Supporting Information

Virtual screening and quantum chemistry analysis for SARS-CoV-2 RNA-dependent RNA polymerase using the ChEMBL database: Reproduction of the remdesivir-RTP and favipiravir-RTP binding modes obtained from cryo-EM experiments with high binding affinity

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Contents

Table S1. Potential anti-SARS-CoV-2 drugs obtained from rDock virtual screening of the ChEMBL database. **S2-S11**

Table S2. Hit compounds obtained by combining the AutoDock Vina and rDock virtual screening results using the ChEMBL database. **S11-S17**

Table S1. Potential anti-SARS-CoV-2 drugs obtained from rDock virtual screening of the ChEMBL database.

ChEMBL ID	Synonym	Status	Target	Action	rDock Score (kcal/mol)	AutoDock Vina Score (kcal/mol)
CHEMBL2106851	NICOMORPHINE		Opioid receptor mu 1	Analgesic	−61.521	−10.2
CHEMBL1371412	TIOXIDAZOLE		Prelamin-A/C	Anthelmintic	−63.708	−6.7
CHEMBL547	ISOTRETINOIN	Approved	Retinoic acid receptor (RAR) agonist	Anti-acne	−60.736	−7.3
CHEMBL23771	TIXANOX		Aldose reductase	Anti-allergic	−60.962	−8.1
CHEMBL296419	ASTEMIZOLE	Approved	H1 receptor antagonist	Anti-allergic	−65.952	−9.2
CHEMBL61301	TECASTEMIZOLE		Histamine receptor H1 antagonist	Anti-allergic	−85.018	−7.7
CHEMBL2104845	ONTAZOLAST		Eukotriene receptor antagonist	Antiasthmatic	−63.044	−8.2
CHEMBL501122	CEFTAROLINE FOSAMIL	Approved	Penicillin binding protein	Antibacterial	−85.659	−10.3
CHEMBL161	CEFTRIAXONE	Approved	Penicillin binding protein	Antibacterial	−67.839	−10.0
CHEMBL2110979	PIRBENICILLIN		Penicillin binding protein	Antibacterial	−64.577	−9.7
CHEMBL2110884	CETOCYCLINE			Antibacterial	−66.912	−9.6
CHEMBL44354	CEFTAZIDIME	Approved	Penicillin binding protein	Antibacterial	−60.388	−9.0
CHEMBL1237124	MECLOCYCLINE		30S ribosomal subunit	Antibacterial	−62.029	−9.0
CHEMBL1697786	CEFUROXIME PIVOXETIL		Penicillin binding protein	Antibacterial	−66.707	−9.0
CHEMBL1433	DOXYCYCLINE	Approved	30S ribosomal subunit	Antibacterial	−63.212	−8.9
CHEMBL1583	BACAMPICILLIN	Approved	Monoamine oxidase A	Antibacterial	−67.654	−8.7
CHEMBL1524273	PHTHALYLSULFATHIAZOLE [1]	Approved	Dihydropteroate synthase	Antibacterial	−96.910	−8.6
CHEMBL1109	SULFAPHENAZOLE	Approved	Dihydropteroate synthase	Antibacterial	−89.002	−8.2
CHEMBL2104908	SULFAZAMET			Antibacterial	−94.032	−8.2
CHEMBL1484857	SUCCINYLSULFATHIAZOLE		Dihydropteroate synthase	Antibacterial	−92.546	−7.9
CHEMBL1167	SPECTINOMYCIN	Approved	30S ribosomal subunit	Antibacterial	−60.601	−7.7
CHEMBL1355299	SULFAETHIDOLE [1]		Putative fructose-1,6-bisphosphate aldolase	Antibacterial	−77.373	−7.6
CHEMBL1191	SULFAMETHIZOLE [1]	Approved	Dihydropteroate synthase	Antibacterial	−85.152	−7.5

CHEMBL453	SULFISOXAZOLE [1]	Approved	Dihydropteroate synthase	Antibacterial	−93.518	−7.4
CHEMBL2105399	SULFAMOXOLE [1]		Dihydropteroate synthase	Antibacterial	−75.727	−7.4
CHEMBL2107088	SULFASOMIZOLE			Antibacterial	−85.069	−7.3
CHEMBL437	SULFATHIAZOLE	Approved	Dihydropteroate synthase	Antibacterial	−95.889	−7.2
CHEMBL4594290	TANIBORBACTAM	Phase1	beta-Lactamase inhibitor	Antibacterial	−60.599	nd [4]
CHEMBL3544919	CIRAPARANTAG	Phase2		Anticoagulant	−64.728	−8.7
CHEMBL549671	SABELUZOLE			Anticonvulsant	−79.056	−9.0
CHEMBL310160	BIPENAMOL		Trypanothione reductase	Antidepressant	−69.331	−6.5
CHEMBL1770248	ERTUGLIFLOZIN	Approved	SGLT-2 inhibitor	Anti-diabetic	−68.404	−9.1
CHEMBL450117	GLYPROTHIAZOL		Monoamine oxidase A	Anti-diabetic	−78.899	−7.6
CHEMBL2107408	GLYBUZOLE [1]			Anti-diabetic	−89.891	−7.3
CHEMBL94087	GLYBUTHIAZOL [1]			Anti-diabetic	−78.713	−7.3
CHEMBL550348	DEFERASIROX	Approved		Antidote	−68.372	−8.9
CHEMBL1950289	TANZISERTIB [1]	Phase2	c-Jun N-terminal kinase inhibitor	Antifibrotic	−86.574	−9.5
CHEMBL4297591	FOSMANOGEPIX	Phase2	Glucosaminylphosphatidylinositol acyltransferase	Antifungal	−65.501	−9.3
CHEMBL333325	FOSRAVUCONAZOLE	Phase2	Sterol 14alpha-demethylase	Antifungal	−63.940	−8.9
CHEMBL2105391	PROTIOFATE			Antifungal	−60.916	−6.2
CHEMBL2105913	BARMASTINE		Histamine receptor H1	Antihistaminic	−93.233	−9.2
CHEMBL539423	SPARSENTAN	Phase3	Angiotensin II receptor type 1	Anti-hypertensive	−84.211	−9.3
CHEMBL2111148	TIPENTOSIN			Anti-hypertensive	−63.007	−8.1
CHEMBL295409	TIAMENIDINE			Anti-hypertensive	−90.127	−5.6
CHEMBL114586	SEPIMOSTAT [1]		Serine protease inhibitor	Anti-inflammatory	−85.231	−9.7
CHEMBL4297477	BREPOCITINIB	Phase2	Janus kinase 1	Anti-inflammatory	−61.358	−9.4
CHEMBL1200342	PARAMETHASONE ACETATE	Approved	Glucocorticoid receptor agonist	Anti-inflammatory	−73.043	−9.3
CHEMBL2105842	CORTIVAZOL	Approved	Glucocorticoid receptor agonist	Anti-inflammatory	−74.903	−9.3
CHEMBL2106520	HALOPREDONE ACETATE		Glucocorticoid receptor partial agonist	Anti-inflammatory	−60.970	−9.2
CHEMBL216981	NAVARIXIN	Phase2	Interleukin-8 receptor B	Anti-inflammatory	−120.782	−8.8
CHEMBL1385514	DICHLORISONE ACETATE		Glucocorticoid receptor agonist	Anti-inflammatory	−72.408	−8.1

CHEMBL2105059	MORNIFLUMATE			Anti-inflammatory	−62.266	−8.1
CHEMBL1413176	NIFENAZONE		Menin/Histone-lysine N-methyltransferase MLL	Anti-inflammatory	−61.214	−7.6
CHEMBL2104561	ELTENAC [1]			Anti-inflammatory	−71.821	−6.7
CHEMBL3809489	BEMCENTINIB	Phase2	Receptor tyrosine kinase inhibitor	Anti-neoplastic	−97.163	−11.2
CHEMBL3989868	TUCATINIB	Approved	erb-B2 receptor tyrosine kinase 2	Anti-neoplastic	−78.569	−11.0
CHEMBL3904602	LEROCICLIB	Phase1	Cyclin-dependent kinase (CDK) inhibitor	Anti-neoplastic	−64.184	−10.7
CHEMBL4582651	PRALSETINIB	Phase3	Replicase polyprotein 1ab	Anti-neoplastic	−90.662	−10.6
CHEMBL4130229	VODOBATINIB	Phase2	BCR-ABL	Anti-neoplastic	−65.358	−10.3
CHEMBL3889654	LAROTRECTINIB	Approved	Tropomyosin receptor kinase inhibitor	Anti-neoplastic	−68.149	−10.1
CHEMBL3218576	COPANLISIB	Approved	Phosphatidylinositol 3-kinase inhibitor	Anti-neoplastic	−71.829	−10.0
CHEMBL3301622	GILTERITINIB	Approved	Tyrosine-protein kinase receptor UFO	Anti-neoplastic	−64.290	−10.0
CHEMBL1908391	MASITINIB	Phase3	Dual specificty protein kinase CLK1	Anti-neoplastic	−90.568	−10.0
CHEMBL522892	DOVITINIB	Phase3	Vascular endothelial growth factor receptor 2	Anti-neoplastic	−60.745	−10.0
CHEMBL2107823	GANDOTINIB	Phase2	Janus kinase (JAK) inhibitor	Anti-neoplastic	−96.129	−10.0
CHEMBL1421	DASATINIB	Approved	Tyrosine kinase inhibitor	Anti-neoplastic	−99.368	−9.9
CHEMBL3265032	ENTOSPLETINIB	Phase2	Tyrosine-protein kinase SYK	Anti-neoplastic	−64.693	−9.9
CHEMBL1091644	LINSITINIB	Phase3	Insulin-like growth factor 1 receptor antagonist	Anti-neoplastic	−62.711	−9.8
CHEMBL4297188	MIRANSERTIB [2]	Phase2	AKT serine/threonine kinase inhibitor	Anti-neoplastic	−67.950	−9.6
CHEMBL4594275	GUSACITINIB	Phase2	Janus kinase 1	Anti-neoplastic	−63.792	−9.5
CHEMBL31965	CANERTINIB	Phase3	Epidermal growth factor receptor erbB1	Anti-neoplastic	−61.274	−9.4
CHEMBL3545369	EPACADOSTAT	Phase3	Indoleamine 2,3-dioxygenase inhibitor	Anti-neoplastic	−93.000	−9.4
CHEMBL1287853	FEDRATINIB	Approved	Janus kinase (JAK) inhibitor	Anti-neoplastic	−65.415	−9.3
CHEMBL4297190	SURUFATINIB	Phase3	Tyrosine kinase inhibitor	Anti-neoplastic	−61.578	−9.3
CHEMBL2103830	FOSTAMATINIB	Approved	Tyrosin kinase inhibitor	Anti-neoplastic	−61.766	−9.2
CHEMBL252164	LUMINESPIB	Phase2	Hsp 90 inhibitor	Anti-neoplastic	−60.834	−9.2

CHEMBL4297595	LISAVANBULIN	Phase1	Tubulin polymerization inhibitor	Anti-neoplastic	−61.208	−9.2
CHEMBL25336	BISANTRENE [1]	Phase3	RPMI-8226	Anti-neoplastic	−101.755	−9.1
CHEMBL2103842	VARLITINIB [1]	Phase2	Receptor protein-tyrosine kinase erbB-2	Anti-neoplastic	−72.031	−9.1
CHEMBL3989970	MAVELERTINIB	Phase2	Epidermal growth factor receptor erbB1	Anti-neoplastic	−76.890	−9.1
CHEMBL2110669	OMTRIPTOLIDE		DNA	Anti-neoplastic	−62.258	−8.9
CHEMBL1094636	NIRAPARIB	Approved	PARP inhibitor	Anti-neoplastic	−60.508	−8.8
CHEMBL3353410	OSIMERTINIB	Approved	Epidermal growth factor receptor erbB1	Anti-neoplastic	−62.621	−8.8
CHEMBL428690	ALVOCIDIB	Phase3	Cyclin-dependent kinase (CDK) inhibitor	Anti-neoplastic	−75.444	−8.8
CHEMBL4558324	LAZERTINIB	Phase1	Epidermal growth factor receptor	Anti-neoplastic	−61.508	−8.7
CHEMBL3422109	AVANBULIN		Tubulin polymerization inhibitor	Anti-neoplastic	−84.936	−8.6
CHEMBL435191	EDOTECARIN	Phase3	Topoisomerase I inhibitor	Anti-neoplastic	−63.426	−8.5
CHEMBL271068	ROSABULIN	Phase1		Anti-neoplastic	−60.832	−8.5
CHEMBL2105946	AMBOMYCIN			Anti-neoplastic	−63.695	−8.0
CHEMBL3544911	PREXASERTIB [2]	Phase2	Checkpoint kinase inhibitor	Anti-neoplastic	−91.788	−7.9
CHEMBL4303782	ZOTATIFIN [2]	Phase1	RNA helicase inhibitor	Anti-neoplastic	−61.715	−7.2
CHEMBL476	DACARBAZINE	Approved	DNA, RNA	Anti-neoplastic	−63.025	−5.6
CHEMBL459505	TALAROZOLE	Phase2	Cytochrome P450 family 26 subfamily A member 1	Antipsoriatic	−93.312	−7.9
CHEMBL53950	INCADRONIC ACID		Farnesyl diphosphate synthase	Antiresorptive	−63.453	−6.6
CHEMBL1350	TILUDRONIC ACID			Antiresorptive	−60.652	−6.5
CHEMBL14249	ADENOSINE TRIPHOSPHATE [3]	Phase2	P2Y purinoceptor 1	Antivertigo	−62.435	−8.8
CHEMBL473882	ENTECAVIR TRIPHOSPHATE [3]		HBV reverse transcriptase	Antiviral	−67.745	−9.7
CHEMBL3818050	FAVIPIRAVIR-RTP [2,3]		Influenza A virus RNA-directed RNA polymerase	Antiviral	−67.292	−9.1
CHEMBL2016761	RDV-TP [3]		Hepatitis C virus	Antiviral	−62.583	−8.9
CHEMBL4594375	PENCICLOVIR TRIPHOSPHATE [3]		Herpesvirus DNA polymerase inhibitor	Antiviral	−66.854	−8.7
CHEMBL290507	ENVIRADENE			Antiviral	−60.236	−8.4
CHEMBL1230	LAMIVUDINE		HIV reverse	Antiviral	−63.543	−8.2

	TRIPHOSPHATE [3]		transcriptase inhibitor			
CHEMBL3039503	LOMIBUVIR	Phase2	HCV NS5B polymerase	Antiviral	−70.808	−8.1
CHEMBL515408	MARIBAVIR	Phase3	HCMV protein kinase	Antiviral	−78.670	−8.0
CHEMBL1162433	ADEFOVIR DIPHOSPHATE		Reverse transcriptase inhibitor	Antiviral	−61.475	−7.9
CHEMBL1214598	UMIFENOVIR	Phase3		Antiviral	−61.709	−7.6
CHEMBL1538	TENOFOVIR DISOPROXIL	Approved	HBV reverse transcriptase	Antiviral	−61.255	−7.5
CHEMBL2111023	NISBUTEROL			Bronchodilator	−63.683	−7.6
CHEMBL436559	CARIPORIDE		Na+/H+ antiport inhibitor	Cardioprotectant	−66.526	−7.3
CHEMBL1014	CANDESARTAN CILEXETIL	Approved	Angiotensin II receptor antagonist	Cardiovascular	−65.673	−10.3
CHEMBL539697	DABIGATRAN ETEXILATE	Approved	Thrombin inhibitor	Cardiovascular	−71.432	−9.2
CHEMBL1697762	NICERITROL			Cardiovascular	−64.854	−8.9
CHEMBL282724	SITAXENTAN	Approved	Endothelin receptor type A antagonist	Cardiovascular	−84.495	−8.6
CHEMBL2107326	DASANTAFIL		Phosphodiesterase V inhibitor	Cardiovascular	−78.105	−8.3
CHEMBL2105424	ROMIFIDINE		Adrenergic receptor agonist	Cardiovascular	−68.171	−7.0
CHEMBL35505	DIHYDRALAZINE			Cardiovascular	−61.789	−6.9
CHEMBL1079	TIZANIDINE [1]		alpha-Adrenergic receptor agonist	Cardiovascular	−90.626	−6.6
CHEMBL19236	MOXONIDINE	Approved	Adrenergic receptor alpha-1	Cardiovascular	−78.408	−6.3
CHEMBL1197578	CYPROQUINATE			Coccidiostat	−62.345	−7.5
CHEMBL2368925	DOLASETRON	Approved	Serotonin 5-HT3 receptor antagonist	Gastrointestinal	−61.293	−8.5
CHEMBL2105496	SUFOTIDINE		Histamine receptor H2 antagonist	Gastrointestinal	−81.234	−8.3
CHEMBL942	BISACODYL	Approved	Prelamin-A/C	Gastrointestinal	−60.770	−7.5
CHEMBL1993793	FANETIZOLE		Luciferin 4-monooxygenase	Immunomodulator	−64.926	−7.3
CHEMBL2105568	LINAROTENE			Keratolytic	−60.847	−9.0
CHEMBL1108	DROPERIDOL [1]	Approved	Dopamine D2-receptor antagonist	Neuropsychiatric	−62.397	−9.2
CHEMBL2105747	TOZADENANT	Phase3	Adenosine A2A receptor antagonist	Neuropsychiatric	−67.688	−8.7
CHEMBL398615	METOPIMAZINE		Dopamine D2 receptor antagonist	Neuropsychiatric	−61.668	−8.6

CHEMBL2107723	ACOTIAMIDE	Phase3	Acetylcholinesterase inhibitor	Neuropsychiatric	−61.609	−8.5
CHEMBL2104165	CYPRAZEPAM			Neuropsychiatric	−64.311	−7.8
CHEMBL1118	DESVENLAFAXINE	Approved	alpha-1a Adrenergic receptor	Neuropsychiatric	−62.187	−6.5
CHEMBL81	RALOXIFENE	Approved	Selective estrogen receptor modulator	Osteoporosis	−60.788	−9.2
CHEMBL122079	LIFARIZINE		Sodium channel alpha subunits; brain (Types I, II, III)	Platelet aggregation inhibitor	−61.327	−9.1
CHEMBL153427	OXAGRELATE		Phosphodiesterase 1	Platelet aggregation inhibitor	−71.034	−7.5
CHEMBL9506	DEVAZEPIDE		Cholecystokinin receptor antagonist	Prokinetic	−60.752	−9.7
CHEMBL2105584	ULDAZEPAM			Sedative-hypnotic	−75.518	−7.5
CHEMBL2364615	LUBABEGRON			Veterinary	−60.795	−8.3
CHEMBL3545378	MK-6592	Phase1	Serine/threonine-protein kinase Aurora-B		−83.808	−11.0
CHEMBL558752	RAF-265	Phase2	Tyrosine-protein kinase receptor FLT3		−67.400	−10.8
CHEMBL2010872	CEP-11981	Phase2			−60.472	−10.5
CHEMBL575448	BMS-754807	Phase2	Insulin-like growth factor I receptor		−74.091	−10.5
CHEMBL4297501	AFABICIN	Phase2			−67.066	−10.4
CHEMBL1742417	POMISARTAN				−60.035	−10.3
CHEMBL3984425	IPI-549	Phase2			−64.454	−10.2
CHEMBL2346976	AZD3514	Phase1			−68.808	−10.1
CHEMBL3128043	PF-03758309				−88.963	−10.1
CHEMBL4297363	UCB-1184197	Phase2			−97.550	−10.0
CHEMBL1967878	CENISERTIB	Phase1	Inhibitor of nuclear factor kappa B kinase epsilon subunit		−60.855	−10.0
CHEMBL2359248	ZEAXANTHIN	Phase3	Tyrosyl-DNA phosphodiesterase 1		−60.523	−9.9
CHEMBL1908394	GSK-461364	Phase1	Dual specificty protein kinase CLK1		−81.373	−9.9
CHEMBL4521078	PLX-51107	Phase1	Bromodomain-containing protein 4		−63.701	−9.9
CHEMBL2105519	ACROCINONIDE				−165.537	−9.9
CHEMBL131854	POSIZOLID				−67.303	−9.8
CHEMBL2338675	FOSDENOPTERIN		MOCS1		−60.184	−9.8

CHEMBL415049	BARASERTIB	Phase3		−69.006	−9.7
CHEMBL1408927	AMARANTH		Thyroid hormone receptor beta-1	−73.728	−9.7
CHEMBL4594255	NICEVERINE			−62.288	−9.7
CHEMBL2107729	ATACIGUAT	Phase2		−63.668	−9.6
CHEMBL482968	ENMD-2076	Phase2	Serine/threonine-protein kinase Aurora-A	−65.872	−9.6
CHEMBL482767	SNS-314	Phase 1	Inhibitor of nuclear factor kappa B kinase epsilon subunit	−71.806	−9.6
CHEMBL1320139	HELIOMYCIN		Menin/Histone-lysine N-methyltransferase MLL	−66.316	−9.6
CHEMBL1614646	SUSALIMOD			−61.119	−9.6
CHEMBL2106914	PHTHALYLSULFAMETHIZOLE [1]			−82.707	−9.6
CHEMBL587723	AEE-788	Phase2		−60.105	−9.5
CHEMBL3989439	NICOFURATE			−60.749	−9.5
CHEMBL4297397	QUERCETIN-3'-O-PHOSPHATE	Phase2		−62.954	−9.4
CHEMBL3182444	MK-5108 [1]	Phase1		−79.062	−9.4
CHEMBL4297470	MAX-40279	Phase1		−94.922	−9.4
CHEMBL457077	SALVIANOLIC ACID A	Phase 1		−67.669	−9.4
CHEMBL1270562	SALAZOSULFATHIAZOLE		PH domain leucine-rich repeat-containing protein phosphatase 2	−88.917	−9.4
CHEMBL3545215	BMS-911543	Phase2	Phosphodiesterase 4	−90.978	−9.3
CHEMBL1939499	MK-6186	Phase1		−62.056	−9.3
CHEMBL2178575	GSK-2239633	Phase1		−94.791	−9.3
CHEMBL1201369	GTP [3]			−68.191	−9.3
CHEMBL292187	ELOPIPRAZOLE		Dopamine D2 receptor	−62.701	−9.3
CHEMBL486231	GS-461203 [3]		Hepatitis C virus	−64.418	−9.3
CHEMBL3545241	AC-430	Phase1	Tyrosine-protein kinase JAK1	−104.425	−9.2
CHEMBL4297451	XL-888	Phase 1		−61.289	−9.2
CHEMBL4297641	SECLIDEMSTAT	Phase 1		−63.420	−9.2
CHEMBL4594423	TP-1287	Phase 1		−64.654	−9.2
CHEMBL4297421	COH-29	Phase1		−69.684	−9.1
CHEMBL2057236	TP-271	Phase 1		−61.562	−9.1
CHEMBL48880	ASULACRINE			−63.785	−9.1

CHEMBL1213492	GIVINOSTAT	Phase3	Histone deacetylase 1	−65.354	−9.0
CHEMBL318191	TONABERSAT	Phase2		−60.055	−9.0
CHEMBL495727	AT-9283	Phase2		−62.873	−9.0
CHEMBL4297473	NP-G2-044	Phase1		−61.646	−9.0
CHEMBL494089	GSK-690693	Phase1	Serine/threonine-protein kinase AKT	−61.825	−9.0
CHEMBL1090173	SD-0006		MAP kinase p38 alpha	−61.633	−9.0
CHEMBL2107195	ISOPREDNIDENE			−66.317	−9.0
CHEMBL142652	PICEID	Phase2		−64.566	−8.9
CHEMBL253969	OSI-632	Phase2	Tyrosine-protein kinase TIE-2	−71.745	−8.9
CHEMBL3545291	JNJ-39393406	Phase2		−89.518	−8.9
CHEMBL3786098	PF-06459988	Phase2	Epidermal growth factor receptor erbB1	−92.876	−8.9
CHEMBL483321	CP-724714	Phase2	Receptor protein-tyrosine kinase erbB-2	−63.732	−8.9
CHEMBL2105118	LIREQUINIL [1]			−61.192	−8.8
CHEMBL276368	TIMEGADINE			−79.662	−8.8
CHEMBL4594368	2-CHLORODEOXYADENOSINE TRIPHOSPHATE [3]			−64.169	−8.8
CHEMBL4297504	BELORANIB	Phase3		−62.185	−8.7
CHEMBL4297399	LY-2608204 [2]	Phase2		−67.265	−8.7
CHEMBL1230607	PHA-793887	Phase1		−69.733	−8.7
CHEMBL3544966	GSK-1059615	Phase1	Adaptor-associated kinase	−63.344	−8.7
CHEMBL4594428	ASP-5878	Phase1		−88.275	−8.6
CHEMBL2106007	COUMETAROL			−63.248	−8.6
CHEMBL2107223	SULFAGUANOLE			−63.498	−8.6
CHEMBL2058833	GANAPLACIDE [1]	Phase2		−94.555	−8.5
CHEMBL4594432	LY-3200882	Phase1		−61.955	−8.5
CHEMBL1201384	DDCTP		Reverse transcriptase	−66.921	−8.5
CHEMBL1205402	OXI-4503	Phase1		−60.250	−8.4
CHEMBL64360	ENIPORIDE		Sodium/hydrogen exchanger 1	−69.610	−8.4
CHEMBL51483	GOSSYPOL	Phase3		−61.311	−8.3
CHEMBL1614710	OSI-930	Phase1	Stem cell growth factor receptor	−93.645	−8.3

CHEMBL2105528	BISFENAZONE [1]		Carboxylesterase	−85.310	−8.3
CHEMBL2106538	DOMOPREDNATE			−60.337	−8.3
CHEMBL2106670	ALESTRAMUSTINE			−62.748	−8.3
CHEMBL2111115	GLUCOSULFAMIDE			−60.309	−8.3
CHEMBL1742458	TUVATIDINE			−61.010	−8.1
CHEMBL2106016	ATRINOSITOL			−63.790	−8.1
CHEMBL338667	DIPERODON		Sodium channel alpha subunits; brain (Types I, II, III)	−64.911	−8.1
CHEMBL3763743	TTC-352		Estrogen receptor alpha	−60.023	−8.1
CHEMBL1416586	BENZPIPERYLON		Inositol monophosphatase 1	−60.255	−8.0
CHEMBL2106807	MALEYLSULFATHIAZOLE [1]			−92.507	−8.0
CHEMBL2104058	CARPRAZIDIL			−69.079	−7.9
CHEMBL2104945	SULFACLORAZOLE			−92.009	−7.9
CHEMBL2105145	NIFURALIDE			−83.434	−7.9
CHEMBL4211107	ATB-346	Phase2		−60.796	−7.8
CHEMBL2104449	SARAKALIM			−63.011	−7.8
CHEMBL26630	SULFATROXAZOLE		Endothelin receptor ET-A	−76.825	−7.8
CHEMBL12552	BIMAKALIM [1]			−79.030	−7.7
CHEMBL3989584	IDRALFIDINE			−64.196	−7.7
CHEMBL1481457	GLYSOBUZOLE		Aldehyde dehydrogenase 1A1	−91.008	−7.6
CHEMBL2106717	BUTADIAZAMIDE			−84.490	−7.6
CHEMBL2106363	ISOSULPRIDE			−60.047	−7.5
CHEMBL2106536	CYCLAZODONE			−67.971	−7.5
CHEMBL2105110	LAMTIDINE			−71.290	−7.4
CHEMBL2105508	SULFATROZOLE			−67.271	−7.4
CHEMBL593262	PARA-NITROSULFATHIAZOLE [1]			−83.527	−7.4
CHEMBL608806	COCAETHYLENE	Phase1	Monoclonal antibody (mAb) 2E2	−60.968	−7.2
CHEMBL2106208	ETASULINE			−91.878	−7.1
CHEMBL2104333	ICODULINUM			−83.698	−7.0
CHEMBL2104022	ACLANTATE			−65.024	−6.9
CHEMBL2105108	ISAGLIDOLE			−85.089	−6.9

CHEMBL2104120	CLANTIFEN			−85.470	−6.5
CHEMBL2106134	DALBRAMINOL [1]			−69.252	−6.5
CHEMBL2105025	IQUINDAMINE			−83.311	−6.2
CHEMBL2105256	PRANOSAL			−61.508	−6.2
CHEMBL2106311	LEUCINOCAINE			−64.900	−6.2
CHEMBL2106760	FLUTONIDINE			−88.413	−6.2
CHEMBL55812	OLPADRONIC ACID		Trypanosoma brucei rhodesiense	−69.980	−5.9
CHEMBL62382	METHYLSELENOCYSTEINE	Phase1	Kynurenine-oxoglutarate transaminase I	−80.956	nd [5]

[1]Potential drugs for SARS-CoV-2 M^{pro} in Ref [1]. [2]Repurposing drugs for SARS-CoV-2.
[3]Nucleoside triphosphate analogs. [4]No data (compound contains an unsupported boron atom).
[5]No data (compound contains an unsupported selenium atom).

Table S2. Hit compounds obtained by combining the AutoDock Vina and rDock virtual screening results using the ChEMBL database.

ChEMBL ID	Target	AutoDock Vina Score (kcal/mol)
CHEMBL4246021	Citrobacter freundii	−13.9
CHEMBL3905018	Serine/threonine-protein kinase mTOR	−13.5
CHEMBL1256418	Receptor protein-tyrosine kinase erbB-2	−13.4
CHEMBL600492		−13.3
CHEMBL4590896	Plasmodium falciparum	−13.1
CHEMBL4552365	MDA-MB-231	−13.0
CHEMBL4457485	Streptococcus gordonii	−13.0
CHEMBL3944416	Tyrosine-protein kinase SYK	−13.0
CHEMBL3940079	MAP kinase p38 alpha	−12.9
CHEMBL4557444	Porphyromonas gingivalis	−12.9
CHEMBL3698432	Tyrosine-protein kinase SYK	−12.9
CHEMBL3641104	Serine/threonine-protein kinase B-raf	−12.8
CHEMBL4434852	TIGK	−12.8
CHEMBL3238193	Protein-tyrosine phosphatase 1B	−12.7

CHEMBL4444544	Stimulator of interferon genes protein	−12.7
CHEMBL3958000	Tyrosine-protein kinase BTK	−12.7
CHEMBL2263277	Xanthomonas campestris	−12.7
CHEMBL3939320	Apoptosis regulator Bcl-X	−12.6
CHEMBL3694020	Serine/threonine-protein kinase B-raf	−12.6
CHEMBL1993470	SN12C	−12.6
CHEMBL178947	Telomerase reverse transcriptase	−12.6
CHEMBL4090562	Tyrosine-protein kinase receptor UFO	−12.6
CHEMBL3898710	Tyrosine-protein kinase SYK	−12.6
CHEMBL1213559		−12.6
CHEMBL3774987		−12.6
CHEMBL3794423		−12.6
CHEMBL3357287	Bcr/Abl fusion protein	−12.5
CHEMBL4579682	MDA-MB-231	−12.5
CHEMBL572749	Micrococcus flavus	−12.5
CHEMBL2037222	Nerve growth factor receptor Trk-A	−12.5
CHEMBL4561646	Plasmodium falciparum	−12.5
CHEMBL580070	Plasmodium falciparum	−12.5
CHEMBL3401277	Rattus norvegicus	−12.5
CHEMBL450266	Serine/threonine-protein kinase AKT	−12.5
CHEMBL3974105	Tyrosine-protein kinase SYK	−12.5
CHEMBL243919	Tyrosine-protein kinase TIE-2	−12.5
CHEMBL1199180		−12.5
CHEMBL3775025		−12.5
CHEMBL4116218		−12.5
CHEMBL11725	Ancylostoma ceylanicum	−12.4
CHEMBL275918	Ancylostoma ceylanicum	−12.4
CHEMBL409500	Autotaxin	−12.4
CHEMBL3309842	Bacillus subtilis	−12.4
CHEMBL272121	BaF3	−12.4
CHEMBL2048347	Beta-secretase 1	−12.4
CHEMBL3899126	Casein kinase II alpha/beta	−12.4

CHEMBL4112597	Coagulation factor IX	−12.4
CHEMBL3922109	MAP kinase p38 alpha	−12.4
CHEMBL298873	Purinergic receptor P2Y12	−12.4
CHEMBL120478	Rattus norvegicus	−12.4
CHEMBL3684453	Serine/threonine-protein kinase AKT	−12.4
CHEMBL561268	Staphylococcus aureus	−12.4
CHEMBL1095051	Staphylococcus epidermidis	−12.4
CHEMBL3964386	Tyrosine-protein kinase SYK	−12.4
CHEMBL297941		−12.4
CHEMBL448196		−12.4
CHEMBL548692		−12.4
CHEMBL3823355	KB	−12.3
CHEMBL4171392	Klebsiella pneumoniae	−12.3
CHEMBL3897917	MAP kinase p38 alpha	−12.3
CHEMBL1160003	Nucleic Acid	−12.3
CHEMBL1092387	Peroxisome proliferator-activated receptor gamma	−12.3
CHEMBL4580177	Plasmodium falciparum	−12.3
CHEMBL3219913	Plasmodium falciparum 3D7	−12.3
CHEMBL4441513	Porphyromonas gingivalis	−12.3
CHEMBL50724	Purinergic receptor P2Y12	−12.3
CHEMBL454210	Serine/threonine-protein kinase AKT2	−12.3
CHEMBL3669598	Serine/threonine-protein kinase PAK 4	−12.3
CHEMBL3933037	Serine/threonine-protein kinase RAF	−12.3
CHEMBL1972753	SN12C	−12.3
CHEMBL278606	Staphylococcus aureus	−12.3
CHEMBL3641673	Tyrosine-protein kinase SYK	−12.3
CHEMBL1205686		−12.3
CHEMBL3306679		−12.3
CHEMBL4595227		−12.3
CHEMBL587109		−12.3
CHEMBL1170512	Acetyl-CoA carboxylase	−12.2
CHEMBL3651843	ALK tyrosine kinase receptor	−12.2

CHEMBL1779459	Aspergillus oryzae	−12.2
CHEMBL3668756	Complement factor D	−12.2
CHEMBL2316899	Dual specificity protein phosphatase 3	−12.2
CHEMBL3604941	Epidermal growth factor receptor erbB1	−12.2
CHEMBL218416	Escherichia coli	−12.2
CHEMBL218721	Escherichia coli	−12.2
CHEMBL4167104	Hepatocyte growth factor receptor	−12.2
CHEMBL3116482	HERG	−12.2
CHEMBL3978486	Insulin-like growth factor I receptor	−12.2
CHEMBL3921959	MAP kinase p38 alpha	−12.2
CHEMBL3964270	MAP kinase p38 alpha	−12.2
CHEMBL4514182	Porphyromonas gingivalis	−12.2
CHEMBL1256422	Receptor protein-tyrosine kinase erbB-2	−12.2
CHEMBL3680780	Rho-associated protein kinase 2	−12.2
CHEMBL3641102	Serine/threonine-protein kinase B-raf	−12.2
CHEMBL1970631	SN12C	−12.2
CHEMBL4520286	Tyrosine-protein kinase ITK/TSK	−12.2
CHEMBL4071242	Tyrosine-protein kinase receptor UFO	−12.2
CHEMBL4161666		−12.2
CHEMBL3905470	Apoptosis regulator Bcl-X	−12.1
CHEMBL3949706	Apoptosis regulator Bcl-X	−12.1
CHEMBL258469	Autotaxin	−12.1
CHEMBL3309844	Bacillus subtilis	−12.1
CHEMBL3663195	DNA gyrase	−12.1
CHEMBL2206745	Dual specificity phosphatase Cdc25B	−12.1
CHEMBL488574	Furin	−12.1
CHEMBL579430	HepG2	−12.1
CHEMBL3661012	Insulin-like growth factor I receptor	−12.1
CHEMBL4583938	L1210	−12.1
CHEMBL1213154	MAP kinase p38 alpha	−12.1
CHEMBL3935885	MAP kinase p38 alpha	−12.1
CHEMBL3946614	MAP kinase p38 alpha	−12.1

CHEMBL574054	Micrococcus flavus	−12.1
CHEMBL2386806	MOLM-13	−12.1
CHEMBL4216323	Mycobacterium tuberculosis	−12.1
CHEMBL4534583	Plasmodium falciparum	−12.1
CHEMBL4555672	Plasmodium falciparum	−12.1
CHEMBL4582854	Plasmodium falciparum	−12.1
CHEMBL534053	Plasmodium falciparum	−12.1
CHEMBL1277758	Plasmodium yoelii nigeriensis	−12.1
CHEMBL1256423	Receptor protein-tyrosine kinase erbB-2	−12.1
CHEMBL1969834	Serine/threonine-protein kinase Aurora-A	−12.1
CHEMBL3689913	Serine/threonine-protein kinase B-raf	−12.1
CHEMBL3909544	Serine/threonine-protein kinase Sgk1	−12.1
CHEMBL1807708	SK-MEL-28	−12.1
CHEMBL1997404	SN12C	−12.1
CHEMBL22723	Staphylococcus aureus	−12.1
CHEMBL235941	Staphylococcus aureus	−12.1
CHEMBL364874	Staphylococcus aureus	−12.1
CHEMBL4090946	Tyrosine-protein kinase BTK	−12.1
CHEMBL4110832	Tyrosine-protein kinase BTK	−12.1
CHEMBL4113946	Tyrosine-protein kinase BTK	−12.1
CHEMBL3698429	Tyrosine-protein kinase SYK	−12.1
CHEMBL3969554	Tyrosine-protein kinase SYK	−12.1
CHEMBL1195620		−12.1
CHEMBL1199215		−12.1
CHEMBL1739538		−12.1
CHEMBL2178272		−12.1
CHEMBL2237058		−12.1
CHEMBL3297827		−12.1
CHEMBL3963814	Apoptosis regulator Bcl-X	−12.0
CHEMBL2314162	Carbonic anhydrase II	−12.0
CHEMBL168162	Corticotropin releasing factor receptor 1	−12.0
CHEMBL3658931	DNA gyrase	−12.0

CHEMBL2206742	Dual specificity phosphatase Cdc25B	−12.0
CHEMBL3604938	Epidermal growth factor receptor erbB1	−12.0
CHEMBL3980253	GroEL/GroES	−12.0
CHEMBL4205192	MAP kinase ERK1	−12.0
CHEMBL3972567	MAP kinase p38 alpha	−12.0
CHEMBL4061895	MGC-803	−12.0
CHEMBL573890	Micrococcus flavus	−12.0
CHEMBL4579172	Mycobacterium tuberculosis	−12.0
CHEMBL3627920	Nucleic Acid	−12.0
CHEMBL32741	P388	−12.0
CHEMBL4447611	Plasmodium falciparum	−12.0
CHEMBL4522857	Plasmodium falciparum	−12.0
CHEMBL4566305	Plasmodium falciparum	−12.0
CHEMBL2430796	Pseudomonas aeruginosa	−12.0
CHEMBL120321	Rattus norvegicus	−12.0
CHEMBL2315364	Rattus norvegicus	−12.0
CHEMBL1256417	Receptor protein-tyrosine kinase erbB-2	−12.0
CHEMBL1256429	Receptor protein-tyrosine kinase erbB-2	−12.0
CHEMBL4579941	Sepiapterin reductase	−12.0
CHEMBL3692214	Serine/threonine-protein kinase Aurora-B	−12.0
CHEMBL3694024	Serine/threonine-protein kinase B-raf	−12.0
CHEMBL1971789	SN12C	−12.0
CHEMBL2018735	TCF4/beta-catenin	−12.0
CHEMBL4090260	Toll-like receptor 4	−12.0
CHEMBL499445	Trypanosoma brucei brucei	−12.0
CHEMBL4210185	Tyrosine kinase non-receptor protein 2	−12.0
CHEMBL1076474	Tyrosine-protein kinase LCK	−12.0
CHEMBL4100738	Tyrosine-protein kinase receptor UFO	−12.0
CHEMBL3891553	Tyrosine-protein kinase SYK	−12.0
CHEMBL3923486	Tyrosine-protein kinase SYK	−12.0
CHEMBL3678955	Vascular endothelial growth factor receptor 2	−12.0
CHEMBL3972455	Vascular endothelial growth factor receptor 2	−12.0

CHEMBL1086295	−12.0
CHEMBL1231573	−12.0
CHEMBL2207914	−12.0
CHEMBL3306628	−12.0
CHEMBL3765281	−12.0
CHEMBL3990330	−12.0
CHEMBL4104974	−12.0
CHEMBL4116805	−12.0
CHEMBL4203222	−12.0
CHEMBL4571014	−12.0

Reference

[1] Tsuji M. Potential anti-SARS-CoV-2 drug candidates identified through virtual screening of the ChEMBL database for compounds that target the main coronavrius protease. FEBS Open Bio **2020**, 10, 995−1004.