

Supplementary Material

Development and Optimization of a High-Throughput Screening Assay for In Vitro Anti SARS-CoV-2 Activity: Evaluation of 5676 Phase One Passed Structures

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Identifier	Name	GFP plate reader anti-viral screen EC50 (µM)	HCl antiviral screen EC50 (µM)	ATPlite toxicity CC50 (µM)
COVC-0134286843	EVP-6124_ENCENICLINE	>100.00	>100.00	20.9
COVC-0135464447	VE-822	> 5.01	8.32	10.2
COVC-0135517367	ORANTINIB STEREOISOMER	2	> 50.10	> 50.10
COVC-0136083474	HALOFANTRINE	> 20.00	9.12	15.1
COVC-0136118120	PECAZINE	> 20.00	>100.00	11.8
COVC-0136318398	CANNABINOR	>100.00	> 50.10	7.67
COVC-0136544954	CYCLOSPORINE	>100.00	>100.00	18.6
COVC-0136580428	ALMOREXANT	18.6	> 25.10	21.4
COVC-0136643402	BEDAQUILINE	> 50.10	> 50.10	13.7
COVC-0138110417	RAVIDASVIR	>100.00	>100.00	12.7
COVC-0139007958	ICI-195739	>100.00	>100.00	25.7
COVC-0139169083	JNJ-18038683	> 25.10;> 20.00	> 25.10	14.6
COVC-0139464749	BP-897	> 25.10	> 25.10	30.2
COVC-0139663433	8-AZAGUANINE	> 50.10	> 50.10	23.7
COVC-0140030971	PIPENDOXIFENE	3.63	> 6.31	4.62
COVC-0140330787	TMC310911	6.92; 2.24	9.55;>100.00	14.30; 11.80
COVC-0140549998	SALMATEROL	19.1	>100.00	18.6
COVC-0140833037	TIOPIRIDONE	9.12	>100.00	7.24
COVC-0140864590	TRIMEPRAZINE	17.4	> 25.10	21.4
COVC-0140958357	TIPIFARNIB	>100.00	>100.00	13.3
COVC-0141087222	CLOMIPRAMINE	14.5	>100.00	16
COVC-0141101284	MCN-5691	4.27	>100.00	4.84
COVC-0141142856	MEQUITAZINE	7.76	>100.00	7.76
COVC-0141155358	FLUSPIRILENE	>100.00	>100.00	7
COVC-0141155434	PHENOXYBENZAMINE HYDROCHLORIDE	20	>100.00	
COVC-0141206740	LESOPITRON	2.34	>100.00	>100.00
COVC-0141212165	NORTRIPTYLIN	15.9	>100.00	24
COVC-0141261705	EVANS-BLUE	>100.00	>100.00	18
COVC-0149442021	MOCRAVIMOD	3.31	>100.00	3.06
COVC-0149674334	BREXPIRAZOLE	>100.00	>100.00	12
COVC-0150976668			> 20.00	
COVC-0150980605	ENECADIN	1.74	21.9	
COVC-0672397984	EVP-0334	>100.00	>100.00	1.55
COVC-0672954843	DULOXETINE	>100.00; 7.24	>100.00;> 10.00	17.80; 14.80
COVC-0674506360	CAMOSTAT	> 20.00	>100.00	
COVC-0675007677	DACLATASVIR	>100.00	>100.00	19.7
COVC-0675868528	METITEPINE	7.24	>100.00	7
COVC-0675878035	SABELUZOLE	18.6	>100.00	15.3
COVC-0675923228	FLUPENTHIXOL	8.71	>100.00	7.67
COVC-0676534350	BAY-B-5369		> 20.00	
COVC-0677008167	AZELASTINE	13.3	>100.00	17.8
COVC-0677194034	REVAPRAZAN	>100.00	10.5	11.5
COVC-0677582639	SAREDUTANT (MIXTURE?)	>100.00	>100.00	23.4
COVC-0677720184	EUPROGIN	>100.00	>100.00	11.4
COVC-0677735491	THIOPROPERAZINE	13.2	>100.00	6.31
COVC-0677952181	BIFEMELANE	>100.00	20.9	26.9
COVC-067795252	METHADONE	> 25.10	> 25.10	13.2
COVC-0677970346	LACIDIPINE	> 10.00		7.24
COVC-0677970490	TIOSPIRONE	>100.00	>100.00	24.6
COVC-0678000383	CURCUMIN	>100.00	>100.00	14.8
COVC-0678006086	ABIRATERONE ACETATE	>100.00	> 25.10	9.89
COVC-0678009973	SEMATILIDE	3.89	>100.00	>100.00
COVC-0678023366	CLOCINIZINE	>100.00	20.9	21.9
COVC-0678033956	PROMETHAZINE	21.9	>100.00	33.1
COVC-0678071379	PIPTHIAZINE	13.8	>100.00	7.33
COVC-0678151537	METHDILAZINE	16.2	>100.00	14.8
COVC-0678170981	INDATRALINE	8.32	>100.00	8.51
COVC-0678171662	THIOTHIXENE	>100.00	5.75	4.96
COVC-0678230812	DRAFLAZINE	>100.00	>100.00	9.66
COVC-0678388189	HALETAZOLE	3.89	>100.00;> 10.00	3.72
COVC-0678849574	SEPROXETINE	7.59	>100.00	10.6

Identifier	Name	GFP plate reader anti-viral screen EC50 (μM)	HCl antiviral screen EC50 (μM)	ATPlite toxicity CC50 (μM)
COVC-0678867755	BENIDIPINE	>100.00	>100.00	14.8
COVC-0678879901	ITRACONAZOLE	>100.00		>100.00
COVC-0686249369	TAK-652		> 20.00	
COVC-0687833464			> 20.00	
COVC-0687841008			> 20.00	
COVC-0687843163			> 20.00	
COVC-0687847569			> 20.00	
COVC-0687852474	BGP-15	0.525	>100.00	
COVC-0687853800	EIDD-2801	14.1	4.43	
COVC-0687854362	ANAMORELIN HYDROCHLORIDE		> 20.00	
COVC-1207972476	DR1289116	>100.00	> 50.10	16
COVC-1207984410	ANDROGRAPHOLIDE	>100.00	>100.00	21.6
COVC-1208049825	GS-938	> 20.00	> 50.10	
COVC-1210360354	METHOTRIMEPRAZINE_LEVOMEPRIMAZINE	11.8	> 50.10	11.6
COVC-1210360383	MONENSIN	> 20.00	1.12	
COVC-1210363295	PRENYLAMINE	8.71	>100.00	8.41
COVC-1210363846	SULCOTIDIL	>100.00	>100.00	3.27
COVC-1211756174	DARIFENACIN	> 25.10	>100.00	56.2
COVC-1212730902	NEBIVOLOL	8.91	>100.00	7
COVC-1212741697	R-167154 ISOMER	>100.00	>100.00	19.5
COVC-1212748902	NEBIVOLOL	> 10.00	>100.00	8.71
COVC-1213406057	PIPERLONGUMINE	> 50.10	> 50.10	9.55
COVC-1214272359	CLEMASTINE	> 50.10	20.4	18.4
COVC-1214358711	BROFAROMINE	14.8	>100.00	19.1
COVC-1214407107	QUININE_QUINIDINE	15.1	> 25.10	> 25.10
COVC-1214563522	BITOLTEROL	8.13	>100.00	5.69
COVC-1214565530	METIXENE	9.55	>100.00	10.1
COVC-1214607586	PROPIPOCAINE	>100.00	>100.00	31.6
COVC-1214614542	CARFENAZINE	>100.00	>100.00	6.31
COVC-1214621709	FENOBAM	> 20.00	> 25.10	
COVC-1214767323	ZOTEPINE	>100.00	>100.00	12.3
COVC-1214826443	GIRISOPAM	>100.00	>100.00	>100.00
COVC-1214829248	HALOFANTRINE	9.55	9.12	11.5
COVC-1214857454	FLUPHENAZINE	>100.00	>100.00	7.76
COVC-1214857892	OXATOMIDE	>100.00	>100.00	12.6
COVC-1214895840	SPIPERONE	20.4	22.4	81.3
COVC-1214897179	PENFLURIDOL	>100.00	>100.00	3.59
COVC-1214903948	INDOMETACIN	>100.00	>100.00; > 50.10	>100.00
COVC-1215023048	METHYPRYLON	18.4	> 25.10	> 25.10
COVC-1215027317	LEVOMEPRIMAZINE	>100.00	>100.00	22.9
COVC-1215738110	CLOMIFENE	> 20.00	> 20.00	
COVC-1222873116	HYDROXYCHLOROQUINE STEREOISOMER(S)	12.7	18.8	> 50.10
COVC-1223085504	CCS-1477 (S*)	>100.00	>100.00	3.16
COVC-1224702964			>100.00	
COVC-1746032955	REMDESIVIR	4.64	3.12	95.5
COVC-1746696265	ATRACURIUM BESYLATE		> 20.00	
COVC-1746967931	TOREFORANT	> 25.10	> 50.10	22.4
COVC-1747138106	BERBAMINE	8.51	> 6.31	10.2
COVC-1747138440	SALINOMYCIN	> 20.00	1.29	
COVC-1747138479	BEBEERINE	> 10.00	5.37	11.5
COVC-1747162848	CASOPITANT	> 25.10	> 25.10	17.8
COVC-1747188285	BI-2536	> 50.10	> 50.10	0.603
COVC-1747231597	DEPTROPINE	7.41	> 50.10	13.5
COVC-1747292777	LYNESTRENOL	> 50.10	> 50.10	10.5
COVC-1747397988	HT-61	> 20.00	4.9	
COVC-1748269057	NERATINIB		> 10.00	
COVC-1751145778	DITHRANOL	>100.00	>100.00	>100.00
COVC-1751409823	SYROSINGOPINE	>100.00	>100.00	8.91
COVC-1751415324	OXAPROZIN	11.8	> 50.10	> 50.10
COVC-1751439919	PERAZINE	14	>100.00	14.6
COVC-1751458750	NOXIPTILINE	14.1	>100.00	77.6

Identifier	Name	GFP plate reader anti-viral screen EC50 (µM)	HCl antiviral screen EC50 (µM)	ATPlite toxicity CC50 (µM)
COVC-1751645509	CARPIPRAMINE	8.91	>100.00	8.61
COVC-1751700625	CLOPIPAZAN	> 20.00	>100.00	15
COVC-1751748815	METHOXYTACRINE	11.5	> 25.10	47.9
COVC-1751763386	PROADIFEN	5.13	>100.00	24
COVC-1751764998	ASTEMIZOLE	>100.00	>100.00	7.5
COVC-1751771027	PROFLAVINE	15	> 25.10	6.61
COVC-1751892074	BBR-3464		> 20.00	
COVC-1751893009	DIPERODON	15.1	> 25.10	> 25.10
COVC-1752607069	SAPERCONAZOLE	>100.00;> 20.00	>100.00	>100.00
COVC-1752620251	3 ALLYL FENTANYL	4.37	4.9	
COVC-1760096432	GSK-921	> 50.10	> 50.10	2.63
COVC-1760099291	AJULEMIC ACID	>100.00	>100.00	21.4
COVC-1760287043	SULFATINIB	> 10.00	> 50.10	4.9
COVC-1761575739			> 20.00	
COVC-1761588262			> 20.00	
COVC-1761590281			> 20.00	
COVC-1761595595	V-GLYCOPEPTIDE		> 20.00	
COVC-1761604319	ADOMEGLIVANT	> 10.00	> 6.31	10.4
COVC-2282947189	VALRUBICIN		> 20.00	
COVC-2283008312	NAVITOCCLAX	>100.00	>100.00	4.73
COVC-2283590314	OSIMERTINIB	>100.00	>100.00	3.09
COVC-2283593123	GSK1070916	>100.00	>100.00	9.33
COVC-2285168592	VINORELBINE		> 20.00	
COVC-2285169276	C-172	19.5	14.5	28.2
COVC-2286471467	LOFENTANIL	20.9	> 25.10	
COVC-2286484880	METHYLDOPA	17.8	>100.00	
COVC-2286491085	NEBIVOLOL	>100.00	>100.00	10.2
COVC-2286528427	CDP-840 (B)	>100.00	>100.00	23.4
COVC-2286535978	PENBUTOLOL	15.1	20	29.5
COVC-2287142567	NORCYCLOBENZAPRINE	> 50.10	> 50.10	23.4
COVC-2287147580	CEFOPERAZONE	> 20.00	> 20.00	
COVC-2287807964	SAQUINAVIR	>100.00	>100.00	18.2
COVC-2288269965	PIPERACETAZINE	16.2	> 12.60	12.2
COVC-2288318596	METHOPROMAZINE	> 20.00	>100.00	14.1
COVC-2288327793	DIAMOCAINE	9.55	22.4	46.8
COVC-2288339516	OXETORONE	18.2	>100.00	12.2
COVC-2288570388	DOSULEPIN	16.6	> 25.10	20
COVC-2288571827	BUCINDOLOL	17	>100.00	30.9
COVC-2288600616	DRONEDARONE	3.02	>100.00	3.85
COVC-2288609209	LOPERAMIDE	11.8	8.91	22
COVC-2288621041	PRENYLAMINE	8.51	>100.00	10.7
COVC-2288636389	ZIMELIDINE	> 20.00		> 10.00
COVC-2288688211	MILENPERONE	>100.00	>100.00	32.4
COVC-2288695035	CARVEDILOL	15.5	10	17
COVC-2288727795	NAFOXIDINE	>100.00	>100.00	3.85
COVC-2288809083	RHODOQUINE	24.6	>100.00	>100.00
COVC-2288955269	LIFIBRATE	>100.00	>100.00	38
COVC-2289454566	BEDAQUILINE	>100.00	15.5	26.9
COVC-2289479927	ZUCLOPENTHIXOL_CLOPENTHIXOL	7.24	>100.00	6.68
COVC-2289732646	PIMETHIXENE	>100.00	>100.00	25.7
COVC-2298439635			> 20.00;> 20.00	
COVC-2298460306			> 20.00	
COVC-2298477237	O-304		> 20.00	
COVC-2819871799	IVACAFTOR	4.57	> 25.10	4.62
COVC-2820438510	LOTEPREDNOL ETABONATE		> 20.00	
COVC-2820464103	VOLASERTIB	> 50.10	> 50.10	0.234
COVC-2820786116	TETRANDRINE_HANFANGCHIN A	3.98	> 50.10	5.17
COVC-2820802843	CRIZOTINIB	6.76	4.47	4.42
COVC-2821037923	FLUORESC EIN		>0.3090	> 20.00
COVC-2821711673	HYDROQUINIDINE	15.5	> 25.10	> 25.10
COVC-2822096521	RENYTOLINE	3.47	>100.00	2.92

Identifier	Name	GFP plate reader anti-viral screen EC50 (µM)	HCl antiviral screen EC50 (µM)	ATPlite toxicity CC50 (µM)
COVC-2823343639	NEBIVOLOL	>100.00	>100.00	7.85
COVC-2823361537	NEBIVOLOL	>100.00	>100.00	7.76
COVC-2824600869	ARIPIRAZOLE	>100.00	>100.00	11.4
COVC-2825210622	BUCLIZINE	>100.00	20.4	81.3
COVC-2825221500	SERCLOREMINE	17.2	>100.00	34.7
COVC-2825327487	PAROXETINE	15.1	>100.00	16.6
COVC-2825450452	CLOSIPIRAMINE	7.41	>100.00	8.13
COVC-2825472328	LIDOFLAZINE	9.55	>100.00	8.41
COVC-2825487070	ARBIDOL	>100.00	>100.00	
COVC-2825507141	ACEPROMAZINE	>100.00	>100.00	22.4
COVC-2825508294	MASOPROCOL	>100.00	>100.00	37.2
COVC-2825514435	CHLOROQUINE	5.86	9.46	38.7
COVC-2825515130	QUINESTROL	8.71	>100.00	7.59
COVC-2825616197	CLOBENZTROPINE	9.77	>100.00	8.13
COVC-2825616302	DIHYDREXIDINE	7.94	>100.00	18.6
COVC-2825622218	OXETHAZAINE	18.6	>100.00	26.3
COVC-2825640648	HOMOCHLORCYCLIZINE	> 20.00	> 25.10	21.1
COVC-2825645391	TERFENADINE	>100.00	>100.00	5.13
COVC-2826330726	ZAMIFENACIN	>100.00	87.1	>100.00
COVC-2826351877	SABELUZOLE	>100.00	>100.00	15.5
COVC-2833485378	HYDROXYCHLOROQUINE (R*)	12.7	> 50.10	> 50.10
COVC-2833739552	QCC-374	17.4	16.6	50.1
COVC-2835343357	LEVOMEFOLATE		> 20.00	
COVC-3356547646	HDAC-42_AR-42	> 20.00		0.851
COVC-3356682871	TEPOTINIB_EMD-1214063	>100.00	>100.00	5.75
COVC-3356809212	CYTARABINE	> 50.10	> 20.00	
COVC-3357305447	TPEN	> 3.09	>100.00	1.93
COVC-3357309398	CEFUROXIME AXETIL		> 20.00	
COVC-3357775383	SUDOTERB	>100.00	>100.00	14.3
COVC-3357844334	TRIBENOSIDE	> 50.10	> 50.10	17.4
COVC-3358854404	PONATINIB_ICLUSIG	> 20.00;>100.00	>100.00	0.9890;< 1.55
COVC-3359139833	ERDAFITINIB	> 10.00;>100.00	> 6.31	5.25; 3.63
COVC-3359217199	MK-0893	>100.00	>100.00	18.8
COVC-3360221789	EPIRUBICIN		>100.00	
COVC-3360223611	CINNARIZINE	18.2	>100.00	14.5
COVC-3360248091	DOXORUBICIN	8.04	33.1	64.6
COVC-3360252970	ALVOCIDIB		> 10.00	
COVC-3360889795	CONESSINE	12	> 25.10	34.7
COVC-3361592863	TMC-353121	> 20.00	> 20.00;> 5.01	9.33
COVC-3361708049	AMG-487-(+/-)	> 20.00	> 20.00	
COVC-3361719627	TANDUTINIB	>100.00	>100.00	11.5
COVC-3362013046	PERICIAZINE	> 20.00	>100.00	12.7
COVC-3362049948	METOFENAZATE	18.6	>100.00	>100.00
COVC-3362050611	ACETOPHENAZINE	>100.00	>100.00	14.6
COVC-3362302644	FLUPIRTINE	>100.00	>100.00	>100.00
COVC-3362312915	PROTRIPTYLINE	>100.00	>100.00	26.3
COVC-3362312957	THIORIDAZINE	6.76	>100.00	6.38
COVC-3362314340	BENZATROPINE	> 25.10	>100.00	46.8
COVC-3362314676	RAUNORMINE_DESERPIDINE	> 20.00	> 25.10	11.5
COVC-3362317361	QUINESTROL	>100.00	>100.00	8.22
COVC-3362343100	TERFLAVOXATE	>100.00	>100.00	63.1
COVC-3362347376	TRIFLUOPERAZINE	6.46	>100.00	7.94
COVC-3362350497	CHLORBENZOXAMINE	>100.00	> 25.10	15.3
COVC-3362350605	LASALOCID	>0.6310	1.07	5.37
COVC-3362375297	NORGESTIMATE	>100.00	>100.00	20.9
COVC-3362380349	CINCHOCAINE	29.1	29.5	39.6
COVC-3362381936	PROMAZINE	16.2	>100.00	25.7
COVC-3362486392	DOTARIZINE	> 20.00	10	17.4
COVC-3363187991	COLCHICINE	>100.00	>100.00	
COVC-3370896893	R-428_BEMCENTINIB	1.78	> 50.10	1.55
COVC-3372196066	ROVAZOLAC		> 20.00	

Identifier	Name	GFP plate reader anti-viral screen EC50 (µM)	HCl antiviral screen EC50 (µM)	ATPlite toxicity CC50 (µM)
COVC-3372202143			> 20.00	
COVC-3372208332	L-1777		> 20.00	
COVC-3372208930	MAVORIXAFOR		> 20.00	
COVC-3893557264	BMS833923	2.95	>100.00	3.09
COVC-3893559927	RIBOCICLIB	>100.00	>100.00	38.9
COVC-3894275940	TECALCET	16.6	>100.00	28.2
COVC-3894718404	DOSULEPIN	14.3	> 25.10	17
COVC-3894856214	GIVINOSTAT	10.5	>100.00	0.767
COVC-3895781309	ALOXISTATIN	34.3	85.1	>100.00
COVC-3897093565	NEBIVOLOL	>100.00	>100.00	7.16
COVC-3897104103	SABELUZOLE	18.6	>100.00	19.5
COVC-3897760602	VITAMINE B2_RIBOFLAVIN	11.2	> 50.10	> 50.10
COVC-3898089676	DARUNAVIR	> 20.00	> 20.00	
COVC-3898253804	LOPINAVIR	22.9	15.7	33.7
COVC-3898420702	NELFINAVIR	5.22	3.50; 4.10	11.2
COVC-3898606637	JNJ-5207852	> 20.00	> 20.00	
COVC-3898674512	IMATINIB_GLEEVEC_	11	21.9	11.9
COVC-3898855212	CHLORPROTHIXENE	7.08	>100.00	13.8
COVC-3898932127	BUTOPROZINE	>100.00	>100.00	6.61
COVC-3898935732	OXAPROTILINE	>100.00	>100.00	28.2
COVC-3898956268	CLOXACEPRIDE	3.63	>100.00	2.85
COVC-3899173551	FLUTROLINE	4.68	>100.00	6.92
COVC-3899185596	RESCINNAMINE	> 50.10	>100.00	5.5
COVC-3899220261	FENRETINIDE	>100.00	2.95	5.01
COVC-3899221661	RESERPINE	> 25.10	> 50.10	11
COVC-3899227081	ALGESTONE ACETOPHENIDE	>100.00	> 12.60	15.5
COVC-3899229498	RG-12915	7.94	> 25.10	21.6
COVC-3899304998	FEZOLAMINE	14.5	>100.00	39.8
COVC-3899357267	DILAZEP	>100.00	>100.00	28.2
COVC-3899382603	HYDROXYCHLOROQUINE	11.6	> 10.00; 18.00	47.9
COVC-3899396989	CYCLOSPORINE	6.61	> 50.10	26.3
COVC-3899449667	SEGANSERIN	7.59	>100.00	10.2
COVC-3900064416	ASENAPINE	> 25.10	>100.00	5.89
COVC-3900085863	POSACONAZOLE	>100.00	>100.00	>100.00
COVC-3900086865	FLUOTRACEN	>100.00	10.5	12
COVC-3900092763	NABILONE	8.91	> 25.10	11.1
COVC-3900101626	TERCONAZOLE	16.6	> 12.60	10
COVC-3900102081	RITONAVIR	> 50.10		37.2
COVC-3900128072	R-167154	>100.00	> 50.10	22.4
COVC-3900346251	ORANTINIB	1.78	> 25.10	> 25.10
COVC-3907440078	CCS-1477 (R*)	>100.00	>100.00	9.12
COVC-3907758471	ANLOTINIB	>100.00	>100.00	5.25
COVC-3909057522			> 20.00	
COVC-3909068638			> 20.00	