2 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Control		[77]
ML188	1.4 ± 0.4 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Control		[77]
6a	11.1 ± 1.5 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
13a	5.3 ± 0.8 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
14a	0.42 ± 0.11 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
16a	0.41 ± 0.13 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
18a	5.2 ± 1.2 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
20a	7.0 ± 0.2 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
22a	12.4 ± 5.2 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
23a	0.85 ± 0.42 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
13b	15.0 ± 9.3 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
13c	9.7 ± 3.8 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
13d	>30 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
16b	0.38 ± 0.09 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
16c	0.92 ± 0.24 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
14b	0.28 ± 0.10 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
14c	0.17 ± 0.07 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	X77 derivatives	[77]
14d	0.24 ± 0.15 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
14e	0.52 ± 0.16 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]

14f	0.22 ± 0.08 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
14g (R,S)	0.32 ± 0.10 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
14h (S,S)	6.0 ± 2.7 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
16e	0.84 ± 0.30 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
16f	0.98 ± 0.35 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
13e	5.0 ± 2.3 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
13p	45.1 ± 18.3 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	X77 derivatives	[77]
Disulfiram	6.1 ± 0.6a μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Control		[78]
Ebselen	1.7 ± 0.4a μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Control		[78]
Ibuprofen	>500 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Control		[78]
1	2.6 ± 0.39 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
2a	5.9 ± 2.2 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
2b	18.5 ± 3.1 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
2c	5.5 ± 0.7 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
2d	3.3 ± 0.5 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]no	[78]

											nane (bispidine) derivatives	
2e	4.8 ± 0.6 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
2f	1.45 ± 0.2 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
2g	4.99 ± 0.8 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
2h	1.4 ± 0.2 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
2i	13.0 ± 2.1 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
2j	0.75 ± 0.2 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
3a	17.9 ± 3.1 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
3e	46.6 ± 3.1 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine)	[78]

											derivatives	
3k	99.6 ± 10 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
4c	8.8 ± 2 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
4d	0.9 ± 0.2 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
4l	5.5 ± 1.2 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
4m	7.1 ± 1.4 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
4n	33.7 ± 5.2 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
4o	5.2 ± 1.1 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
4p	2.02 ± 0.41 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]

4q	0.83 ± 0.17 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
4r	2.2 ± 0.5 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
4s	16.3 ± 3.1 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
4t	13.6 ± 1.4 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	3,7-diazabicyclo[3.3.1]nonane (bispidine) derivatives	[78]
Leupeptin	92 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[79]
Telaprevir	18 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[79]
Narlaprevir	5.1 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[79]
Boceprevir	3.1 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[79]
AT7519	ND*	ND*	ND*	25.16 μM	Vero E6	>100 μM	ND*	ND*	ND*	ND*	Repurposed	[80]
Calpeptin	ND*	ND*	ND*	0.072 μM	Vero E6	>100 μM	ND*	ND*	ND*	ND*	Repurposed	[80]
HEAT	ND*	ND*	ND*	24.05 μM	Vero E6	55.42 μM	ND*	ND*	ND*	ND*	Repurposed	[80]
Ifenprodil	ND*	ND*	ND*	46.86 μM	Vero E6	>100 μM	ND*	ND*	ND*	ND*	Repurposed	[80]
Isofloxythepin	ND*	ND*	ND*	4.8 μM	Vero E6	17 μM	ND*	ND*	ND*	ND*	Repurposed	[80]
MUT056399	ND*	ND*	ND*	38.24 μM	Vero E6	>100 μM	ND*	ND*	ND*	ND*	Repurposed	[80]
Pelitinib	ND*	ND*	ND*	1.25 μM	Vero E6	13.96 μM	ND*	ND*	ND*	ND*	Repurposed	[80]
Quipazine meleate	ND*	ND*	ND*	31.64 μM	Vero E6	>100 μM	ND*	ND*	ND*	ND*	Repurposed	[80]
RS-102895	ND*	ND*	ND*	19.8 μM	Vero E6	54.98 μM	ND*	ND*	ND*	ND*	Repurposed	[80]
Tolperisone	ND*	ND*	ND*	19.17 μM	Vero E6	>100 μM	ND*	ND*	ND*	ND*	Repurposed	[80]

Triglycidyl isocyanurate	ND*	ND*	ND*	30.02 µM	Vero E6	>100 µM	ND*	ND*	ND*	ND*	Repurposed	[80]
GC376	13.8 µM	ND*	Enzymatic assay	74 ± 35 nM	Vero E6	ND*	ND*	ND*	ND*	Control		[80]
Entrectinib	10.6 µM	ND*	Enzymatic assay	198 ± 116 nM	Vero E6	ND*	ND*	ND*	ND*	Experimental	Repurposed	[80]
Simeprevir	2.46 ± 0.26 µM	High throuput screenion g	ND*	1.40 ± 0.09 µM	Vero E6	18.58 ± 0.70 µM	ND*	ND*	ND*	Hit	Repurposed	[80]
Cinacalcet	5.99 ± 1.32 µM	High throuput screenion g	ND*	2.93 ± 0.38 µM	Vero E6	21.23 ± 1.62 µM	ND*	ND*	ND*	Hit	Repurposed	[80]
Ethacridine	3.54 ± 0.66 µM	High throuput screenion g	ND*	0.08 ± 0.01 µM	Vero E6	>40 µM	ND*	ND*	ND*	Experimental	Repurposed	[80]
ABT-199 (veneotclax)	3.18 ± 0.55 µM	High throuput screenion g	ND*	1.18 ± 0.12 µM	Vero E6	20.56 ± 2.56 µM	ND*	ND*	ND*	Hit	Repurposed	[80]
Hydroxyprogesterone	2.47 ± 0.30 µM	High throuput screenion g	ND*	2.77 ± 0.49 µM	Vero E6	>40 µM	ND*	ND*	ND*	Hit	Repurposed	[80]
Butoconazole	5.07 ± 0.58 µM	High throuput screenion g	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[80]
Remdesivir	ND*	ND*	ND*	0.52 ± 0.09 µM	Vero E6	>40 µM	ND*	ND*	ND*	Control	FDA approved	[80]
CDD-1777	NI	2400 ± 230 nM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	DNA-encoded chemistry technology	[81]
CDD-1713	5.19 µM	24 ± 3 nM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	DNA-encoded chemistry technology	[81]
CDD-1976	2.50 µM	42 ± 5 nM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	DNA-encoded chemistry technology	[81]
PUG	4.62 ±	ND*	FRET assay	7.20 ±	Vero E6	>100 µm	ND*	ND*	ND*	Experimental	Repurposed	[82]

	0.27 µM			1.08 µM								
CHLA	9.09 ± 0.87 µM	ND*	FRET assay	9.76 ± 0.42 µM	Vero E6	>100 µM	ND*	ND*	ND*	Hit	Repurposed	[82]
GC376	0.47 ± 0.03 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Control	Repurposed	[83]
Bismuth Gluconate	0.96 ± 0.02 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[83]
CBS	0.93 ± 0.04 µM	ND*	FRET assay	177.3 ± 32 µM	Vero E6	>200 µM	ND*	ND*	ND*	Experimental	Repurposed	[83]
GC376	160 ± 34 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Control		[84]
Compound 4	151 ± 15 nM	ND*	Enzymatic assay	2.883 ± 0.227 µM	Vero E6	ND*	ND*	ND*	ND*	Experimental		[84]
MAC-5576	81 ± 12 nM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit		[84]
Ebselen	0.67 ± 0.09 µM	ND*	Enzymatic assay	4.67 ± 0.80 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	Repurposed	[40]
Disulfiram	9.35 ± 0.18 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[40]
Tideglusib	1.55 ± 0.30 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[40]
Carmofur	1.82 ± 0.06 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[40]
Shikonin	15.75 ± 8.22 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[40]
PX-12	21.39 ± 7.06 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[40]
N3		ND*	ND	16.77 ± 1.7 µM	Vero E6	ND*	ND*	ND*	ND*	Experimental	Repurposed	[40]
6a	0.82 ± 0.1 µM	ND*	FRET enzyme assay	ND	Vero E6	>100 µM	ND*	ND*	ND*	Hit	Broad-spectrum inhibitors	[85]
7a	0.65 ± 0.06 µM	ND*	FRET enzyme assay	ND	Vero E6	>100 µM	ND*	ND*	ND*	Hit	Broad-spectrum inhibitors	[85]
6c	0.28 ± 0.05 µM	ND*	FRET enzyme assay	0.25 ± 0.15 µM	Vero E6	>100 µM	ND*	ND*	ND*	Hit	Broad-spectrum inhibitors	[85]

7c	0.23 ± 0.05 μM	ND*	FRET enzyme assay	ND	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Broad-spectrum inhibitors	[85]
6e	0.17 ± 0.06 μM	ND*	FRET enzyme assay	0.15 ± 0.14 μM	Vero E6	63.3 ± 2.3 μM	ND*	ND*	ND*	Experimental	Broad-spectrum inhibitors	[85]
7e	0.20 ± 0.06 μM	ND*	FRET enzyme assay	ND	Vero E6	59.1 ± 3.5 μM	ND*	ND*	ND*	Hit	Broad-spectrum inhibitors	[85]
6h	0.43 ± 0.1 μM	ND*	FRET enzyme assay	0.9 ± 0.8 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Broad-spectrum inhibitors	[85]
7h	0.41 ± 0.1 μM	ND*	FRET enzyme assay	ND	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Broad-spectrum inhibitors	[85]
6j	0.48 ± 0.08 μM	ND*	FRET enzyme assay	0.8 ± 0.7 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Broad-spectrum inhibitors	[85]
7j	0.45 ± 0.1 μM	ND*	FRET enzyme assay	ND	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Broad-spectrum inhibitors	[85]
GC376	0.62 ± 0.08 μM	ND*	FRET enzyme assay	ND	Vero E6	>100 μM	ND*	ND*	ND*	Control		[85]
13B-H (12)	>5 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit		[86]
13b-K (13)	0.12 ± 0.03 μM	ND*	ND*	1.3 μM	Vero E6	ND*	ND*	ND*	ND*	Experimental		[86]
YH-53	0.124 μM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	benzothiazolyl ketone warhead	[87]
GRL-1720	0.32 ± 0.02 μM	2.15 ± 0.49 μM	FRET-based assay	15 ± 4 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Indole based	[88]
Compound 5h	ND*	17.6 ± 3.2 nM	FRET-based assay	4.2 ± 0.7 μM	Vero E6	>100 μM	ND*	ND*	ND*	Experimental	Indole based	[88]
GC376	0.052 ± 0.007 μm	ND*	FRET assay	>50 μM	Vero E6	10 ± 4.2 μM	ND*	ND*	ND*	Hit	Repurposed	[89]
Calpain Inhibitor II	8.98 ± 2.0 μM	ND*	FRET assay	>100 μM	Vero E6	27 ± 1.4 μM	ND*	ND*	ND*	Hit	Repurposed	[89]
Calpain Inhibitor XII	6.48 ± 3.4 μM	ND*	FRET assay	>50 μM	Vero E6	1.3 ± 0.57 μM	ND*	ND*	ND*	Hit	Repurposed	[89]
Ebselen	>100 μM	ND*	FRET assay	8.23 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Repurposed	[89]
Disulfiram	>100 μM	ND*	FRET assay	8.35 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Repurposed	[89]

Shikonin	15.0 ± 3.0 μM	ND*	FRET assay	0.32 μM	Vero E6	>100 μM	ND*	ND*	ND*	Experimental	Repurposed	[89]
Remdesivir	ND*	ND*	ND*	≥50 μM	Vero E6	ND*	ND*	ND*	ND*	Control	FDA approved	[89]
GS-441524	ND*	ND*	ND*	ND*	Vero E6	<0.8 μM	ND*	ND*	ND*	Control		[89]
GC376	0.19 ± 0.04 μM	ND*	FRET assay	0.9 ± 0.2 μM	Vero E6	>200 μM	ND*	ND*	ND*	Experimental		[90]
GC373	0.40 ± 0.05 μM	ND*	FRET assay	1.5 μM	Vero E6	>200 μM	ND*	ND*	ND*	Hit		[90]
Ebselen	0.67 ± 0.033 μM	ND*	FRET assay	4.67 ± 0.024 μM	Vero E6	ND*	ND*	ND*	ND*	Control	Repurposed	[91]
MR6-7-2	0.363 ± 0.044 μM	ND*	FRET assay	4.50 ± 0.086 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Ebselen derivatives	[91]
MR6-17-2	0.70 ± 0.032 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Ebselen derivatives	[91]
MR6-18-4	0.345 ± 0.034 μM	ND*	FRET assay	3.74 ± 0.066 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Ebselen derivatives	[91]
MR6-26-2	0.467 ± 0.038 μM	ND*	FRET assay	3.17 ± 0.112 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Ebselen derivatives	[91]
MR6-31-2	0.824 ± 0.044 μM	ND*	FRET assay	1.78 ± 0.073 μM	Vero E6	ND*	ND*	ND*	ND*	Experimental	Ebselen derivatives	[91]
PF-00835231 (4)	0.27 ± 0.1 nM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	clinical candidate	Ketone-Based Covalent Inhibitors	[92]
Mastinib	2.5 μM	ND*	Enzymatic assay	3.2 μM	A549	>10 μM	ND*	ND*	ND*	Experimental	Repurposed	[93]
GRL-0496	3.8 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposed	[93]
FB2001	0.053 μM	ND*		0.39 ± 0.01 μM	Vero E6	274.4 μM	ND*	ND*	ND*	Experimental		[94]
Chloroquinine phosphate	ND*	ND*	ND*	4.17 ± 0.05 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit		[94]
PF-07304814					Vero E6					lead		[95]
PF-00835231	0.0069 μM	0.27 ± 0.1 μM		39.8 μM	Vero E6	>100 μM		P450	14 μL/min/mg	lead		[95]
PF-07321332	ND*	ND*	ND*	0.88 μM	TMPRSS2	>10 μM	ND*	ND*	ND*	Control	narlaprevir- and bocepr	[95]

											evir-derived hybrid inhibitors	
BBH-1	ND*	ND*	ND*	16.1 μM	HEK293-ACE2-TMPRSS2	>10 μM		ND*	ND*	Hit	narlaprevir- and boceprevir-derived hybrid inhibitors	[95]
BBH-2	ND*	ND*	ND*	15.4 μM	HEK293-ACE2-TMPRSS2	>10 μM		ND*	ND*	Hit	narlaprevir- and boceprevir-derived hybrid inhibitors	[95]
NBH-2	ND*	ND*	ND*	13.9 μM	HEK293-ACE2-TMPRSS2	>10 μM		ND*	ND*	Experimental	narlaprevir- and boceprevir-derived hybrid inhibitors	[95]
Compound 9	1.4 μM		Fluorescence 3CLpro Inhibition assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Deep learning-based screening	[96]
Compound 13	4.9 μM		Fluorescence 3CLpro Inhibition assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Deep learning-based screening	[96]
Compound 20	5.2 μM		Fluorescence 3CLpro Inhibition assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Deep learning-based screening	[96]
Compound 21	10.7 μM		Fluorescence 3CLpro Inhibition assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Deep learning-based screening	[96]
Compound 22	11.9 μM		Fluorescence 3CLpro Inhibition assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Deep learning-based screening	[96]
Compound 27	5.5 μM		Fluorescence 3CLpro Inhibition assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Deep learning-based screening	[96]
Tideglusib	0.3 ± 0.02 μM		Fluorescence 3CLpro Inhibition assay	ND*	ND*	ND*	ND*	ND*	ND*	Control		[96]

1	100–250a μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of Triarylpyridinone Inhibitors	[97]
2	0.140 ± 0.020 μM	ND*	Enzymatic assay	1.51 ± 0.01 μM	Vero E6	22 ± 7.2 μM	ND*	ND*	ND*	Hit	Optimization of Triarylpyridinone Inhibitors	[97]
3	0.170 ± 0.022 μM	ND*	Enzymatic assay	1.76 ± 0.31 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Optimization of Triarylpyridinone Inhibitors	[97]
4	0.120 ± 0.006 μM	ND*	Enzymatic assay	1.20 ± 0.20 μM	Vero E6	22 ± 8 μM	ND*	ND*	ND*	Hit	Optimization of Triarylpyridinone Inhibitors	[97]
5	0.120 ± 0.016 μM	ND*	Enzymatic assay	ND8	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of Triarylpyridinone Inhibitors	[97]
6	0.037 ± 0.004 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of Triarylpyridinone Inhibitors	[97]
7	0.025 ± 0.003 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of Triarylpyridinone Inhibitors	[97]
8	0.328 ± 0.061 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of Triarylpyridinone Inhibitors	[97]
9	0.083 ± 0.023 μM	ND*	Enzymatic assay	0.73 ± 0.26 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Optimization of Triarylpyridinone Inhibitors	[97]
10	0.085 ± 0	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of	[97]

	.005 μM										Triaryl pyridinone Inhibitors	
11	0.131 ± 0.009 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of Triaryl pyridinone Inhibitors	[97]
12	0.027 ± 0.004 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of Triaryl pyridinone Inhibitors	[97]
13	0.042 ± 0.015 μM	ND*	Enzymatic assay	>40 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Optimization of Triaryl pyridinone Inhibitors	[97]
14	0.105 ± 0.013 μM	ND*	Enzymatic assay	NAd	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Optimization of Triaryl pyridinone Inhibitors	[97]
15	0.038 ± 0.015 μM	ND*	Enzymatic assay	NAd	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Optimization of Triaryl pyridinone Inhibitors	[97]
16	0.061 ± 0.007 μM	ND*	Enzymatic assay	0.53 ± 0.23 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Optimization of Triaryl pyridinone Inhibitors	[97]
17	0.059 ± 0.014 μM	ND*	Enzymatic assay	0.82 ± 0.28 μM	Vero E6	82 μM	ND*	ND*	ND*	Hit	Optimization of Triaryl pyridinone Inhibitors	[97]
18	0.028 ± 0.007 μM	ND*	Enzymatic assay	3.2 ± 1.0 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Optimization of Triaryl pyridinone Inhibitors	[97]
19	0.044 ± 0.009 μM	ND*	Enzymatic assay	0.175 ± 0.005 μM	Vero E6	>80 μM	ND*	ND*	ND*	Experimental	Optimization of Triaryl pyridinone	[97]

											Inhibitors	
20	0.130 ± 0.018 μM	ND*	Enzymatic assay			>32.5 μM	ND*	ND*	ND*	Hit	Optimization of Triarylpyridinone Inhibitors	[97]
21	0.061 ± 0.011 μM	ND*	Enzymatic assay	1.08 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Optimization of Triarylpyridinone Inhibitors	[97]
Remdesivir	ND*	ND*	ND*	0.59 ± 0.25 μM	Vero E6	72 ± 28 μM	ND*	ND*	ND*	Control		[97]
ML 188 (1)	10.96 ± 1.58 Mm	ND*	Enzymatic assay	>20 μM	Vero E6	>125 μM	ND*	ND*	ND*	Hit	Rational design of non-covalent inhibitors	[98]
GC376	0.033 ± 0.003 μM	ND*	Enzymatic assay	1.51 ± 0.27 μM	Vero E6	>125 μM	ND*	ND*	ND*	Hit	Aldehyde prodrug	[98]
20	0.94 ± 0.33 μM	ND*	Enzymatic assay	1.73 ± 0.19 μM	Vero E6	>200 μM	ND*	ND*	ND*	Hit	Rational design of non-covalent inhibitors	[98]
23	0.66 ± 0.07 μM	ND*	Enzymatic assay	1.61 ± 0.26 μM	Vero E6	>200 μM	ND*	ND*	ND*	Hit	Rational design of non-covalent inhibitors	[98]
24	0.96 ± 0.09 μM	ND*	Enzymatic assay	13.06 ± 2.30 μM	Vero E6	129.38 ± 25.12 μM	ND*	ND*	ND*	Hit	Rational design of non-covalent inhibitors	[98]
37	0.67 ± 0.15 μM	ND*	Enzymatic assay	4.54 ± 0.69 μM	Vero E6	147.8 ± 13.9 μM	ND*	ND*	ND*	Hit	Rational design of non-covalent inhibitors	[98]
38	0.28 ± 0.07 μM	ND*	Enzymatic assay	0.82 ± 0.65 μM	Vero E6	>200 μM	ND*	ND*	ND*	Hit	Rational design of non-covalent inhibitors	[98]

40	1.05 ± 0.09 μM	ND*	Enzymatic assay	2.04 ± 1.08 μM	Vero E6	>200 μM	ND*	ND*	ND*	Hit	Rational design of non-covalent inhibitors	[98]
23R	0.20 ± 0.01 μM	ND*	Enzymatic assay	1.27 ± 0.09 μM	Vero E6	>100 μM	ND*	ND*	ND*	Experimental	Rational design of non-covalent inhibitors	[98]
23S	>20 μM	ND*	Enzymatic assay	ND*	Vero E6	ND*	ND*	ND*	ND*	Hit	Rational design of non-covalent inhibitors	[98]
E01	0.33 ± 0.03 Mm	ND*	FRET assay	>20 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl-1,2-benzoselenazol-3-one analogues	[99]
E02	2.78 ± 1.0 μM	ND*	FRET assay	16.7 ± 4.8	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl-1,2-benzoselenazol-3-one analogues	[99]
E03	>10 μM	ND*	FRET assay	>20 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl-1,2-benzoselenazol-3-one analogues	[99]
E04	0.90 ± 0.17 μM	ND*	FRET assay	11.2 ± 1.3 μM	Vero E6	ND*	ND*	ND*	3.19	Hit	2-Phenyl-1,2-benzoselenazol-3-one analogues	[99]
E05	>10 μM	ND*	FRET assay	12.2 ± 1.7 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl-1,2-benzoselenazol-3-one analogues	[99]
E06	1.00 ± 0.29 μM	ND*	FRET assay	>20 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl-1,2-benzoselenazol-3-one analogues	[99]
E07	0.61 ±	ND*	FRET assay	26.5 ± 1.2 μM	Vero E6	ND*	ND*	ND*	0.85	Hit	2-Phenyl-1,2-	[99]

	0.44 μM										benzos elenazo l-3-one analog ues	
E08	>10 μM	ND*	FRET assay	>20 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E09	>10 μM	ND*	FRET assay	11.2 ± 3.7 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E10	>10 μM	ND*	FRET assay	>20 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E11	2.09 ± 0.97 μM	ND*	FRET assay	>20 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E12	>10 μM	ND*	FRET assay	>20 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E13	>10 μM	ND*	FRET assay	>20 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E14	>10 μM	ND*	FRET assay	>20 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E15	6.40 ± 0.78 μM	ND*	FRET assay	11.2 ± 1.3 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E16	3.30 ± 0.74 μM	ND*	FRET assay	>20 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl -1,2-benzos elenazo l-3-one	[99]

											analog ues	
E17	1.80 ± 0.88 µM	ND*	FRET assay	>20 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E18	6.18 ± 1.74 µM	ND*	FRET assay	6.5 ± 2.0 µM	Vero E6	ND*	ND*	ND*	2.87	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E19	0.68 ± 0.28 µM	ND*	FRET assay	17.4 ± 3.5 µM	Vero E6	ND*	ND*	ND*	1.53	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E20	0.64 ± 0.10 µM	ND*	FRET assay	18.2 ± 3.6 µM	Vero E6	ND*	ND*	ND*	1.67	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E21	2.77 ± 0.67 µM	ND*	FRET assay	5.2 ± 1.8 µM	Vero E6	ND*	ND*	ND*	1.46	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E22	2.29 ± 0.95 µM	ND*	FRET assay	15.4 ± 1.5 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E23	7.43 ± 0.77 µM	ND*	FRET assay	20.7 ± 2.6 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E24	2.77 ± 0.51 µM	ND*	FRET assay	0.8 ± 0.3 µM	Vero E6	ND*	ND*	ND*	3.18	Experime ntal	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]
E25	0.38 ± 0.08 µM	ND*	FRET assay	2.0 ± 1.1 µM	Vero E6	ND*	ND*	ND*	1.45	Hit	2-Phenyl -1,2-benzos elenazo l-3-one analog ues	[99]

E26	>10 μM	ND*	FRET assay	15.1 ± 3.1 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl-1,2-benzoselenazol-3-one analogues	[99]
E27	1.25 ± 0.35 μM	ND*	FRET assay	1.7 ± 2.7 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl-1,2-benzoselenazol-3-one analogues	[99]
E28	5.56 ± 1.85 μM	ND*	FRET assay	17.3 ± 3.7 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl-1,2-benzoselenazol-3-one analogues	[99]
E29	2.69 ± 0.24 μM	ND*	FRET assay	>20 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl-1,2-benzoselenazol-3-one analogues	[99]
E30	>10 μM	ND*	FRET assay	>20 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	2-Phenyl-1,2-benzoselenazol-3-one analogues	[99]
Ebselen	ND*	ND*	ND*	>20 μM	Vero E6	ND*	ND*	ND*	0.92	Lead	Repurposed	[99]
Remdesivir	ND*	ND*	ND*	1.8 μM	Vero E6	ND*	ND*	ND*	ND*	Control	FDA approved	[99]
10	6.6 ± 2.7 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]
20e	9.0 ± 1.3 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]
20f	7.9 ± 1.4 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]
20g	5.2 ± 0.6 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]
20h	3.0 ± 0.4 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]
20i	9.7 ± 3.3 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]
25h	5.3 ± 3.3 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]

25k	2.8 ± 1.2 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]
25l	2.3 ± 1.2	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]
25m	4.1 ± 0.1 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]
28	0.7 ± 0.1 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]
31	0.6 ± 0.1 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]
32	0.5 ± 0.1 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Penecillin V derivatives	[100]
Disulfiram	1.04 ± 0.03 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Control	Repurposed	[101]
B1	8.54 ± 0.94 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B2	2.46 ± 0.14 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B3	9.82 ± 1.16 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B4	4.79 ± 0.22 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B5	10.26 ± 0.66 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B6	3.32 ± 0.25 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B7	1000 ± 0.47 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B8	11.23 ± 0.70 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene	

											derivatives	
B9	7.39 ± 0.11 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B10	5.25 ± 0.24 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B11	4.29 ± 0.62 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B12	2.72 ± 0.23 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B13	6.73 ± 1.29 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B14	2.78 ± 0.18 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B15	8.89 ± 3.34 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B16	6.65 ± 0.26 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B17	5.83 ± 0.34 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B18	3.66 ± 0.17 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B19	8.28 ± 1.88 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
B20	3.31 ± 0.36 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]

C1	1.55 ±0.21 μM	6.09 μM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	9,10-dihydrophenanthrene derivatives	[101]
C2	1.81 ± 0.17 μM	7.64 μM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
C3	10.23 ± 3.50 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
C4	5.39 ± 0.65 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
C5	4.71 ± 0.20 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
C6	10.68 ± 0.46 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
C7	5.50 ± 0.35 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	9,10-dihydrophenanthrene derivatives	[101]
Atovaquone	ND*	ND*	ND*	1.20 ± 0.84 μM	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Repurposed	[41]
Mebendazole	19.94 ± 1.06 μM	ND*	Enzymatic assay	1.30 ± 0.95 μM	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Repurposed	[41]
Dronedarone	18.03 ± 1.15 μM	ND*	Enzymatic assay	1.50 ± 0.86 μM	Vero E6	22.70 ± 0.91 μM	ND*	ND*	ND*	Hit	Repurposed	[41]
Ouabain	ND*	ND*	ND*	0.03 ± 0.89 μM	Vero E6	> 100 μM	ND*	ND*	ND*	Experimental	Repurposed	[41]
Digoxin	ND*	ND*	ND*	0.07 ± 0.91 μM	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Repurposed	[41]
Entacapone	9.04 ± 1.04 μM	ND*	Enzymatic assay	ND*	Vero E6	> 100 μM	ND*	ND*	ND*	Hit	Repurposed	[41]
1	ND*	ND*	ND*	16.8 μM	Vero E6	>133 μM	ND*	ND*	ND*	Hit	Targeting proteases and polymerase	[102]
2	0.18 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Targeting	[102]

											proteases and polymerase	
3	0.67 μM	ND*	Enzymatic assay	4-5 μM	Calu3	ND*	ND*	ND*	ND*	Hit	Targeting proteases and polymerase	[102]
4	1.34 μM	ND*	Enzymatic assay	>40 μM	Calu3	ND*	ND*	ND*	ND*	Hit	Targeting proteases and polymerase	[102]
5	53 nM	ND*	Enzymatic assay	0.52 μM	Vero E6	>100 μM	ND*	ND*	ND*	Experimental	Targeting proteases and polymerase	[102]
6	40 nM	ND*	Enzymatic assay	0.72 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Targeting proteases and polymerase	[102]
7 (GC376)	30 nM	ND*	Enzymatic assay	3.37 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Targeting proteases and polymerase	[102]
Boceprevir	4.13 μM	1.18 μM	Enzymatic assay	1.95 a μM	Vero E6	>100 μM	ND*	ND*	ND*	Lead	Clinical candidate	[102]
Baicalein	0.94 μM	ND*	Enzymatic assay	1.69 μM	Vero E6	>200 μM	ND*	ND*	ND*	Hit	Repurposed	[102]
Baicalin	6.41 μM	ND*	Enzymatic assay	10.27 μM	Vero E6	>200 μM	ND*	ND*	ND*	Hit	Repurposed	[102]
A1	194.8 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.34*	Hit	Pyrimidone derivatives	[103]
A2	20.9 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.48*	Hit	Pyrimidone derivatives	[103]
A3	37.0 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.63*	Hit	Pyrimidone derivatives	[103]
A4	18.8 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.78*	Hit	Pyrimidone derivatives	[103]
A5	226.8 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.93*	Hit	Pyrimidone derivatives	[103]
A6	38.3 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.36*	Hit	Pyrimidone derivatives	[103]
A7	60.8 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.19*	Hit	Pyrimidone derivatives	[103]
A8	185.6 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.76*	Hit	Pyrimidone derivatives	[103]

A9	287.1 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	5.09*	Hit	Pyrimidone derivatives	[103]
S-217622b	20.3 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.11*	Control	Clinical candidate	[103]
A10	24.7 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.78	Hit	Pyrimidone derivatives	[103]
A11	>1000 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.96	Hit	Pyrimidone derivatives	[103]
A12	>1000 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.63	Hit	Pyrimidone derivatives	[103]
A13	>1000 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.19	Hit	Pyrimidone derivatives	[103]
A14	>1000 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.31	Hit	Pyrimidone derivatives	[103]
A15	81.9 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.91	Hit	Pyrimidone derivatives	[103]
A16	>1000 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.35	Hit	Pyrimidone derivatives	[103]
A17	>1000 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.87	Hit	Pyrimidone derivatives	[103]
A18	>1000 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	0.70	Hit	Pyrimidone derivatives	[103]
A19	>1000 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	2.69	Hit	Pyrimidone derivatives	[103]
A20	15.7 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.74	Hit	Pyrimidone derivatives	[103]
A21	26.8 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.35	Hit	Pyrimidone derivatives	[103]
A22	555.6 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.21	Hit	Pyrimidone derivatives	[103]
A23	206.4 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.54	Hit	Pyrimidone derivatives	[103]
A24	14.1 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	5.88	Hit	Pyrimidone derivatives	[103]
A25	42.2 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	5.46	Hit	Pyrimidone derivatives	[103]

A26	24.3 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	5.04	Hit	Pyrimidone derivatives	[103]
A27	48.8 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.62	Hit	Pyrimidone derivatives	[103]
A28	26.5 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.13	Hit	Pyrimidone derivatives	[103]
A29	30.7 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.93	Hit	Pyrimidone derivatives	[103]
A30	33.3 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	5.14	Hit	Pyrimidone derivatives	[103]
A31	31.8 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.66	Hit	Pyrimidone derivatives	[103]
A32	105.4 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	7.34	Hit	Pyrimidone derivatives	[103]
A33	27.1 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	5.84	Experimental	Pyrimidone derivatives	[103]
A34	11.4 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	5.77	Hit	Pyrimidone derivatives	[103]
A35	55.6 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	5.35	Hit	Pyrimidone derivatives	[103]
A36	51.3 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.54	Hit	Pyrimidone derivatives	[103]
A37	29.2 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	5.50	Hit	Pyrimidone derivatives	[103]
A38	55.2 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	5.79	Hit	Pyrimidone derivatives	[103]
A39	51.9 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	5.37	Hit	Pyrimidone derivatives	[103]
A40	40.5 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.95	Hit	Pyrimidone derivatives	[103]
A41	27.4 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.62	Hit	Pyrimidone derivatives	[103]
A42	17.7 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	4.60	Hit	Pyrimidone derivatives	[103]
A43	29.6 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	3.55	Hit	Pyrimidone derivatives	[103]

WU-01	648 ± 68 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	DNA encoded library	[104]
WU-02	71 ± 4 nM	ND*	FRET-based assay	54 ± 10 nM	A549-hACE2	>20	ND*	ND*	ND*	Hit	DNA encoded library	[104]
WU-03	ND*	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	DNA encoded library	[104]
WU-04	72 ± 6 nM	ND*	FRET-based assay	12 ± 1 nM	A549-hACE2	>20	ND*	ND*	ND*	Experimental	DNA encoded library	[104]
WU-05	122 ± 16 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	DNA encoded library	[104]
WU-06	ND*	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of WU-04	[104]
WU-07	239 ± 16 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of WU-04	[104]
WU-08	467 ± 64 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of WU-04	[104]
WU-09	221 ± 35 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of WU-04	[104]
WU-10	135 ± 8 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of WU-04	[104]
WU-11	849 ± 161 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of WU-04	[104]
WU-12	6112 ± 2635 nM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Analogues of WU-04	[104]
PF-07321332	ND*	ND*	FRET-based assay	117 ± 9 nM	A549-hACE2	ND*	ND*	ND*	ND*	Control	FDA approved	[104]
2c	ND*	2.95 ± 0.29 μM	Enzymatic assay	10.3 ± 3.9 μM	Huh-7-ACE2	>100 μM	ND*	ND*	ND*	Hit	Dual inhibitors	[52]
2f	ND*	1.61 ± 0.21 μM	Enzymatic assay	ND*	Huh-7-ACE2	12.6 ± 7.7 μM	ND*	ND*	ND*	Hit	Dual inhibitors	[52]
3f	ND*	3.66 ± 0.23 μM	Enzymatic assay	ND*	Huh-7-ACE2	22.6 ± 2.3 μM	ND*	ND*	ND*	Hit	Dual inhibitors	[52]
4b	ND*	5.58 ± 0.32 μM	Enzymatic assay	7.63 ± 2.2 μM	Huh-7-ACE2	>100 μM	ND*	ND*	ND*	Hit	Dual inhibitors	[52]
4d	ND*	5.54 ± 0.31 μM	Enzymatic assay	3.50 ± 1.1 μM	Huh-7-ACE2	>100 μM	ND*	ND*	ND*	Experimental	Dual inhibitors	[52]
4e	ND*	10.72 ± 0.84 μM	Enzymatic assay	ND*	Huh-7-ACE2	>100 μM	ND*	ND*	ND*	Hit	Dual inhibitors	[52]
4f	ND*	3.14 ± 0.33 μM	Enzymatic assay	ND*	Huh-7-ACE2	46.9 ± 11.2 μM	ND*	ND*	ND*	Hit	Dual inhibitors	[52]
SPR3926	ND*	1.8 μM	Enzymatic assay	1.5 μM	Huh-7-ACE2	100 μM	ND*	ND*	ND*	Control	Dual inhibitors	[52]
Nirmatrelvir	ND*	0.003 μM	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	FDA-approved	Peptidomimetic	[52]

											derivative	
1 (Nirmatrelvir)	ND*	0.26 nM	FRET-based assay	2.0 μM	Vero E6	ND*	ND*	ND*	ND*	FDA-approved	Exploring P1 and P4 of Nirmatrelvir	[105]
5a	ND*	0.44 nM	FRET-based assay	4.0 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
5b	ND*	36.9 nM	FRET-based assay	17 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
5c	ND*	22.1 nM	FRET-based assay	2.3 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
5d	ND*	0.2 nM	FRET-based assay	1.6 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
5e	ND*	0.04 nM	FRET-based assay	0.26 μM	Vero E6	ND*	ND*	ND*	ND*	Experimental	Exploring P1 and P4 of Nirmatrelvir	[105]
5f	ND*	1.1 nM	FRET-based assay	0.27 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
5g	ND*	323 nM	FRET-based assay	100 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
5h	ND*	7.7 nM	FRET-based assay	30.7 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
5i	ND*	0.02 5 nM	FRET-based assay	0.29 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
5j	ND*	32.2 nM	FRET-based assay	29.7 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
5k	ND*	0.09 nM	FRET-based assay	0.03 5 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]

5l	ND*	0.49 nM	FRET-based assay	40.1 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
5m	ND*	3.3 nM	FRET-based assay	100 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
5n	ND*	0.094 nM	FRET-based assay	3.4 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
5o	nD*	7.8 nM	FRET-based assay	27.1 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	Exploring P1 and P4 of Nirmatrelvir	[105]
Compound 9	5.7 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based optimization of S2 binding	[51]
Compound 14	4.4 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based optimization of S2 binding	[51]
Compound 18	1.9 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based optimization of S2 binding	[51]
Compound 19	0.7 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based optimization of S2 binding	[51]
Compound 20	1.2 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based optimization of S2 binding	[51]
Compound 21	10 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based optimization of S2 binding	[51]
Compound 23	1.9 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based optimization of S2 binding	[51]
Compound 25	6.6 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-	[51]

											Based optimization of S2 binding	
Compound 26	1.5 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based optimization of S2 binding	[51]
Compound 27	3.5 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based optimization of S2 binding	[51]
Compound 28	0.9 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based optimization of S2 binding	[51]
Compound 29	2.7 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based optimization of S2 binding	[51]
Compound 33	7.6 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based optimization of S2 binding	[51]
Compound 36	8.8 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 37	0.66 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 37a	0.33 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 38	0.28 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 38a	0.16 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]

Compound 39	2.8 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 40	1.9 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 61	0.19 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 62	0.21 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 63	0.92 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 64	0.27 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 65	1.3 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 66	0.63 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 67	1.0 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 68	0.25 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 69	0.52 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane	[51]

											Analogues	
Compound 70	10 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 71	0.62 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 76	0.2 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 77	5.6 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 78	0.39 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 79	4.7 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 80	2.2 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 81	1.9 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 82	7.2 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 85	8.1 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 87	3.7 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted	[51]

											Diazepane Analogues	
Compound 90	9.2 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 91	8.9 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 92	9.9 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 94	7.2 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 96	1.5 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 97	9.2 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 98	0.23 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 99	0.26 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 100	0.15 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 101	0.54 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]

Compound 102	0.12 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 103	0.31 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 104	0.27 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 105	0.04 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 106	0.06 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 107	5.1 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 108	0.39 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 109	0.36 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 110	0.24 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 111	2.3 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 119	15.7 nM	ND*	FRET assay	ND*	ND*	ND*	2011	ND*	ND*	Experimental	Tri-Substituted Diazepane	[51]

											Analogues	
Compound 112	21.3 nM	ND*	FRET assay	ND*	ND*	ND*	1100	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 121	51.2 nM	ND*	FRET assay	ND*	ND*	ND*	451	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
Compound 123	74.4 nM	ND*	FRET assay	ND*	ND*	ND*	633	ND*	ND*	Hit	Tri-Substituted Diazepane Analogues	[51]
9a	138 ± 13 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Thioamide-linked spiropyrrolidine derivatives	[106]
9d	115 ± 6 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Thioamide-linked spiropyrrolidine derivatives	[106]
9f	681 ± 47 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Thioamide-linked spiropyrrolidine derivatives	[106]
9g	35 ± 1 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	Thioamide-linked spiropyrrolidine derivatives	[106]
SD-9bb	25 ± 1 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Lead compound	Thioamide-linked spiropyrrolidine derivatives	[106]
Nirmatrelvir	54 ± 3 nM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Control	FDA approved	[106]
1	8.6 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	7.3 mL/min/kg	ND*	Hit	HTP screening	https://doi.org/10.1021/acs.jmedchem.2c00117

2	0.096 μM	ND*	Enzymatic assay	12.5 μM	Vero E6	ND*	ND*	4.9 mL/min/kg	ND*	Hit	Structure-based optimization	
3 (S-217622)	0.013 μM	ND*	Enzymatic assay	0.37 μM	Vero E6	ND*	ND*	1.7 mL/min/kg	ND*	Phase 3 (NCT05330547)	Structure-based optimization	
1	143 nM	ND*	Enzymatic assay	264 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
2	335 nM	ND*	Enzymatic assay	1490 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
3	179 nM	ND*	Enzymatic assay	191 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
4	0.760 nM	ND*	Enzymatic assay	4.94 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
5	11.8 nM	ND*	Enzymatic assay	20.4 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
6	1.51 nM	ND*	Enzymatic assay	9.41 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
7	14.0 nM	ND*	Enzymatic assay	41.9 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
8	5.63 nM	ND*	Enzymatic assay	14.4 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
9	8.37 nM	ND*	Enzymatic assay	18.4 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
10	8.27 nM	ND*	Enzymatic assay	25.3 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
11	19.6 nM	ND*	Enzymatic assay	41.8 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent	[107]

											warhead	
12	99.6 nM	ND*	Enzymatic assay	117 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
13	7.16 nM	ND*	Enzymatic assay	23.1 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
14	0.403 nM	ND*	Enzymatic assay	1.57 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
15	0.493 nM	ND*	Enzymatic assay	4.48 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
16	2.36 nM	ND*	Enzymatic assay	7.79 nM	HEK 293T	ND*	ND*	ND*	ND*	Hit	Reversible covalent warhead	[107]
17 (S-892216)	0.655 nM	ND*	Enzymatic assay	2.48 nM	HEK 293T	ND*	ND*	6.79/2.52/11.4 mL/min/kg	ND*	Experimental	Reversible covalent warhead	[107]
18	0.391 nM	ND*	Enzymatic assay	3.82 nM	HEK 293T	ND*	ND*	6.69/4.59/19.7 mL/min/kg	ND*	Hit	Reversible covalent warhead	[107]
AC1115	2.44 nM	ND*		0.96 μM		ND*	ND*	ND*	ND*			[108]
Nirmatrelvir	5.38 nM	ND*		2.23 μM		ND*	ND*	41.2 mL/mL/kg	ND*	FDA-approved		[108]
Olgotrelvir	ND*	ND*		1.38 μM		ND*	ND*	11.0 mL/min/kg	ND*	Experimental		[108]
Nirmatrelvir	0.031 ± 0.001 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Lead compound	Varying nirmatrelvir warheads	[109]
2	0.010 ± 0.001 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Varying nirmatrelvir warheads	[109]
5	0.008 ± 0.001 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	Varying nirmatrelvir warheads	[109]
7	0.044 ± 0.	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Varying nirmatrelvir	[109]

	002 μM										warheads	
8	0.019 ± 0.001 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Varying nirmatrelvir warheads	[109]
9	0.027 ± 0.001 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Varying nirmatrelvir warheads	[109]
10	0.027 ± 0.001 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Varying nirmatrelvir warheads	[109]
4 (GC-3760	190 ± 40 nM	ND*	FRET assay	0.9 ± 0.2 μM	Vero E6	>200 μM	ND*	ND*	ND*	Control	Aldehyde prodrug	[110]
7	60 ± 10 nM	ND*	FRET assay	0.9 ± 0.1 μM	Vero E6	>200 μM	ND*	ND*	ND*	Experimental	Aldehyde and bisulfate derivatives	[110]
17a	40 ± 8 nM	ND*	FRET assay	>5 μM	Vero E6	>200 μM	ND*	ND*	ND*	Hit	Nitrile warhead	[110]
18a	13 ± 3 nM	ND*	FRET assay	2.7 ± 0.7	Vero E6	>200 μM	ND*	ND*	ND*	Hit	Nitrile warhead	[110]
18b	9.1 ± 2.5 nM	ND*	FRET assay	2.2 ± 0.5 μM	Vero E6	>200 μM	ND*	ND*	ND*	Hit	Nitrile warhead	[110]
19b	14 ± 2 nM	ND*	FRET assay	1.5 ± 0.4 μM	Vero E6	>200 μM	ND*	ND*	ND*	Hit	Nitrile warhead	[110]
18c	24 ± 4 nM	ND*	FRET assay	4.8 ± 0.5 μM	Vero E6	>200 μM	ND*	ND*	ND*	Hit	Nitrile warhead	[110]
18d	13.7 ± 1.5 nM	ND*	FRET assay	2.6 ± 0.3 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Nitrile warhead	[110]
18e	49 ± 10 nM	ND*	FRET assay	>10 μM	Vero E6	>200 μM	ND*	ND*	ND*	Hit	Nitrile warhead	[110]
GC376	35 nM	ND*	qRT-PCR assay	51 nM	Huh-7ACE2	ND*	ND*	ND*	ND*	Control		[111]
EB46	23 nM	ND*	qRT-PCR assay	14 nM	Huh-7ACE3	>100 μM	ND*	ND*	ND*	Hit	GC376 analogs	[111]
EB48	200 nM	ND*	qRT-PCR assay	16 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	GC376 analogs	[111]
EB54	29 nM	ND*	qRT-PCR assay	5 nM	Huh-7ACE2	>100 μM	ND*	ND*	ND*	Hit	GC376 analogs	[111]
EB55	72 nM	ND*	qRT-PCR assay	11 nM	Huh-7ACE2	ND*	ND*	ND*	ND*	Hit	GC376 analogs	[111]
EB56	50 nM	ND*	qRT-PCR assay	28 nM	Huh-7ACE2	ND*	ND*	ND*	ND*	Hit	GC376 analogs	[111]
SL-4-241	75 nM	ND*	qRT-PCR assay	17 μM	Vero E6	ND*	ND*	ND*	ND*	Hit	GC376 analogs	[111]

NK01-14	22 nM	ND*	qRT-PCR assay	26 nM	Huh-7ACE2	ND*	ND*	ND*	ND*	Hit	GC376 analogs	[111]
NK01-48	92 nM	ND*	qRT-PCR assay	15 nM	Huh-7ACE2	ND*	ND*	ND*	ND*	Hit	GC376 analogs	[111]
NK01-57	13 nM	ND*	qRT-PCR assay	92 nM	Huh-7ACE2	ND*	ND*	ND*	ND*	Hit	GC376 analogs	[111]
NK01-63	16 nM	ND*	qRT-PCR assay	6 nM	Huh-7ACE2	>100 μM	ND*	ND*	ND*	Experimental	GC376 analogs	[111]
NK01-69	24 nM	ND*	qRT-PCR assay	35 nM	Huh-7ACE2	ND*	ND*	ND*	ND*	Hit	GC376 analogs	[111]
GC376	31 ± 4 nM	ND*	fluorescent peptide assay	ND*	ND*		ND*	ND*	ND*	Control	Opal-based dipeptidyl and tripeptidyl inhibitors	[112]
MPI1	100 ± 23 nM	ND*	fluorescent peptide assay	ND*	ND*		ND*	ND*	ND*	Hit	Opal-based dipeptidyl and tripeptidyl inhibitors	[112]
MPI2	103 ± 14 nM	ND*	fluorescent peptide assay	ND*	ND*		ND*	ND*	ND*	Hit	Opal-based dipeptidyl and tripeptidyl inhibitors	[112]
MPI3	8.5 ± 1.5 nM	ND*	fluorescent peptide assay	ND*	Vero E6		ND*	ND*	ND*	Hit	Opal-based dipeptidyl and tripeptidyl inhibitors	[112]
MPI4	15.5 ± 5 nM	ND*	fluorescent peptide assay	ND*	ND*		ND*	ND*	ND*	Hit	Opal-based dipeptidyl and tripeptidyl inhibitors	[112]
MPI5	33 ± 2 nM	ND*	fluorescent peptide assay	ND*	Vero E6		ND*	ND*	ND*	Hit	Opal-based dipeptidyl and tripeptidyl inhibitors	[112]
MPI6	60 ± 4 nM	ND*	fluorescent peptide assay	ND*	ND*		ND*	ND*	ND*	Hit	Opal-based dipeptidyl and tripeptidyl inhibitors	[112]
MPI7	47 ± 3 nM	ND*	fluorescent peptide assay	ND*	ND*		ND*	ND*	ND*	Hit	Opal-based dipeptidyl and	[112]

											tripeptidyl inhibitors	
MPI8	105 ± 22 nM	ND*	fluorescent peptide assay	ND*	Vero E6		ND*	ND*	ND*	Hit	Opal-based dipeptidyl and tripeptidyl inhibitors	[112]
MPI9	56 ± 14 nM	ND*	fluorescent peptide assay	ND*	ND*		ND*	ND*	ND*	Hit	Opal-based dipeptidyl and tripeptidyl inhibitors	[112]
11a	31 ± 3 nM	ND*	fluorescent peptide assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	Opal-based dipeptidyl and tripeptidyl inhibitors	[112]

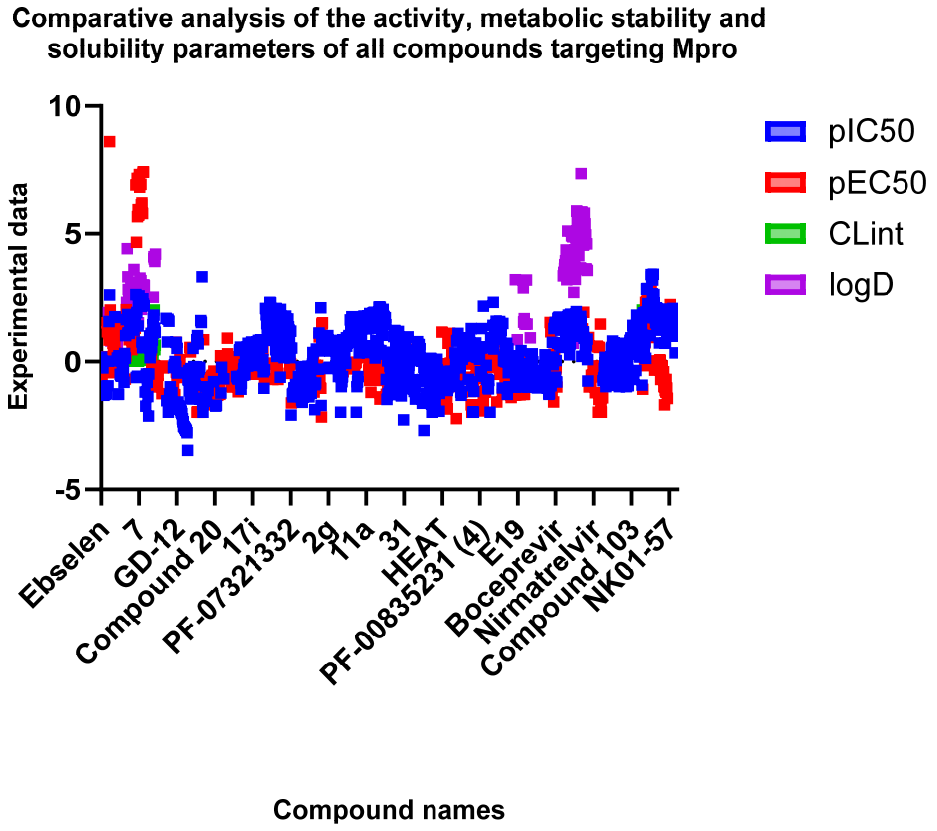


Figure S1. Comparative analysis of the activity, metabolic stability and solubility parameters of all reported compounds targeting Mpro.

Table S5. Pharmacological and physicochemical profiles of inhibitors targeting SARS-CoV-2 PLpro

No.	Name	IC_{50}	K_i	Type of PLpro assay	EC_{50}	Type of viral assay	CC_{50}	Metabolic profiling (CL_{int}) (μl/min/mg)/μL/min/10 cells	Metabolite ID	Log D	Approval status	Design strategy	References
1	7724772	23.5 μM	ND*	SARS-CoV-2 PLpro Inhibition assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Original HTS hit containing 2-naphtalene moiety	[113]
2	GRL-0617	2.4 ± 0.2 μM	ND*	Enzymatic assay	27.6 ± 1.2 μM	Vero E6	>60 μM	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[113]
2a	GRL-0617	2.1 ± 0.2 μM	ND*	Enzymatic assays	21.2 μM	Vero E6 cell	ND*	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[114]
2b	GRL0617	ND*	1800 nM	Enzymatic assay	68200 nM	Vero E6	ND*	20.9	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[115]
2c	GRL-0617	ND*	ND*	ND*	35.43 ± 15.02 μM	Vero E6	48.28± 20. 74 μM	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[116]
2d	GRL-0617	1.66 ± 0.36 μM	ND*	Enzymatic assay	33.9 ± 6.5 μM	Calu-3 cells	>40 μM	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[117]
2e	GRL-0617	1.39 ± 0.26 μM	ND*	High-throughput screening	3.18 ± 0.71	Vero E6	~500 μM	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[118]
2f	GRL-0617	0.82 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[119]
2g	GRL-0617	6.97 ± 1.34 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[120]

2h	GRL-0617	1.60 ± 0.13	ND*	FRET-based assay	23.64 ± 4.72 μM	Vero E6	>60 μM	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[121]
2i	GRL-0617	1.2 μM	ND*	Fluorogenic peptide assay	ND*	ND*	ND*	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[122]
2j	GRL-0167	1.61 μM	ND*	Enzymatic assays	>20 μM	ND*	>80 μM	13.13	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[123]
2k	GRL-0617	1.113 ± 0.175 ng/μL	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[124]
2l	GRL-0617	0.65 μM	ND*	High-throughput screening	ND*	ND*	ND*	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[125]
2m	GRL-0617	ND*	ND*	ND*	25.47 μM	Caco-2	ND*	67.4	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[126]
2n	GRL-0617	1.43 ± 0.26 μM	ND*	Enzymatic assay	15.68 ± 1.97 μM	Cell-based assay (Flip GFP)	>40 μM	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[127]
2o	GRL-0617	1.88 μM	ND*	FRET assay	74.42 μM	ND*	ND*	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[128]
2p	GRL-0617	2.4 ± 1.2 μM	ND*	Enzymatic assay	17.6 ± 1.2 μM	Vero-E6	ND*	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[113]
2q	GRL-0617	ND*	ND*	ND*	19.56 ± 1.75 μM	Flip GFP assay/Ck8 assay	>200 μM	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[129]
2r	GRL-0617	4.82 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl	[130]

												and amino-methylbenzene groups	
2s	GRL-0617	2.12 µM	ND*	Enzymatic activity	ND*	ND*	ND*	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[131]
2t	GRL-0617	1918.0 ±150.0 nM	1374 ± 58 nM	FRET enzymatic assay	>20 µM	Vero E6	107.3 ±10.9 µM	ND*	ND*	ND*	Lead	7724772 derivative with 1-naphthyl and amino-methylbenzene groups	[132]
3	2	ND*	116 nM	Enzymatic assay	1850 nM	Vero E6	ND*	13.9	CYP 3A4	ND*	hit	N-methyl pyrazole derivative	[115]
4	3	ND*	9 nM	Enzymatic assay	652 nM	Vero E6	ND*	12.8	CYP 3A5	ND*	hit	N-methyl pyrazole derivative	[115]
5	4(PF-07957472)	28 µM	2 nM	Enzymatic assay	147 nM	Vero E6	69.3 µM	8.84	CYP 3A4	2.5	Experimental	N-methyl pyrazole derivative	[115]
6	JUN12129	90.9±4.6 nM	75.5± 2.0 nM	FRET enzymatic assay	ND*	Vero E6	8.3 ± 1.2 µM	ND*	CYP 450	ND*	Hit	Thiophene-containing	[132]
7	JUN11875	66.2 ±2 nM	13.2 ±2 nM	FRET enzymatic assay	ND*	Vero E6	4.5 ± 1.6 µM	ND*	CYP 450	ND*	Hit	Thiophene-containing	[132]
8	JUN12303	121.5 ± 4.0 nM	88.2 ± 6.0 nM	FRET enzymatic assay	0.32 µM	Vero E6	56.8 ± 7.4 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]
9	JUN12162	98.3 ± 7.0 nM	33.6 ± 3.0 nM	FRET enzymatic assay	0.23 µM	Vero E6	42.3 ± 2.3 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]
10	JUN12682	106.8±5.0 nM	37.7 nM	FRET enzymatic assay	0.42 µM	Vero E6	61.3 ± 4.5 µM	10.5	CYP 450	ND*	Experimental	Pyrazole-containing	[132]
11	JUN11941	151.4 ± 4.0 nM	34.3 ± 3.0 nM	FRET enzymatic assay	0.31 µM	Vero E6	54.8 ± 8.3 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]
12	JUN12199	108.8 ± 10.2 nM	47.6 ± 3.0 nM	FRET enzymatic assay	0.45 µM	Vero E6	63.2 ± 11.3 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]
13	JUN12197	102.7 ± 10.2 nM	33.2 ± 3.0 nM	FRET enzymatic assay	0.35 µM	Vero E6	43.7 ± 5.1 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]
14	JUN12603	112.2 ± 6.0 nM	39.8 ± 4.0 nM	FRET enzymatic assay	0.50 µM	Vero E6	61.0 ± 19.3 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]
15	JUN12351	98.8 ± 5.2 nM	29.3 ± 3.0	FRET enzym	0.59 µM	Vero E6	>125 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]

			n M	atic assay									
16	JUN12145	108.5 ± 6.2 nM	35.2 ± 2.0 n M	FRET enzymatic assay	0.58 µM	Vero E6	31.3 ± 2.0 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]
17	JUN12682	106.8 ± 5.0 nM	37.7 ± 3.0 n M	FRET enzymatic assay	0.42 µM	Vero E6	61.3 ± 4.5 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]
18	JUN12763	164.6 ± 23.0 nM	37.2 ± 4.0 n M	FRET enzymatic assay	0.96 µM	Vero E6	>125 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]
19	JUN12395	121.9 ± 8.0 nM	47.1 ± 4.0 n M	FRET enzymatic assay	1.15 µM	Vero E6	109.4 ± 16.2 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]
20	JUN12713	86.7 ± 6.0 nM	34.0 ± 3.0 n M	FRET enzymatic assay	0.86 µM	Vero E6	107.2 ± 6.2 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]
21	JUN12602	116.2 ± 9.2 nM	46.9 ± 3.0 n M	FRET enzymatic assay	0.80 µM	Vero E6	>125 µM	ND*	CYP 450	ND*	Hit	Pyrazole-containing	[132]
22	2 (XR8-24)	0.58 µM	N D*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Lead	Aminoazetidine-substituted phenylthiophenes	[133]
23	10 (XR8-23)	0.39 µM	N D*	Enzymatic assay	2.5 ± 0.15 µM	A549-hACE2	43 ± 1.8 µM	ND*	ND*	ND*	Experimental	Aminoazetidine-substituted phenylthiophenes	[133]
24	11 (XR8-89)	0.11 µM	N D*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
25	12 (XR8-65)	0.33 µM	N D*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
26	13 (XR8-69)	0.37 µM	N D*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
27	14 (XR8-83)	0.21 µM	N D*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
28	15	0.92 µM	N D*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
29	16	0.65 µM	N D*	Enzymatic assay	2.3 ± 0.22 µM	A549-Hace2	27 ± 1.4 µM	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]

30	17	0.33 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
31	18	1.48 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
32	19	1.96 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
33	20	3.17 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
34	21	1.56 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
35	22	1.13 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
36	23	5.53 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
37	24	1.93 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
38	25	1.19 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
39	26	4.75 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
40	27	4.43 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
41	28	6.12 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
42	29	1.08 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
43	30	0.82 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
44	31	0.79 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted	[133]

												phenylthiophenes	
45	32	0.38 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
46	33	0.82 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
47	34	0.69 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
48	35	2.40 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
49	36	1.14 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
50	37	0.96 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
51	38	0.55 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
52	39	0.32 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
53	40	0.49 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
54	41	0.96 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
55	42	0.81 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
56	43	0.43 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
57	44	0.75 µM	ND*	Enzymatic assay	787 ± 68 nM	A549-Hace2	22 ± 0.9 µM	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
58	45	1.6 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]

59	46	0.36 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
60	47	0.26 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
61	48	0.57 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
62	49	1.2 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
63	50	1.79 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
64	51	2.42 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
65	52	1.52 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
66	53	1.39 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
67	54	1.69 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
68	55	0.60 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
69	56	2.82 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
70	57	1.39 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
71	58	1.56 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
72	59	9.78 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
73	60	0.56 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted	[133]

												phenylthiophenes	
74	61	0.50 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
75	62	0.60 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
76	63	0.47 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
77	64	0.62 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Aminoazetidine-substituted phenylthiophenes	[133]
78	F0213	7.4 µM	ND*	HTS fluorescence-based Plpro Cleavage assay	4.549 µM	Vero E6-TMPRSS2 cells	ND*	ND*	ND*	ND*	Experimental	HTS lead	[134]
79	F0326	8.2 µM	ND*	HTS fluorescence-based Plpro Cleavage assay	7.62 µM	Vero E6-TMPRSS2 cells	ND*	ND*	ND*	ND*	Hit	HTS hit	[134]
80	F0393	ND*	ND*	HTS fluorescence-based Plpro Cleavage assay	15.59 µM	Vero E6-TMPRSS2 cells	ND*	ND*	ND*	ND*	Hit	HTS hit	[134]
81	Compound 6	5 ± 1.9 µM	ND*	Enzymatic assay	21 ± 1.9 µM	Vero E6	>60 µM	ND*	ND*	ND*	Experimental	Lead containing 1-naphthyl and acetyl amino moeities	[113]
82	7724772	23.5 ± 1.7 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit containing 1-naphthyl and acetyl amino moeities	[113]
83	6577871	100.7 ± 4.76 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Insertion of a 4-piperidinecarboxa-mide oxalate moiety	[113]
84	9247873	>200 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Insertion of a 4-piperidinecarboxa-mide oxalate moiety	[113]

88	1c	2.64 ± 0.34 μM	ND*	HEK293T	ND*	ND*	ND*	ND*	ND*	ND*	Lead	peptide–drug conjugate	[135]
89	Ac-EM-C	7.4 ± 0.37 μM	ND*	HEK293T	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	peptide–drug conjugate	[135]
90	Ac-ELRGG	15.38 ± 1.63 μM	ND*	HEK293T	ND*	ND*	ND*	ND*	ND*	ND*	Hit	peptide–drug conjugate	[135]
91	Ac-EC-M	8.63 ± 0.55 μM	ND*	HEK293T	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	peptide–drug conjugate	[135]
92	Cryptotanshinone	5.63 ± 1.45 μM	ND*	HTS fluorescence-based enzymatic assay	0.70 ± 0.09 μM	Vero E6	>300 μM	ND*	ND*	ND*	Hit	HTS of a library containing diverse compounds	[135]
93	Tanshinone I	2.1 ± 0.1 μM	ND*	HTS fluorescence-based enzymatic assay	2.26 ± 0.11 μM	Vero E6	>300 μM	ND*	ND*	ND*	Hit	HTS of a library containing diverse compounds	[135]
94	YM155	2.47 ± 0.46 μM	ND*	HTS fluorescence-based enzymatic assay	0.17 ± 0.22 μM	Vero E6	~400 μM	ND*	ND*	ND*	Experimental	HTS of a library containing diverse compounds	[135]
95	Rac5c	0.81 μM	ND*	HTS fluorescence-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	Repurposing of known drugs and clinical candidates	[136]
96	Rac3j	1.4 μM	ND*	HTS fluorescence-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposing of known drugs and clinical candidates	[136]
97	Rac3k	1.15 μM	ND*	HTS fluorescence-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Repurposing of known drugs and clinical candidates	[136]
98	EACC	8.28 ± 1.11 μM	ND*	Enzymatic assay	>40 μM	Calu-3 cells	41.9 ± 7.1 μM	ND*	ND*	ND*	Hit	HTS Screening of a MedChemExpress bioactive compound library	[117]
99	KY226	3.39 ± 0.59 μM	ND*	Enzymatic assay	28.4 ± 2.3 μM	Calu-3 cells	49.3 ± 13.5 μM	ND*	ND*	ND*	Hit	HTS Screening of a MedChemExpress bioactive compound library	[117]
100	Tropifexor	5.11 μM	ND*	Enzymatic assay	4.03 ± 0.5 μM	Calu-3 cells	26.6 ± 1.4 μM	ND*	ND*	ND*	Experimental	HTS Screening of a MedChemExpress	[117]

												bioactive compound library	
101	Proanthocyanidin	2.4 ± 0.3 μM	ND*	HTS fluorescence-based enzymatic assay	2.5 ± 0.4 μM	Vero E6	56.4 ± 0.7 μM	ND*	ND*	ND*	Experimental	Screening of FDA approved drugs	[137]
102	Manidipine-2HCl	14.2 ± 1.7 μM	ND*	HTS fluorescence-based enzymatic assay	14.5 ± 0.8 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Screening of FDA approved drugs	[137]
103	Loperamide	33.5 ± 5.8 μM	ND*	HTS fluorescence-based enzymatic assay	11.4 ± 1.6 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Screening of FDA approved drugs	[137]
104	Levothyroxine	15.3 ± 4.2 μM	ND*	HTS fluorescence-based enzymatic assay	7.0 ± 2.2 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Screening of FDA approved drugs	[137]
105	Maprotiline	9.7 ± 0.3 μM	ND*	HTS fluorescence-based enzymatic assay	9.3 ± 0.1 μM	Vero E6	31.8 ± 0.4 μM	ND*	ND*	ND*	Hit	Screening of FDA approved drugs	[137]
106	Reserpine	5.7 ± 0.7 μM	ND*	HTS fluorescence-based enzymatic assay	6.6 ± 1.5 μM	Vero E6	>100 μM	ND*	ND*	ND*	Hit	Screening of FDA approved drugs	[137]
209	Chloroxine	7.24 ± 0.68 μM	ND*	PLpro protease-activity-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library of clinically approved drugs	[138]
210	Tashinone IIA sulfonate sodium	1.65±0.13 μM	ND*	PLpro protease-activity-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library of clinically approved drugs	[138]
107	Compound 1	93.7 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tanshinone IIA sulfonate sodium analogues	[139]
108	Compound 2	>100 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tanshinone IIA sulfonate sodium analogues	[139]

111	Compound 5	>100 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tanshinone IIA sulfonate sodium analogues	[139]
112	Compound 6	68.3 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Tanshinone IIA sulfonate sodium analogues	[139]
113	Compound 7	6.0 µM	ND*	Fluorescence Polarization Assay	4.59 ± 1.22 µM	Vero E6	>800 µM	ND*	ND*	ND*	Experimental	Chloroxine derivative	[139]
115	Compound 9	8.9 µM	ND*	Fluorescence Polarization Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Chloroxine derivative	[139]
116	Compound 10	9.7 µM	ND*	Fluorescence Polarization Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Chloroxine derivative	[139]
117	Compound 11	7.6 µM	ND*	Fluorescence Polarization Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Chloroxine derivative	[139]
118	Compound 12	9.5 µM	ND*	Fluorescence Polarization Assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Chloroxine derivative	[139]
119	4	43.2 ± 9.4 µM	ND*	Biochemical assay	1.7 ± 4.4 µM	Vero E6	ND*	ND*	ND*	ND*	Hit	Derivative of GRL-0617	[140]
120	7	12.7 ± 1.3 µM	ND*	Biochemical assay	5.2 ± 4.2 µM	Vero E6	ND*	ND*	ND*	ND*	Experimental	Amine-functionalized derivatives of GRL-0617	[140]
121	6	7.0 ± 0.6 µM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Amine-functionalized derivatives of GRL-0617	[140]
122	5	16.8 ± 2.9 µM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Amine-functionalized derivatives of GRL-0617	[140]
123	3	6.4 ± 4.2 µM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Amine-functionalized derivatives of GRL-0617	[140]
124	2	5.1 ± 0.7 µM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Amine-functionalized derivatives of GRL-0617	[140]
125	1	2.3 ± 0.2 µM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivative of GRL-0617	[140]

126	HE9	0.2 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Natural phenolic compounds	[119]
127	HBA	1 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Natural phenolic compounds	[119]
128	YRL	1.3 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Natural phenolic compounds	[119]
129	1d	236 ± 107 nM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	Optimization of Ebselen's derivatives substituted on the phenyl ring	[141]
130	1e	256 ± 35 nM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	Optimization of Ebselen's derivatives substituted on the phenyl ring	[141]
131	2d	339 ± 109 nM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of Ebselen's derivatives substituted on the phenyl ring	[141]
132	2e	263 ± 121 nM	ND*	Biochemical assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of Ebselen's derivatives substituted on the phenyl ring	[141]
133	11	2.64 ± 0.29 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse compounds	[120]
134	12	2.69 ± 0.34 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse compounds	[120]
135	13	4.32 ± 0.20 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse compounds	[120]
136	14	1.76 ± 0.06 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse compounds	[120]
137	15	3.75 ± 0.82 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse compounds	[120]
138	16	1.37 ± 0.40 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse compounds	[120]
139	17	0.82 ± 0.16 µM	ND*	Enzymatic assay	ND*	hACE2-HeLa	>10 µM	ND*	ND*	ND*	Hit	HTS of a library containing diverse compounds	[120]

140	18	0.80 ± 0.24 μM	ND*	Enzymatic assay	ND*	hACE2-HeLa	~10 μM	ND*	ND*	ND*	Lead	HTS of a library containing diverse compounds	[120]
141	19	0.44 ± 0.05 μM	ND*	Enzymatic assay	ND*	hACE2-HeLa	>10 μM	ND*	ND*	ND*	Experimental	HTS of a library containing diverse compounds	[120]
142	Jun9-10-1	16.7 ± 2.48 μM	ND*	FRET-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
143	Jun9-10-2	98.8 ± 13.2 μM	ND*	FRET-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
144	Jun9-10-3	19.6 ± 1.6 μM	ND*	FRET-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
145	Jun9-10-4	16.2 ± 5.9 μM	ND*	FRET-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
146	Jun9-10-5	12.8 ± 2.3 μM	ND*	FRET-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
147	Jun9-10-6	23.7 ± 10.1 μM	ND*	FRET-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
148	Jun9-10-7	17.4 ± 2.2 μM	ND*	FRET-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
149	Jun9-10-8	20.5 ± 5.1 μM	ND*	FRET-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
150	Jun9-10-9	38.7 ± 2.9 μM	ND*	FRET-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
151	Jun9-13-1	78.1 ± 28.1 μM	ND*	FRET-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
152	Jun9-13-2	>200 μM	ND*	FRET-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
153	Jun9-13-7	7.29 ± 1.03 μM	ND*	FRET-based enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
154	Jun9-13-9	6.67 ± 0.55 μM	ND*	FRET-based enzym	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from	[121]

				atic assay								Enamine Collection	
155	GC376	ND*	ND*	FRET-based assay	>60 µM	Vero E6	>60 µM	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
156	Jun9-53-2	0.89 ± 0.12 µM	ND*	FRET-based assay	25.19 ± 9.32 µM	Vero E6	>60 µM	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
157	Jun9-72-2	0.67 ± 0.08 µM	ND*	FRET-based assay	6.62 ± 1.31 µM	Vero E6	>60 µM	ND*	ND*	ND*	Lead	Hit Optimization from Enamine Collection	[121]
158	Jun9-75-4	0.62 ± 0.06 µM	ND*	FRET-based assay	7.88 ± 1.44 µM	Vero E6	47.48 ±14.63 µM	ND*	ND*	ND*	Lead	Hit Optimization from Enamine Collection	[121]
159	Jun9-75-5	0.56 ± 0.03 µM	ND*	FRET-based assay	>60 µM	FRET-based assay	>60 µM	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
160	Jun9-84-3	ND*	ND*	FRET-based assay	8.31 ± 2.68 µM	Vero E6	>60 µM	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
161	Jun9-85-1	0.66 ± 0.03 µM	ND*	FRET-based assay	7.81 ± 2.55 µM	Vero E6	>60 µM	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
162	Jun9-87-1	ND*	ND*	FRET-based assay	10.14 ± 3.52 µM	Vero E6	>60 µM	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
163	Jun9-87-2	0.90 ± 0.24 µM	ND*	FRET-based assay	55.07 ± 9.77 µM	FRET-based assay	>60 µM	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
164	Jun9-87-3	0.80 ± 0.10 µM	ND*	FRET-based assay	22.34 ± 9.75 µM	Vero E6	49.52 ± 17.28 µM	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
165	Jun9-13-7	7.29 ± 1.03 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
166	Jun9-13-9	6.67 ± 0.55 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
167	Jun9-81-1	19.23 ± 1.70 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]

168	Jun9-67-2	7.10 ± 2.47 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
169	Jun9-68-1	11.71 ± 2.05 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
170	Jun9-80-4	1.58 ± 0.26 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
171	Jun9-68-3	5.13 ± 0.74 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
172	Jun9-68-2	1.30 ± 0.14 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
173	Jun9-75-2	1.54 ± 0.30 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
174	Jun9-84-2	2.47 ± 0.44 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
175	Jun9-86-2	6.49 ± 1.14 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
176	Jun9-87-3	0.80 ± 0.10 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Ht	Hit Optimization from Enamine Collection	[121]
177	Jun9-75-3	8.89 ± 2.23 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
178	Jun9-67-1	2.72 ± 0.28 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
179	Jun9-86-8	5.50 ± 0.27 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
180	Jun9-86-5	6.12 ± 0.51 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
181	Jun9-81-3	1.85 ± 0.15 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
182	Jun9-85-5	16.59 ± 2.60 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from	[121]

												Enamine Collection	
183	Jun9-85-6	4.42 ± 1.22 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
184	Jun9-81-2	1.44 ± 0.22 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
185	Jun9-86-4	9.22 ± 3.31 µM	ND*	FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Hit Optimization from Enamine Collection	[121]
189	1	159 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
190	2	226 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
191	3	227 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
192	4	248 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
193	5	270 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
194	6	287 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
195	7	303 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	Structure-Based Screening of ENAMINE Real Database	[142]
196	8	324 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE	[142]

												Real Database	
197	9	359 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
198	10	370 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
199	11	383 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
200	12	385 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
201	13	420 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
202	14	432 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
203	15	433 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
204	16	446 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
205	17	476 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
206	18	483 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE	[142]

												Real Database	
207	19	498 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
208	20	505 nM	ND*	Predicted	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Structure-Based Screening of ENAMINE Real Database	[142]
211	Acriflavine	1.66 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	HTS of a library containing diverse clinical compounds	[125]
214	Proflavine Hemisulfate	2.77 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse clinical compounds	[125]
215	PHA-665752	3.92 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse clinical compounds	[125]
216	Chlorophyllin	>100 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse clinical compounds	[125]
217	Clofazimine	>100 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse clinical compounds	[125]
218	Dithranol	24.83 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse clinical compounds	[125]
219	Protoporphyrinix	3.335 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse clinical compounds	[125]
220	Tannic acid	6.039 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse clinical compounds	[125]
221	Evans Blue	5.88 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse clinical compounds	[125]

222	Hpericin	7.02 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse clinical compounds	[125]
223	Verteporfin	4.201 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	HTS of a library containing diverse clinical compounds	[125]
224	Acridine orange base	15.10 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Acriflavine analogue	[125]
225	Acridine-3,6-diamine sulfate	3.728 µM	ND*	HTS FRET-based assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Acriflavine analogue	[125]
226	1	73.60 ± 11.94 µM	ND*	In vitro enzymatic assay	ND*	Vero	23.77 µM	ND*	ND*	ND*	Hit	Retention of naphthyridine core from a vHTS hit compound 1	[143]
227	82	79.77 ± 20.37 µM	ND*	In vitro enzymatic assay	ND*	Vero	>50 µM	ND*	ND*	ND*	Hit	Retention of naphthyridine core from a vHTS hit compound 1	[143]
228	83	54.8 ± 20.68 µM	ND*	In vitro enzymatic assay	ND*	Vero	43.58 µM	ND*	ND*	ND*	Hit	Retention of naphthyridine core from a vHTS hit compound 1	[143]
229	84	39.5 ± 4.62 µM	ND*	In vitro enzymatic assay	ND*	Vero	47.32 µM	ND*	ND*	ND*	Hit	Retention of naphthyridine core from a vHTS hit compound 1	[143]
230	85	15.06 ± 2.19 µM	ND*	In vitro enzymatic assay	ND*	Vero	7.47 µM	ND*	ND*	ND*	Experimental	Retention of naphthyridine core from a vHTS hit compound 1	[143]
231	Compound 6	11±3 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Acetamide derivative of GRL0617	

232	3	>100 µM	ND*	Fluorogenic peptide assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 Redesign with N,N'-Acetylacetohydrazine Linker	
234	5	24 µM	ND*	Fluorogenic peptide assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 Redesign with N,N'-Acetylacetohydrazine Linker	
236	7	0.094 µM	ND*	Fluorogenic peptide assay	1.1 µM	ND*	ND*	38.9	ND*	ND*	Experimental	GRL-0617 Redesign with N,N'-Acetylacetohydrazine Linker	
237	8	0.23 µM	ND*	Fluorogenic peptide assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 Redesign with N,N'-Acetylacetohydrazine Linker	
238	9	5.4 µM	ND*	Fluorogenic peptide assay	34 µM	ND*	ND*	689.4	ND*	ND*	Hit	GRL-0617 Redesign with N,N'-Acetylacetohydrazine Linker	
239	10	4.4 µM	ND*	Fluorogenic peptide assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 Redesign with N,N'-Acetylacetohydrazine Linker	
240	11	8 µM	ND*	Fluorogenic peptide assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 Redesign with N,N'-Acetylacetohydrazine Linker	
241	12	0.098 µM		Fluorogenic peptide assay	ND*	ND*	1.3 µM	ND*	ND*	ND*	Hit	GRL-0617 Redesign with N,N'-Acetylacetohydrazine Linker	

242	13	>200 μM		Fluoro genic peptide assay	ND*	ND*	5.0 μM	ND*	ND*	ND*	Hit	GRL-0617 Redesign with N,N'-Acetylaceto hydrazine Linker	
243	14	100 μM	N D*	Fluoro genic peptide assay	ND*	ND*	ND*	<38.5	ND*	ND*	Hit	GRL-0617 Redesign with N,N'-Acetylaceto hydrazine Linker	
244	15	6.2 μM	N D*	Fluoro genic peptide assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 Redesign with N,N'-Acetylaceto hydrazine Linker	
246	ZN-2-180 (101)	6.08 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
247	ZN-2-181 (2)	1.1 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
248	ZN-2-182 (3)	5.5 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
249	ZN-2-183 (4)	6.0 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
250	ZN-2-184 (5)	1.01 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
251	ZN-2-185 (6)	0.6 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
252	ZN-2-186 (7)	1.2 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
253	ZN-2-187 (8)	0.8 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
254	ZN-2-189 (9)	0.7 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]

255	ZN-2-188-1 (10)	1.6 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
256	ZN-2-188-2 (11)	4.3 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
257	ZN-2-197 (12)	2.4 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
258	ZN-3-56 (13)	3.9 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
259	DY2-144 (14)	1.3 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
260	DY2-137 (15)	3.3 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
261	DY2-138-2 (16)	6.1 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
265	ZN-2-192 (20)	4.8 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
269	DY2-115 (24)	7 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
272	DY-3-15 (27)	0.8 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
273	DY-3-65 (28)	6.3 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
274	DY-3-70 (29)	6.4 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
276	ZN-3-55 (31)	7.4 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
278	ZN-3-66 (33)	4.1 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine group of GRL-0617	[123]
279	ZN-3-70 (34)	10.7 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Extention of the amine	[123]

												group of GRL-0617	
290	XDY 2-62 (45)	3.3 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimizatio n of GRL-0617 (methyl, naphthalene , and aniline groups)	[123]
293	YF4-136 (48)	4.7 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimizatio n of GRL-0617 (methyl, naphthalene , and aniline groups)	[123]
297	ZN-3-45 (52)	5.7 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimizatio n of GRL-0617 (methyl, naphthalene , and aniline groups)	[123]
298	DY-3-59 (53)	6.7 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimizatio n of GRL-0617 (methyl, naphthalene , and aniline groups)	[123]
299	DY-3-66 (54)	3.3 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimizatio n of GRL-0617 (methyl, naphthalene , and aniline groups)	[123]
300	ZN-3-79 (55)	1.9 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimizatio n of GRL-0617 (methyl, naphthalene , and aniline groups)	[123]
301	ZN-3-67 (56)	8.5 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimizatio n of GRL-0617 (methyl, naphthalene , and aniline groups)	[123]
302	ZN-3-71 (57)	10.9 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimizatio n of GRL-0617 (methyl, naphthalene , and aniline groups)	[123]
303	DY2-149 (58)	1.6 μM	N D*	Enzym atic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimizatio n of GRL-0617 (methyl, naphthalene , and	[123]

												aniline groups)	
304	ZN-3-79 (59)	1.9 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
305	DY-2-153 (60)	1.8 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
309	ZN-3-74 (64)	2.8 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
310	ZN-3-80 (65)	0.59 μM	ND*	Enzymatic assays	ND*	ND*	ND*	5.64	ND*	ND*	Experimental	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
311	XR8-8 (66)	1.3 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
312	XR8-9 (67)	1.8 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
313	XR8-14 (68)	1.2 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
314	XR8-15 (69)	0.9 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
315	XR8-16 (70)	1.6 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and	[123]

												aniline groups)	
316	XR8-17 (71)	2.7 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
317	XR8-23 (72)	0.39 μM	ND*	Enzymatic assays	1.4 ± 0.1 μM	A549-hACE2	21.6 ± 1.1 μM	5.89	ND*	ND*	Experimental	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
318	XR8-24 (73)	0.56 μM	ND*	Enzymatic assays	1.2 ± 0.2 μM	A549-hACE2	>50 μM	9.60	ND*	ND*	Experimental	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
319	XR8-30 (74)	0.75 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
320	XR8-32-1 (75)	0.97 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
321	XR8-32-2 (76)	0.81 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
322	XR8-35 (77)	1.79 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
323	XR8-38 (78)	0.76 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
324	XR8-39 (79)	1.1 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and	[123]

												aniline groups)	
325	XR8-40 (80)	0.82 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
326	XR8-49 (81)	0.64 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
327	XR8-51 (82)	1.1 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
328	XR8-56 (83)	2.2 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
329	XR8-57 (84)	0.70 µM	ND*	Enzymatic assays	ND*	ND*	ND*	0.27	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
330	XR8-61 (85)	6.5 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
331	XR8-65 (86)	0.33 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
332	XR8-66 (87)	0.62 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
333	XR8-67 (88)	0.17 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and	[123]

												aniline groups)	
334	XR8-69 (89)	0.37 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
335	XR8-77 (90)	0.64 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
336	XR8-79 (91)	0.41 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
337	XR8-83 (92)	0.21 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
338	XR8-84 (93)	0.43 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
339	XR8-89 (94)	0.113 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
340	XR8-96 (95)	0.25 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
341	XR8-98 (96)	0.81 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
342	XR8-101 (97)	1.8 µM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and	[123]

												aniline groups)	
343	XR8-103 (98)	1.1 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
344	XR8-104 (99)	2.3 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
345	XR8-106 (100)	1.4 μM	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of GRL-0617 (methyl, naphthalene, and aniline groups)	[123]
347	SIMR 1440	4.117 + 1.410 ng/μL	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Exploiting shallow pockets	[124]
349	SIMR 1489	33.224 + 5.78 ng/μL	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Exploiting shallow pockets	[124]
350	SIMR 1493	0.0659 ± 0.007 1 ng/μL	ND*	Enzymatic assays	ND*	Vero E6	43.12 μg/mL	ND*	ND*	ND*	Hit	Exploiting shallow pockets	[124]
351	SIMR 1783	27.577 ± 2.27 ng/μL	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Exploiting shallow pockets	[124]
352	SIMR 1888	4.094 ± 2.40 ng/μL	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Exploiting shallow pockets	[124]
355	SIMR 2593	0.852 ± 0.89 ng/μL	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Exploiting shallow pockets	[124]
356	SIMR 3030	0.0399 ± 0.081 ng/μL	ND*	Enzymatic assays	ND*	Vero E6	55.63 μg/mL	ND*	ND*	ND*	Experimental	Exploiting shallow pockets	[124]
357	SIMR 7088	6.0726 ± 0.65 ng/μL	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Exploiting shallow pockets	[124]
358	SIMR 7109	12.8315 ± 2.057 ng/μL	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Exploiting shallow pockets	[124]
359	SIMR 7111	13.947 ± 0.69 ng/μL	ND*	Enzymatic assays	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Exploiting shallow pockets	[124]
360	Jun9722	0.67 ± 0.08 μM	ND*	ND*	ND*	ND*	23.69 ± 1.58 μM	778.8	ND*	ND*	Lead	Quinoline-based optimization of GRL-0617	[126]
361	Jun9871	0.87 ± 0.12 μM	ND*	ND*	ND*	ND*	14.43 ± 0.77 μM	2485.8	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]

362	Jun9851	0.66 ± 0.12 μM	ND*	ND*	4.11 ± 0.64 μM	Caco-2 cells	35.47 ± 1.52 μM	429.1	ND*	ND*	Lead	Quinoline-based optimization of GRL-0617	[126]
366	Jun11213	0.69 μM	ND*	ND*	5.30 ± 1.26 μM	Caco-2 cells	ND*	25.7	ND*	ND*	Lead	Quinoline-based optimization of GRL-0617	[126]
367	Jun11165	0.63 μM	ND*	ND*	6.04 ± 0.84 μM	Caco-2 cells	ND*	11.8	ND*	ND*	Lead	Quinoline-based optimization of GRL-0617	[126]
368	Jun11243	0.50 ± 0.10	ND*	ND*	ND*	Caco-2 cells	15.20 ± 0.30	<9.6	ND*	ND*	Lead	Quinoline-based optimization of GRL-0617	[126]
369	Jun10714	2.81 ± 0.48 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
370	Jun10725	0.58 ± 0.08 μM	ND*	ND*	ND*	Vero E6	31.5 ± 2.70 μM	ND*	ND*	ND*	Lead	Quinoline-based optimization of GRL-0617	[126]
371	Jun10132	4.97 ± 1.30 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
372	Jun10827	1.23 ± 0.24 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
373	Jun10828	2.36 ± 0.15 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
374	Jun10713	>20 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
375	Jun10836	>20 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
376	Jun10872	>20 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]

377	Jun10 873	>20 μM	N D*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
378	Jun10 837	0.48 ± 0.04 μM	N D*	ND*	ND*	Vero E6 cell	>100 μM	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
379	Jun-43	0.67 ± 0.14 μM	N D*	ND*	ND*	Vero E6 cell	24.69 ± 1.3 μM	ND*	ND*	ND*	Experimental	Quinoline-based optimization of GRL-0617	[126]
380	Jun10 711	0.60 ± 0.08 μM	N D*	ND*	ND*	Vero E6	31.80 ± 1.22 μM	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
381	Jun10 712	0.53 ± 0.09 μM	N D*	ND*	ND*	Vero E6	32.5 ± 1.52 μM	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
382	Jun10 715	6.45 ± 1.94 μM	N D*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
383	Jun10 716	5.17 ± 1.24 μM	N D*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
384	Jun10 722	0.63 ± 0.10 μM	N D*	ND*	ND*	Vero E6	28.30 ± 1.50 μM	ND*	ND*	ND*	Hit	Quinoline-based optimization of GRL-0617	[126]
385	Jun-21	0.96 ± 0.11 μM	N D*	ND*	ND*	Vero E6	13.67 ± 3.60 μM	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
386	Jun10 888	2.50 ± 0.37 μM	N D*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
387	Jun11 76	1.66 ± 0.19 μM	N D*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]

388	Jun11114	1.27 ± 0.09 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
389	Jun10889	>20 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
390	Jun10823	2.45 ± 0.14 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
391	Jun-95	2.03 ± 0.33 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
392	Jun10824	1.76 ± 0.33 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
393	Jun-91	5.89 ± 0.44 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
394	Jun10821	2.66 ± 0.35 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
395	Jun10822	2.34 ± 0.22 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
396	Jun10825	5.03 ± 0.52 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
397	Jun10826	2.36 ± 0.27 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
398	Jun-92	3.00 ± 0.52 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended	[126]

												the amino group	
399	Jun-93	7.09 ± 1.50 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
400	Jun-94	3.39 ± 0.34 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Retention of naphthalene ring and extended the amino group	[126]
401	Jun1183	0.69 ± 0.08 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
402	Jun11115	0.89 ± 0.11 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
403	Jun11217	0.99 ± 0.10 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
404	Jun11168	1.41 ± 0.54 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
405	Jun11278	2.82 ± 0.36 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
406	Jun11164	>20 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
407	Jun11166	1.22 ± 0.10 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
408	Jun11184	1.54 ± 0.18 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
409	Jun11273	0.69 ± 0.17 µM	ND*	ND*	Vero E6	45.2 ± 2.40 µM	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
410	Jun11287	2.25 ± 0.54 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
411	Jun11185	0.89 ± 0.05 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
412	Jun11167	>20 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
413	Jun11251	1.08 ± 0.08 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
414	Jun11253	0.97 ± 0.07 µM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]

415	Jun11165	0.53 ± 0.18 μM	ND*	ND*	ND*	Vero E6	>30	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
416	Jun11846	>10 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
417	Jun11813	1.30 ± 0.24 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
418	Jun11814	3.07 ± 0.23 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
419	Jun11275	0.59 ± 0.06 μM	ND*	ND*	ND*	Vero E6	15.00 ± 0.80 μM	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
420	Jun11276	0.94 ± 0.09 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
421	Jun11213	0.63 ± 0.14 μM	ND*	ND*	ND*	Vero E6	103.40 ± 5.60 μM	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
422	Jun11244	0.96 ± 0.08 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
423	Jun11288	1.14 ± 0.06 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
424	Jun11289	1.51 ± 0.15 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
425	Jun11246	1.48 ± 0.32 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
426	Jun11247	1.16 ± 0.06 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
427	Jun11277	3.35 ± 0.51 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
428	Jun11248	1.49 ± 0.18 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
429	Jun11249	1.03 ± 0.05 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
430	Jun11252	1.96 ± 0.61 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
431	Jun11274	2.78 ± 0.38 μM	ND*	ND*	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Derivatives of Jun9722 and XR8-23	[126]
432	Jun11924	177.7 ± 10.0 nM	ND*	FRET-based enzymatic assay	ND*	ND*	36.4 ± 1.3 μM	ND*	ND*	ND*	Experimental	Biarylphenyl benzamide scaffolds	[132]

433	Jun11 922	171.2 ± 14.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	11.0 ± 0.4 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
434	Jun12 38	339.8 ± 29.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	5.9 ± 0.7 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
435	Jun12 112	184.1 ± 22.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	7.9 ± 1.4 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
436	Jun12 71	116.6 ± 16.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	4.6 ± 0.4 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
437	Jun11 923	147.2 ± 7.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	11.6 ± 0.7 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
438	Jun12 111	118.2 ± 12.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	8.23 ± 0.26 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
439	Jun11 945	162.8 ± 0.5 nM	N D*	FRET-based enzymatic assay	ND*	ND*	13.5 ± 0.7 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
440	Jun11 874	65.1 ± 1.4 nM	N D*	FRET-based enzymatic assay	ND*	ND*	7.0 ± 1.1 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
441	Jun11 875	66.2 ± 2.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	4.5 ± 1.6 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
442	Jun11 899	75.9 ± 2.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	6.5 ± 0.3 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
443	Jun11 8910	367.1 ± 3.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	96.8 ± 3.6 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
444	Jun11 898	132.6 ± 4.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	19.1 ± 4.2 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
445	Jun11 931	99.3 ± 4.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	9.4 ± 1.0 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
446	Jun11 9415	143.2 ± 9.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	7.6 ± 0.3 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
447	Jun11 903	202.2 ± 8.0 nM	N D*	FRET-based enzym	ND*	ND*	7.7 ± 0.4 μM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]

				atic assay									
448	Jun11 932	83.7 ± 6.0 nM	N D*	FRET-based enzym atic assay	ND*	ND*	16.0 ± 1.2 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
449	Jun11 34	109.0 ± 7.0 nM	N D*	FRET-based enzym atic assay	ND*	ND*	37.1 ± 4.4 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
450	Jun11 933	103.0 ± 7.0 nM	N D*	FRET-based enzym atic assay	ND*	ND*	13.8 ± 1.9 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
451	Jun11 943	167.3 ± 7.0 nM	N D*	FRET-based enzym atic assay	ND*	ND*	9.1 ± 0.3 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
452	Jun12 18	1.95 ± 0.08 µM	N D*	FRET-based enzym atic assay	ND*	ND*	89.8 ± 3.0 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
453	Jun11 941	151.1 ± 4.0 nM	N D*	FRET-based enzym atic assay	1.8 ± 0.3 µM	Flip GFP	54.8 ± 8.3 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
454	Jun11 942	178.5 ± 8.0 nM	N D*	FRET-based enzym atic assay	2.2 ± 0.2 µM	Flip GFP	160.4 ± 59.2 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
455	Jun12 12	390.3 ± 25.0 nM	N D*	FRET-based enzym atic assay	ND*	ND*	17.8 ± 0.3 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
456	Jun12 15	181.7 ± 6.0 nM	N D*	FRET-based enzym atic assay	4.7 ± 0.5 µM	Flip GFP	77.6 ± 5.5 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
457	Jun12 47	165.3 ± 9.0 nM	N D*	FRET-based enzym atic assay	>60 µM	Flip GFP	>125 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
458	Jun12 382	443.4 ± 44 nM	N D*	FRET-based enzym atic assay	ND*	ND*	31.0 ± 2.1 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
459	Jun12 46	463.6 ± 39.1 nM	N D*	FRET-based enzym atic assay	ND*	ND*	39.6 ± 4.7 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
460	Jun12 11	152.7 ± 6.0 nM	N D*	FRET-based enzym atic assay	ND*	ND*	9.8 ± 1.0 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]
461	Jun12 44	81.9 ± 8.0 nM	N D*	FRET-based enzym atic assay	ND*	ND*	9.0 ± 0.7 µM	ND*	ND*	ND*	Hit	Biarylphen yl benzamide scaffolds	[132]

462	Jun12 51	74.7 ± 4.0 nM	ND*	FRET-based enzymatic assay	ND*	ND*	7.6 ± 0.4 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
463	Jun12 52	116.4 ± 10.0 nM	ND*	FRET-based enzymatic assay	ND*	ND*	8.2 ± 0.2 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
464	Jun12 54	111.8 ± 11.0 nM	ND*	FRET-based enzymatic assay	ND*	ND*	9.7 ± 2.2 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
465	Jun12 57	113.5 ± 8.0 nM	ND*	FRET-based enzymatic assay	ND*	ND*	18.0 ± 1.0 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
466	Jun12 1210	81.9 ± 5.7 nM	ND*	FRET-based enzymatic assay	13.6 ± 1.9 µM	Flip GFP	>125 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
467	Jun12 149	73.8 ± 3.0 nM	ND*	FRET-based enzymatic assay	ND*	ND*	6.3 ± 1.1 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
468	Jun12 129	90.9 ± 4.6 nM	ND*	FRET-based enzymatic assay	ND*	ND*	8.3 ± 1.2 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
469	Jun12 1910	66.4 ± 3.0 nM	ND*	FRET-based enzymatic assay	1.1 ± 0.2 µM	Flip GFP	17.7 ± 2.1 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
470	Jun12 511	91.5 ± 17.0 nM	ND*	FRET-based enzymatic assay	ND*	ND*	6.2 ± 0.2 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
471	Jun12 145	108.5 ± 6.2 nM	ND*	FRET-based enzymatic assay	1.3 ± 0.3 µM	Flip GFP	31.3 ± 5.4 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
472	Jun12 681	120.2 ± 5.1 nM	ND*	FRET-based enzymatic assay	1.8 ± 0.3 µM	Flip GFP	114.5 ± 3.4 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
473	Jun12 1911	73.2 ± 6.4 nM	ND*	FRET-based enzymatic assay	>60 µM	Flip GFP	>125 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
474	Jun12 336	118.2 ± 6.4 nM	ND*	FRET-based enzymatic assay	ND*	ND*	>125 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
475	Jun12 467	73.26 ± 6 nM	ND*	FRET-based enzymatic assay	1.7 ± 0.4 µM	Flip GFP	165.2 ± 26.5 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
476	jun12 351	98.8 ± 5.2 nM	ND*	FRET-based enzym	2.0 ± 0.4 µM	Flip GFP	>125 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]

				atic assay									
477	Jun12 199	108.8 ± 10.2 nM	N D*	FRET-based enzymatic assay	0.8 ± 0.2 µM	Flip GFP	63.2 ± 11.3 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
478	Jun12 197	102.7 ± 10.2 nM	N D*	FRET-based enzymatic assay	0.6 ± 0.1 µM	Flip GFP	43.7 ± 5.1 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
479	Jun12 603	112.2 ± 6.0 nM	N D*	FRET-based enzymatic assay	2.4 ± 0.4 µM	Flip GFP	61.0 ± 19.3 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
480	Jun12 446	132.5 ± 4.2 nM	N D*	FRET-based enzymatic assay	ND*	ND*	8.6 ± 0.5 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
481	Jun12 278	88.1 ± 11.5 nM	N D*	FRET-based enzymatic assay	1.0 ± 0.4 µM	Flip GFP	37.3 ± 3.8 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
482	Jun12 162	98.3 ± 7.0 nM	N D*	FRET-based enzymatic assay	2.1 ± 0.2 µM	Flip GFP	42.3 ± 2.3 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
483	Jun12 208	91.6 ± 6.0 nM	N D*	FRET-based enzymatic assay	16.9 ± 3.3 µM	Flip GFP	167.8 ± 15.8 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
484	Jun12 235	162.2 ± 10.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	16.5 ± 6.8 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
485	Jun12 281	111.9 ± 9.0 nM	N D*	FRET-based enzymatic assay	1.8± 0.5 µM	Flip GFP	59.2 ± 10.0 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
486	Jun12 303	121.5 ± 4.0 nM	N D*	FRET-based enzymatic assay	2.6 ± 0.2 µM	Flip GFP	56.8 ± 7.4 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
487	Jun12 284	96.6 ± 6.0 nM	N D*	FRET-based enzymatic assay	2.1 ± 0.4 µM	Flip GFP	30.4 ± 9.5 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
488	Jun12 165	145.0 ± 10.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	>125 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
489	Jun12 168	72.4 ± 3.0 nM	N D*	FRET-based enzymatic assay	9.7 ± 1.5 µM	Flip GFP	34.5 ± 10.2 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
490	Jun12 163	102.0 ± 7.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	>125 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]

491	Jun12 164	92.4 ± 4.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	>125 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
492	Jun12 198	142. 0 ± 19.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	>125 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
493	Jun12 242	90.47 ± 4.0 nM	N D*	FRET-based enzymatic assay	>60 µM	Flip GFP	>125 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
494	Jun12 147	110.3 ± 9.0 nM	N D*	FRET-based enzymatic assay	2.1 ± 0.5 µM	Flip GFP	65.0 ± 9.2 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
495	Jun12 759	206.7 ± 8.2 nM	N D*	FRET-based enzymatic assay	ND*	ND*	80.3 ± 14.6 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
496	Jun12 379	147.8 ± 10.0 nM	N D*	FRET-based enzymatic assay	2.8 ± 0.5 µM	Flip GFP	194.2 ± 15.9 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
497	Jun12 528	98.4 ± 6.2 nM	N D*	FRET-based enzymatic assay	4.5 ± 1.2 µM	Flip GFP	>125 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
498	Jun12 529	96.8 ± 13.5 nM	N D*	FRET-based enzymatic assay	2.1 ± 0.2 µM	Flip GFP	28.1 ± 4.7 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
499	Jun12 531	112.4 ± 10.3 nM	N D*	FRET-based enzymatic assay	3.3 ± 0.5 µM	Flip GFP	49.9 ± 5.3 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
500	Jun12 584	123.9 ± 4.3 nM	N D*	FRET-based enzymatic assay	1.6 ± 0.3 µM	Flip GFP	49.1 ± 2.7 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
501	Jun12 602	116.7 ± 9.2 nM	N D*	FRET-based enzymatic assay	14.7 ± 2.5 µM	Flip GFP	442.6 ± 38.4 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
502	Jun12 703	83.1 ± 4.2 nM	N D*	FRET-based enzymatic assay	4.9 ± 0.8 µM	Flip GFP	ND*	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
503	Jun12 713	86.70 ± 6 nM	N D*	FRET-based enzymatic assay	ND*	ND*	107.2 ± 6.2 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
504	Jun12 395	121.9 ± 8.0 nM	N D*	FRET-based enzymatic assay	2.9 ± 0.3 µM	Flip GFP	109.38 ± 16.16 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
505	Jun12 827	324.9 ± 46.3 nM	N D*	FRET-based enzym	ND*	ND*	23.7 ± 2.0 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]

				atic assay									
506	Jun12 831	202.5 ± 18.3 nM	N D*	FRET-based enzymatic assay	ND*	ND*	27.8 ± 1.3 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
507	Jun12 833	207.9 ± 9.3 nM	N D*	FRET-based enzymatic assay	ND*	ND*	17.6 ± 4.1 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
508	Jun12 834	263.8 ± 26.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	158.8 ± 10.9 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
509	Jun12 835	232.7 ± 10.4 nM	N D*	FRET-based enzymatic assay	ND*	ND*	33.1 ± 2.6 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
510	Jun12 836	336.1 ± 14.2 nM	N D*	FRET-based enzymatic assay	ND*	ND*	70.5 ± 4.3 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
511	Jun12 837	435.7 ± 78.6 nM	N D*	FRET-based enzymatic assay	ND*	ND*	10.3 ± 0.6 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
512	Jun13 14	222.7 ± 23.2 nM	N D*	FRET-based enzymatic assay	2.8 ±0.6 µM	Flip GFP	45.8 ± 3.6 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
513	Jun12 839	270.4 ± 12.3 nM	N D*	FRET-based enzymatic assay	ND*	ND*	14.7 ± 1.0 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
514	Jun12 682	106.8 ± 5.0 nM	N D*	FRET-based enzymatic assay	1.1 ± 0.1 µM	Flip GFP	61.3 ± 4.5 µM	ND*	ND*	ND*	Experimental	Biarylphenyl benzamide scaffolds	[132]
515	Jun12 924	240.2 ± 10.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	180.6 ± 9.2 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
516	Jun12 763	164.6 ± 23.0 nM	N D*	FRET-based enzymatic assay	ND*	ND*	>125 µM	ND*	ND*	ND*	Hit	Biarylphenyl benzamide scaffolds	[132]
517	A0	2.71 ± 0.18 µM	N D*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Lead	Hit identification using HTS	[127]
518	1	16.60 ± 3.18 µM	N D*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
519	2	>20 µM	N D*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
520	3	>20 µM	N D*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]

521	4	>20 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
522	5	>20 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
523	6	7.09 ± 0.43 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
524	7	>20 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
525	8	>20 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
526	9	>20 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
527	XR8-89	0.163 ± 0.045 μM	ND*	Enzymatic assay	>40 μM	Cell-based assay (FlipGFP)	>40 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
528	10	1.07 ± 0.13 μM	ND*	Enzymatic assay	13.63 ± 3.13 μM	Cell-based assay (FlipGFP)	>40 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
529	11	8.15 ± 0.50 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
530	12	6.08 ± 0.44 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
531	13	14.11 ± 0.70 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
532	14	>20 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
533	15	19.82 ± 0.85 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
534	16	13.75 ± 0.52 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
535	17	2.63 ± 9.14 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
536	18	>20 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
537	19	>20 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
538	20	3.58 ± 0.29 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
539	21	4.61 ± 0.33 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]

540	22	3.51 ± 0.31 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
541	23	>20 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
542	24	16.33 ± 1.47 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
543	25	4.82 ± 0.22 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
544	26	5.09 ± 0.49 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
545	27	8.77 ± 0.08 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
546	28	0.144 ± 0.018 μM	ND*	Enzymatic assay	12.44 ± 2.19 μM	Cell-based assay (FlipGFP)	30.67 ± 6.63 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
547	29	0.141 ± 0.054 μM	ND*	Enzymatic assay	8.00 ± 2.00 μM	Cell-based assay (FlipGFP)	32.51 ± 5.41 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
548	30	0.342 ± 0.224 μM	ND*	Enzymatic assay	10.59 ± 3.46 μM	Cell-based assay (FlipGFP)	>40 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
549	31	0.672 ± 0.224 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
550	32	0.275 ± 0.058 μM	ND*	Enzymatic assay	10.8 ± 1.85 μM	Cell-based assay (FlipGFP)	33.47 ± 1.60 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
551	33	0.231 ± 0.019 μM	ND*	Enzymatic assay	8.79 ± 2.19 μM	Cell-based assay (FlipGFP)	30.67 ± 6.63 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
552	34	0.436 ± 0.036 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
553	35	1.86 ± 0.68 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
554	36	1.40 ± 0.09 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]

555	37	0.095 ± 0.034 μM	ND*	Enzymatic assay	4.22 ± 0.89 μM	Cell-based assay (FlipGFP)	17.76 ± 0.68 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
556	38	0.074 ± 9.025 μM	ND*	Enzymatic assay	4.30 ± 1.21 μM	Cell-based assay (FlipGFP)	25.30 ± 9.87 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
557	39	0.078 ± 0.014 μM	ND*	Enzymatic assay	2.41 ± 0.12 μM	Cell-based assay (FlipGFP)	12.91 ± 3.55 μM	105 mL/min/gprot	ND*	ND*	Experimental	Optimization of HTS hit A0	[127]
558	(S)-39	0.035 ± 0.006 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
559	(R)-39	4.266 ± 0.013 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
560	40	0.169 ± 0.035 μM	ND*	Enzymatic assay	6.09 ± 0.45 μM	Cell-based assay (FlipGFP)	>40 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
561	41	0.523 ± 0.147 μM	ND*	Enzymatic assay	6.64 ± 1.73 μM	Cell-based assay (FlipGFP)	>40 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
562	42	0.070 ± 0.025μM	ND*	Enzymatic assay	4.11 ± 1.82 μM	Cell-based assay (FlipGFP)	18.79 ± 0.71 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
563	43	0.044 ± 0.007 μM	ND*	Enzymatic assay	2.33 ± 0.33 μM	Cell-based assay (FlipGFP)	9.40 ± 0.54 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
564	44	0.052 ± 0.008 μM	ND*	Enzymatic assay	3.81 ± 0.59 μM	Cell-based assay (FlipGFP)	11.64 ± 0.35 μM	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
565	45	0.246 ± 0.044 μM	ND*	Enzymatic assay	3.13 ± 0.75 μM	Cell-based assa	>40 μM	2503 mL/min/gprot	ND*	ND*	Experimental	Optimization of HTS hit A0	[127]

						y (Flip GFP)							
566	(S)-45	0.097 ± 0.013 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
567	(R)-45	>20 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
568	46	0.511 ± 0.090 μM	ND*	Enzymatic assay	5.33 ± 1.54 μM	Cell-based assay (Flip GFP)	>40	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
569	47	0.594 ± 0.108 μM	ND*	Enzymatic assay	5.52 ± 0.77 μM	Cell-based assay (Flip GFP)	>40	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
570	48	0.714 ± 0.128 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
571	49	1.482 ± 0.234 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
572	50	1.355 ± 0.230 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
573	51	1.741 ± 0.545 μM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Optimization of HTS hit A0	[127]
574	Jun9-53-1	2.71 μM	NN	FRET assay	ND*	Vero-E6	32.18 μM	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
575	Jun9-53-2	0.89 μM	ND*	FRET assay	25.19 μM	Vero-E6	25.70 ± 0.46 μM	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
576	Jun9-44-3	0.76 μM	ND*	FRET assay	11.23 ± 6.72 μM	Calu-3/Vero-E6	27.71 ± 1.05 μM	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
577	Jun9-28-6	2.66 μM	ND*	FRET assay	5.17 μM	Huh7-ACE2 cells	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
578	Jun9-26-5	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
579	Jun9-25-5 (Jun9-13-9)	4.98 μM	ND*	FRET assay	3.10 μM	Huh7-ACE2/Vero E6	38.76 μM	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]

580	Jun9-26-2	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
581	Jun9-13-7	7.29 μM	ND*	FRET assay	ND*	Vero E6	23.27 μM	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
582	Jun9-29-1	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
583	Jun9-13-8	71.8 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
584	Jun9-13-4	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
585	Jun9-13-6	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
586	Jun9-26-5	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
587	Jun9-29-6	26.9 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
588	Jun9-29-7	42.9 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
589	Jun9-14-5	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
590	Jun9-29-3	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
591	Jun9-25-4	49.3 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
592	Jun9-26-2	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]

593	Jun9-29-4	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
594	Jun9-47-2	6.72 μM	ND*	FRET assay	ND*	Vero E6	62.08 ± 2.53 μM	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
595	Jun9-47-3	2.44 μM	ND*	FRET assay	ND*	Vero E6	118.6 ± 2.14 μM	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
596	Jun9-87-1	0.87 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
597	Jun9-87-2	0.90 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
598	Jun9-87-3	0.80 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
599	Jun9-81-2	1.44 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
600	Jun9-81-3	1.85 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
601	Jun9-81-1	19.23 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
602	Jun9-75-5	0.56 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Experimental	QSAR of GRL-0617	[128]
603	Jun9-75-3	8.89 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
604	Jun9-75-2	1.54 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
605	Jun9-87-1	0.87 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]

606	Jun9-87-2	0.90 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
607	Jun9-87-3	0.80 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
608	Jun9-81-2	1.44 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
609	Jun9-81-3	1.85 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
610	Jun9-81-1	19.23 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
611	Jun9-75-5	0.56 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
612	ZX-136-2	9.29 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
613	ZX-136-3	10.11 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
614	ZX-136-4	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
615	ZX-136-5	8.32 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
616	ZX-136-6	11.71 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
617	ZX-136-7	1.30 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
618	Jun9-80-4	1.58 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]

619	ZX-136-8	5.13 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
620	ZX-136-9	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
621	ZX-136-10	14.35 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
622	ZX-128	2.72 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
623	ZX-129	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
624	Jun9-75-4	0.62 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
625	Jun9-84-2	2.47 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
626	Jun9-84-3	0.67 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
627	Jun9-84-4	1.30 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
628	Jun9-84-5	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
629	Jun9-84-6	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
630	Jun9-84-7	5.62 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
631	Jun9-85-1	0.66 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]

632	Jun9-85-2	1.15 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
633	Jun9-85-4	2.84 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
634	Jun9-85-5	16.59 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
635	Jun9-85-6	4.42 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
636	Jun9-85-7	6.41 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
637	Jun9-85-8	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
638	Jun9-86-1	3.99 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
639	Jun9-86-2	6.49 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
640	Jun9-86-3	7.01 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
641	Jun9-86-4	9.22 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
642	Jun9-86-5	6.12 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
643	Jun9-86-6	0.37 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
644	Jun9-86-7	>20 μM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]

645	Jun9-86-8	5.50 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
646	Jun9-87-1	0.87 µM	ND*	FRET assay	ND*	Vero-E6	14.43 ± 0.77 µM	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
647	Jun9-87-2	0.90 µM	ND*	FRET assay	ND*	Vero-E6	60.96 ± 6.79 µM	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
648	Jun9-87-3	0.80 µM	ND*	FRET assay	ND*	Vero-E6	25.97 ± 2.99 µM	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
649	Jun 10-69-2	3.99 ± 0.74 µM	ND*	FRET assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	QSAR of GRL-0617	[128]
650	VIR251	ND*	ND*	Enzymatic assay	~5 µM	ND*	ND*	ND*	ND*	ND*	Hit	Covalent peptidomimetics	[129]
651	Compound 1	ND*	ND*	Enzymatic assay	2.69 ± 0.34 µM	ND*	ND*	ND*	ND*	ND*	Hit	Covalent peptidomimetics	[129]
652	Compound 2	0.39 µM	ND*	Enzymatic assay	3.61 ± 0.52 µM	Flip GFP assay/CCk8 assay	~179.9 µM	ND*	ND*	ND*	Experimental	Covalent peptidomimetics	[129]
653	Compound 3	ND*	ND*	Enzymatic assay	2.97 ± 0.16 µM	Flip GFP assay/CCk8 assay	58.32 ± 22.11 µM	ND*	ND*	ND*	Hit	Covalent peptidomimetics	[129]
654	Compound 4	ND*	ND*	Enzymatic assay	>200 µM	Flip GFP assay/CCk8 assay	>200 µM	ND*	ND*	ND*	Hit	Covalent peptidomimetics	[129]
655	Compound 6	5.0 ± 1.9 µM	ND*	Enzymatic assay	21.0 ± 1.9 µM	Vero-E6	ND*	ND*	ND*	ND*	Experimental	Covalent peptidomimetics	[129]
656	7724772	23.5 ± 1.7 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Covalent peptidomimetics	[113]
657	6577871	100.7 ± 4.76 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Covalent peptidomimetics	[113]
658	9247873	>200 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Covalent peptidomimetics	[113]
659	GNZL-P1	2.8310 µM	ND*	Enzymatic assay	µM	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]

660	GNZ L-P2	6.9000 µM	N D*	Enzym atic assay	µM	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
661	GNZ L-P3	0.1858 µM	N D*	Enzym atic assay	µM	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
662	GNZ L-P4	0.0363 µM	Ve ro E6	Enzym atic assay	µM	ND*	24.57 µM	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
663	GNZ L-P5	0.0210 µM	N D*	Enzym atic assay	µM	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
664	GNZ L-P13	0.0900 µM	N D*	Enzym atic assay	µM	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
665	GNZ L-P17	0.00291 µM	Ve ro E6	Enzym atic assay	µM	ND*	36.68 µM	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
666	GNZ L-P20	0.1150 µM	N D*	Enzym atic assay	µM	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
667	GNZ L-P25	0.4700 µM	N D*	Enzym atic assay	µM	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
668	GNZ L-P28	0.01464 µM	N D*	Enzym atic assay	µM	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
669	GNZ L-P29	0.0420 µM	Ve ro E6	Enzym atic assay	µM	ND*	12.23 µM	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
670	GNZ L-P30	0.0440 µM	N D*	Enzym atic assay	µM	ND*	ND*	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
671	GNZ L-P31	0.00846 µM	Ve ro E6	Enzym atic assay	µM	ND*	157.4 µM	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
672	GNZ L-P35	0.00815 µM	Ve ro E6	Enzym atic assay	µM	ND*	67.67 µM	ND*	ND*	ND*	Hit	GRL-0617 analogue	[130]
673	GNZ L-P36	0.00645 µM	Ve ro E6	Enzym atic assay	111. 0 ± 9.95 nM	ND*	888.41 µM	ND*	ND*	ND*	Experi mental	GRL-0617 analogue	[130]

674	S-217622	ND*	ND*	ND*	171.9 ± 8.65 nM	ND*	ND*	ND*	ND*	ND*	Lead	GRL-0617 analogue	[130]
675	WEHI-P1	2.6 µM	ND*	Enzymatic assay	>20 µM	FRET assay	ND*	ND*	ND*	ND*	Hit	Methoxynaphtalene containing	[144]
676	WEHI-P2	397 nM	ND*	Enzymatic assay	11 µM	FRET assay	ND*	ND*	ND*	ND*	Hit	Methoxynaphtalene containing	[144]
677	WEHI-P4	19 nM	ND*	Enzymatic assay	0.31 µM	FRET assay	ND*	ND*	ND*	ND*	Hit	Methoxynaphtalene containing	[144]
678	WEHI-P8	12 nM	ND*	Enzymatic assay	0.36 µM	FRET assay	ND*	ND*	16.8	ND*	Experimental	Methoxynaphtalene containing	[144]
679	WEHI-P70	98 nM	ND*	Enzymatic assay	298 nM	FRET assay	ND*	ND*	ND*	ND*	Hit	Methoxynaphtalene containing	[144]
680	WEHI-P24		ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Methoxynaphtalene containing	[144]
681	Sennoside A	7.01 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Biochemical HTS screening	[131]
682	Sepimod (EOS)	1.21 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Biochemical HTS screening	[131]
683	Sepimod (FhG)	5.23 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Biochemical HTS screening	[131]
684	SRT 1720	>20 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Biochemical HTS screening	[131]
685	PR-619	1.39 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Lead	Biochemical HTS screening	[131]
686	CPI-169 (FhG)	14.17 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Biochemical HTS screening	[131]
687	CPI-169 (EOS)	19.8 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Biochemical HTS screening	[131]
688	DOM_SIM_710	>20 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Biochemical HTS screening	[131]
689	Purpurogallin	>20 µM	ND*	Enzymatic assay	ND*	ND*	ND*	ND*	ND*	ND*	Hit	Biochemical HTS screening	[131]

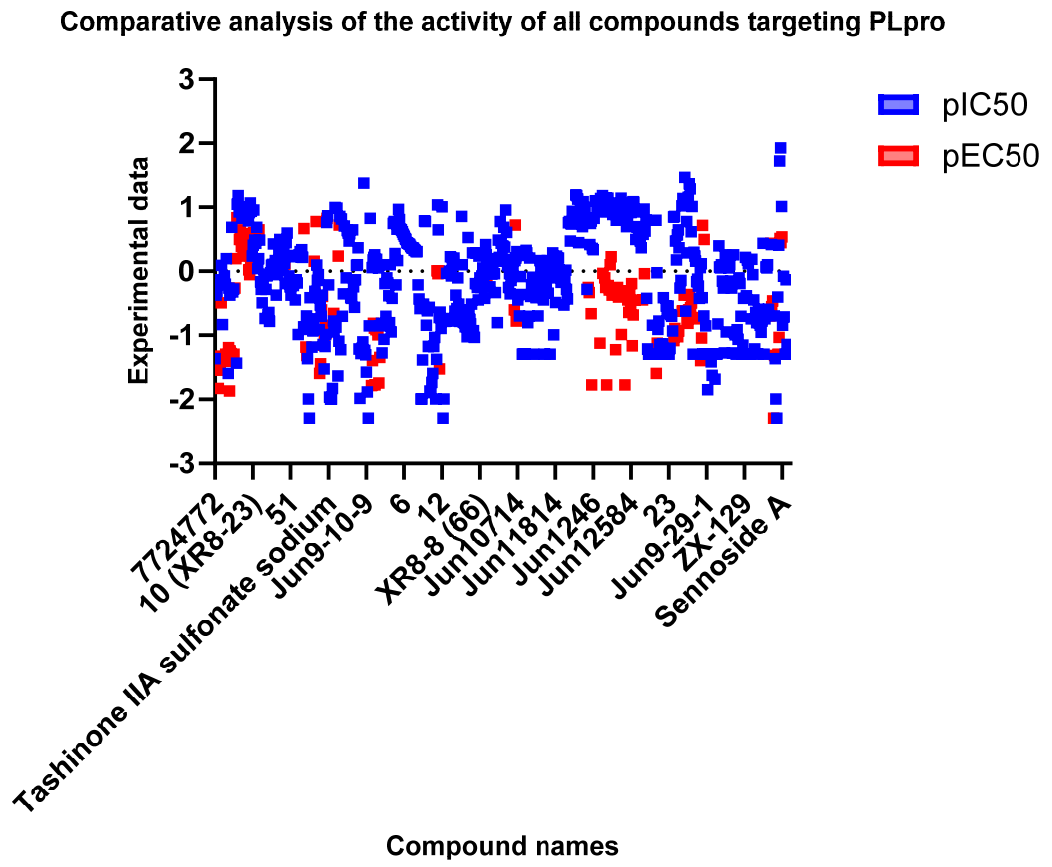


Figure S2. Comparative analysis of activity of all reported compounds targeting PLpro.

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