

Supplementary data Table 1: The COVID-19 clinical trial drugs as an external data set.

Number	DrugBankID	DrugName
1	DB08877	Ruxolitinib
2	DB00619	imatinib
3	DB00358	mefloquine
4	DB00608	Chloroquine
5	DB00112	Bevacizumab
6	DB00051	Adalimumab
7	DB01109	heparin
8	DB00788	naproxen
9	DB01050	ibuprofen
10	DB00482	celecoxib
11	DB00020	Sargramostim
12	DB11569	Ixekizumab
13	DB00026	Anakinra
14	DB01167	itraconazole
15	DB00879	emtricitabine
16	DB01041	thalidomide
17	DB00207	azithromycin
18	DB09036	Siltuximab
19	DB00848	Levamisole
20	DB05511	Piclidenoson
21	DB00203	sildenafil
22	DB01394	Colchicine
23	DB09079	Nintedanib
24	DB09035	Nivolumab
25	DB07615	Tranilast
26	DB04932	Defibrotide
27	DB00811	Ribavirin
28	DB04786	Suramin
29	DB09037	Pembrolizumab
30	DB01257	Eculizumab
31	DB01410	ciclesonide
32	DB00331	Metformin
33	DB00864	tacrolimus
34	DB06273	Tocilizumab
35	DB00959	methylprednisolone
36	DB08868	Fingolimod
37	DB00633	dexmedetomidine
38	DB01601	lopinavir
39	DB00503	ritonavir
40	DB08934	Sofosbuvir

Supplementary data Table 3: Predicted top 50 drugs related to HCoV-s-host proteins and coronavirus-related research literatures among these drugs.

Number	DrugID	DrugName	research literatures
1	DB06616	Bosutinib	
2	DB07159	Tamatinib	[1]
3	DB01268	Sunitinib	[2]
4	DB08568	A-674563	
5	DB08877	Ruxolitinib	[1]
6	DB03496	Alvocidib	[3]
7	DB08865	Crizotinib	[4, 5]
8	DB02567	PD173955	
9	DB01254	dasatinib	[6]
10	DB05294	Vandetanib	[7]
11	DB03044	Doramapimod	[8]
12	DB08094	RO-4584820	
13	DB00530	erlotinib	[7]
14	DB06999	PLX-4720	
15	DB05424	Canertinib	[9]
16	DB04849	Cediranib	[10]
17	DB08142	AT-7519	
18	DB06589	Pazopanib	[11, 12]
19	DB04716	2-tert-butyl-9-fluoro-1,6-dihydrobenzo[h]imidazo[4,5-f]isoquinolin-7-one	
20	DB04868	AMN107	[13]
21	DB00317	gefitinib	[14]
22	DB00398	sorafenib	[7]
23	DB08916	Afatinib	[7, 15]
24	DB07149	(7S)-2-(2-aminopyrimidin-4-yl)-7-(2-fluoroethyl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one	
25	DB07995	H-89	[16]
26	DB08901	Ponatinib	[17, 18]
27	DB07235	N-[(1S)-2-AMINO-1-(2,4-DICHLOROBENZYL)ETHYL]-5-[2-(METHYLAMINO)PYRIMIDIN-4-YL]THIOPHENE-2-CARBOXAMIDE	
28	DB08059	Wortmannin	[19, 20]
29	DB00619	imatinib	[21, 22]
30	DB02482	Phosphonothreonine	[23]

31	DB08067	4-[(2-{4-[(CYCLOPROPYLCARBAMOYL)AMINO]-1H-PYRAZOL-3-YL}-1H-BENZIMIDAZOL-6-YL)METHYL]MORPHOLIN-4-IUM	
32	DB01238	aripiprazole	[24]
33	DB08846	Ellagic acid	[25]
34	DB00246	ziprasidone	[26]
35	DB00734	risperidone	[27]
36	DB06144	Sertindole	[28]
37	DB01224	quetiapine	[29]
38	DB04216	Quercetin	[30]
39	DB02010	Staurosporine	[31]
40	DB05465	Tandutinib	[32]
41	DB02656	LY-294002	[33]
42	DB00477	Chlorpromazine	[34]
43	DB03444	6-bromoindirubin-3'-oxime	[2]
44	DB07107	(1S)-2-(1H-INDOL-3-YL)-1-[(5-{(E)-2-PYRIDIN-4-YLVINYLYL}PYRIDIN-3-YL)OXY)METHYL]ETHYLAMINE	
45	DB08073	(2S)-1-(1H-INDOL-3-YL)-3-[[5-(3-METHYL-1H-INDAZOL-5-YL)PYRIDIN-3-YL]OXY}PROPAN-2-AMINE	
46	DB00502	haloperidol decanoate	[35]
47	DB07266	AKI-001	
48	DB07274	N-cyclopropyl-6-[(6,7-dimethoxyquinolin-4-yl)oxy]naphthalene-1-carboxamide	
49	DB01267	paliperidone	[36]
50	DB01100	Pimozide	[37]

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Supplementary data Table 2: The top 100 drug-protein associations in the prediction results of 119

HCoVs-host proteins.

DrugID	DrugName	Gene Entrez ID	Gene Symbol	Z_Score	Known Link
DB06616	Bosutinib	2932	GSK3B	1.3022	0
DB07159	Tamatinib	2932	GSK3B	1.1843	1
DB01268	Sunitinib	2932	GSK3B	1.1494	0
DB08568	A-674563	2932	GSK3B	1.1459	1
DB08877	Ruxolitinib	2932	GSK3B	1.1389	0
DB06616	Bosutinib	2931	GSK3A	1.122	0
DB03496	Alvocidib	2932	GSK3B	1.0881	0
DB08865	Crizotinib	2932	GSK3B	1.0836	0
DB02567	PD173955	2932	GSK3B	1.0725	0
DB01254	dasatinib	2932	GSK3B	1.0257	0
DB05294	Vandetanib	2932	GSK3B	1.0223	0
DB03044	Doramapimod	2932	GSK3B	1.0081	1
DB01268	Sunitinib	2931	GSK3A	1.0073	0
DB08094	RO-4584820	2932	GSK3B	1.0032	1
DB07159	Tamatinib	2931	GSK3A	0.98811	1
DB06616	Bosutinib	634	CEACAM1	0.97344	0
DB00530	erlotinib	2932	GSK3B	0.97328	0
DB06616	Bosutinib	3551	IKBKB	0.94968	0
DB06999	PLX-4720	2932	GSK3B	0.94818	0
DB08877	Ruxolitinib	2931	GSK3A	0.94724	0
DB06616	Bosutinib	4140	MARK3	0.94131	0
DB08865	Crizotinib	2931	GSK3A	0.92627	0
DB05424	Canertinib	2932	GSK3B	0.90195	0
DB04849	Cediranib	2932	GSK3B	0.90018	0
DB05294	Vandetanib	2931	GSK3A	0.89943	0
DB03496	Alvocidib	2931	GSK3A	0.89351	0
DB01254	dasatinib	2931	GSK3A	0.89315	0
DB02567	PD173955	2931	GSK3A	0.89058	0
DB01268	Sunitinib	634	CEACAM1	0.8836	0
DB08142	AT-7519	2932	GSK3B	0.88008	1
DB06589	Pazopanib	2932	GSK3B	0.8684	0
DB01268	Sunitinib	3551	IKBKB	0.85594	0
DB08568	A-674563	2931	GSK3A	0.8557	1
DB07159	Tamatinib	634	CEACAM1	0.85558	0
DB01268	Sunitinib	4140	MARK3	0.85301	1
DB04716	2-tert-butyl-9-fluoro-1,6-	2932	GSK3B	0.84643	0

	dihydrobenzo[h]imidazo[4,5-f]isoquinolin-7-one				
DB06616	Bosutinib	11200	CHEK2	0.84397	1
DB03044	Doramapimod	2931	GSK3A	0.84181	0
DB04868	AMN107	2932	GSK3B	0.84161	0
DB07159	Tamatinib	3551	IKBKB	0.83962	1
DB00317	gefitinib	2932	GSK3B	0.83695	0
DB00530	erlotinib	2931	GSK3A	0.83483	0
DB00398	sorafenib	2932	GSK3B	0.83353	1
DB08916	Afatinib	2932	GSK3B	0.83179	0
DB07159	Tamatinib	4140	MARK3	0.82193	1
DB08877	Ruxolitinib	634	CEACAM1	0.8165	0
DB08865	Crizotinib	634	CEACAM1	0.80738	0
DB08877	Ruxolitinib	3551	IKBKB	0.8044	1
DB07149	(7S)-2-(2-aminopyrimidin-4-yl)-7-(2-fluoroethyl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one	2932	GSK3B	0.80285	1
DB06999	PLX-4720	2931	GSK3A	0.80096	0
DB08865	Crizotinib	3551	IKBKB	0.78955	1
DB06589	Pazopanib	2931	GSK3A	0.7895	0
DB05294	Vandetanib	634	CEACAM1	0.78935	0
DB08877	Ruxolitinib	4140	MARK3	0.78667	0
DB01254	dasatinib	634	CEACAM1	0.78479	0
DB08865	Crizotinib	4140	MARK3	0.77675	0
DB05424	Canertinib	2931	GSK3A	0.77544	0
DB07995	H-89	2932	GSK3B	0.77339	0
DB08901	Ponatinib	2932	GSK3B	0.77214	1
DB02567	PD173955	634	CEACAM1	0.77154	0
DB03496	Alvocidib	634	CEACAM1	0.77007	0
DB08094	RO-4584820	2931	GSK3A	0.76871	1
DB07235	N-[(1S)-2-AMINO-1-(2,4-DICHLOROBENZYL)ETHYL]-5-[2-(METHYLAMINO)PYRIMIDIN-4-YL]THIOPHENE-2-CARBOXAMIDE	2932	GSK3B	0.76745	0
DB04849	Cediranib	2931	GSK3A	0.76645	0
DB05294	Vandetanib	3551	IKBKB	0.76417	0
DB08059	Wortmannin	2932	GSK3B	0.76283	0
DB02567	PD173955	3551	IKBKB	0.76103	0
DB01254	dasatinib	3551	IKBKB	0.76064	0
DB05294	Vandetanib	4140	MARK3	0.7601	0
DB00619	imatinib	2932	GSK3B	0.7595	0
DB03496	Alvocidib	3551	IKBKB	0.75928	0
DB01268	Sunitinib	11200	CHEK2	0.75872	1

DB02482	Phosphonothreonine	2932	GSK3B	0.75843	0
DB01254	dasatinib	4140	MARK3	0.75346	0
DB07159	Tamatinib	11200	CHEK2	0.74223	0
DB06616	Bosutinib	4836	NMT1	0.74055	0
DB02567	PD173955	4140	MARK3	0.74028	1
DB00530	erlotinib	634	CEACAM1	0.73828	0
DB03496	Alvocidib	4140	MARK3	0.73777	0
DB08067	4-[(2-[4- [(CYCLOPROPYLCARBAMOYL)AMINO]- 1H-PYRAZOL-3-YL]-1H- BENZIMIDAZOL-6- YL)METHYL]MORPHOLIN-4-IUM	2932	GSK3B	0.7372	1
DB01238	aripiprazole	3832	KIF11	0.73667	0
DB03044	Doramapimod	634	CEACAM1	0.72986	0
DB08846	Ellagic acid	2932	GSK3B	0.72599	1
DB00398	sorafenib	2931	GSK3A	0.72298	0
DB00246	ziprasidone	3832	KIF11	0.72084	0
DB00530	erlotinib	3551	IKBKB	0.71882	0
DB00734	risperidone	3832	KIF11	0.71752	0
DB03044	Doramapimod	3551	IKBKB	0.716	0
DB00317	gefitinib	2931	GSK3A	0.7151	0
DB06144	Sertindole	3832	KIF11	0.71337	0
DB01224	quetiapine	3832	KIF11	0.71172	0
DB08568	A-674563	3551	IKBKB	0.71165	0
DB04216	Quercetin	2932	GSK3B	0.71133	0
DB08877	Ruxolitinib	11200	CHEK2	0.71024	0
DB02010	Staurosporine	2932	GSK3B	0.70886	1
DB08916	Afatinib	2931	GSK3A	0.70736	0
DB06589	Pazopanib	634	CEACAM1	0.70644	0
DB05465	Tandutinib	2932	GSK3B	0.70641	0
DB06616	Bosutinib	4869	NPM1	0.70596	1
DB00530	erlotinib	4140	MARK3	0.70544	0

41	DB08895	Tofacitinib
42	DB09065	Cobicistat
43	DB00177	valsartan
44	DB00300	tenofovir
45	DB00198	oseltamivir