

Table S1. Top Ranked Link Prediction Nodes for Potential COVID-19 Treatment. Predicted nodes are primarily based on analyzing connections in the knowledge graph from older coronavirus literature on SARS and MERS. Lower hetesim score is better. Standardize hetesim score used for comparison. Predicted link shows predicted relationship type. DOI, validation label, pharmacokinetic label determined by human in the loop validation using multiple trained human reviewers with quality control examining existing COVID-19 specific data sets.

node	Drug Class	node type	hetesim score	standardized								pharmacokinetics	
				hetesim score	novelty score	count score	predicted link 1	predicted link 2	predicted link 3	predicted link 4	DOI(s)		
Glycyrrhetic Acid	anti-inflammatory	OrganicChemical	33.748	0.074	0.681	9.403	treats	prevents	part of	neg prevent	10_1016/i.phy med.2020.1533	PROVEN	Primary
Quinine	anti-inflammatory	OrganicChemical	35.013	0.077	0.665	9.297	treats	prevents	neg treats	neg prevent	10_1016/i.tmai d.2020.101873	PROVEN	Primary
ebselen	anti-inflammatory	OrganicChemical	35.015	0.077	0.679	9.583	treats	prevents	neg treats	inhibits	10_1016/i.freera	UNCLEAR	N/A
Fluticasone propionate	anti-inflammatory	OrganicChemical	36.184	0.079	0.670	9.603	treats	prevents	neg treats	part of	10_3390/v1204	UNCLEAR	N/A
Esters	anti-inflammatory	OrganicChemical	32.110	0.070	0.650	8.510	N/A	N/A	N/A	N/A	10_1016/i.cbi.2	MISSING	N/A
Flavonoids	anti-inflammatory	OrganicChemical	35.868	0.079	0.637	8.867	prevents	treats	part of	neg treats	020.109211	PROVEN	Primary
Quinolone Antibacterial Agents	anti-inflammatory	OrganicChemical	37.309	0.082	0.654	9.472	prevents	treats	part of	neg treats	10_3389/fmed. 2020.00420	UNCLEAR	N/A
Morphine	anti-inflammatory	OrganicChemical	38.213	0.084	0.592	8.359	treats	prevents	neg treats	part of	10_1016/i.dsx.2 020.05.022	UNCLEAR	N/A
Curcumin	anti-inflammatory	OrganicChemical	38.445	0.084	0.594	8.432	treats	prevents	part of	neg treats	7-020-00598-8	UNCLEAR	N/A
Hydroxymethylglutaryl-CoA Reductase Inhibitors	anti-inflammatory	OrganicChemical	36.662	0.080	0.619	8.641	prevents	treats	neg treats	part of	10_1002/phar.2 397	PROVEN	Side-Effect
salicylate	anti-inflammatory	OrganicChemical	38.471	0.084	0.643	9.441	treats	prevents	neg treats	part of	10_1080/22221 751.2020.1785 336	UNCLEAR	N/A
baicalin	anti-inflammatory	OrganicChemical	37.024	0.081	0.658	9.501	treats	prevents	part of	inhibits	1-020-0483-6	PROVEN	Primary
Albuterol	anti-inflammatory	OrganicChemical	37.647	0.083	0.645	9.345	treats	prevents	neg treats	part of	10_1186/s1002 0-020-00215-w	PROVEN	Adjunctive
Levamisole	anti-inflammatory	OrganicChemical	38.954	0.085	0.624	9.143	prevents	treats	neg treats	part of	10_3855/iidc.13	UNCLEAR	N/A
ethyl pyruvate	anti-inflammatory	OrganicChemical	36.503	0.080	0.679	9.829	treats	prevents	neg prevent	part of	N/A	MISSING	N/A
Chlorpromazine	anti-inflammatory	OrganicChemical	38.653	0.085	0.626	9.118	treats	prevents	part of	neg treats	p.2020.05.006	PROVEN	Primary
Tretinoin	anti-inflammatory	OrganicChemical	37.341	0.082	0.579	7.941	treats	prevents	neg treats	part of	N/A	MISSING	N/A
Indometheacin	anti-inflammatory	OrganicChemical	38.826	0.085	0.592	8.459	treats	prevents	part of	neg treats	10_1111/iicp.13	PROVEN	Adjunctive
Sulfonamides	anti-inflammatory	OrganicChemical	38.098	0.084	0.641	9.332	treats	prevents	neg treats	part of	N/A	MISSING	N/A
SB 203580	anti-inflammatory	OrganicChemical	38.160	0.084	0.653	9.599	treats	prevents	neg treats	part of	N/A	MISSING	N/A
Chloroquine	antimalarial	OrganicChemical	25.420	0.077	0.648	7.470	treats	prevents	neg treats	neg prevent	10_1016/i.viro. 2020.08.011	PROVEN	Primary
Fluoroquinolones	antimalarial	OrganicChemical	25.554	0.077	0.682	8.125	treats	prevents	neg treats	part of	10_1016/i.ctim. 2020.102473	PROVEN	Adjunctive
Polyamines	antimalarial	OrganicChemical	26.260	0.080	0.656	7.759	treats	prevents	part of	neg treats	10_1021/acsinf ecdis.0c00491	DISPROVEN	Other
Ciprofloxacin	antimalarial	OrganicChemical	27.756	0.084	0.647	7.878	treats	prevents	neg treats	part of	10_1136/bmjga st-2020-000434	PROVEN	Side-Effect
Tannic Acid	antimalarial	OrganicChemical	28.577	0.087	0.666	8.391	treats	prevents	part of	neg treats	10_1111/ifbc.13 432	UNCLEAR	N/A
Vitamin A	antimalarial	OrganicChemical	29.413	0.089	0.599	7.291	prevents	treats	neg treats	part of	10_18632/aging .103888	UNCLEAR	N/A

Validation Label
PROVEN
DISPROVEN
UNCLEAR
MISSING

Pharmacokinetic Label
Primary
Adjunctive
Side-Effect
Other

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Methotrexate	antimalarial	OrganicChemical	28.656	0.087	0.602	7.211	treats	prevents	neg treats	part of	10.1002/imv.26	PROVEN	Primary	
Esters	antimalarial	OrganicChemical	27.856	0.084	0.629	7.554	N/A	N/A	N/A	N/A	N/A	MISSING	N/A	
artemisinine	antimalarial	OrganicChemical	28.721	0.087	0.666	8.416	treats	prevents	neg treats	part of	10.1021/acsinf	PROVEN	Primary	
Alkaloids	antimalarial	OrganicChemical	29.719	0.090	0.652	8.342	prevents	treats	part of	neg treats	1-020-09723-3	PROVEN	Primary	
Camptothecin	antimalarial	OrganicChemical	28.953	0.088	0.669	8.510	treats	prevents	part of	neg treats	N/A	MISSING	N/A	
Aldehydes	antimalarial	OrganicChemical	29.544	0.090	0.644	8.151	N/A	N/A	N/A	N/A	N/A	MISSING	N/A	
Vitamin K 3	antimalarial	OrganicChemical	29.556	0.090	0.666	8.573	treats	prevents	part of	neg treats	N/A	MISSING	N/A	
Flavonoids	antimalarial	OrganicChemical	29.755	0.090	0.630	7.937	prevents	treats	part of	neg treats	10.1016/j.cbi.2	PROVEN	Primary	
Amantadine	antimalarial	OrganicChemical	30.196	0.092	0.655	8.487	prevents	treats	neg treats	neg prevent	10.1186/s4073	UNCLEAR	N/A	
favor	antimalarial	OrganicChemical	29.810	0.090	0.591	7.211	prevents	treats	part of	neg treats	N/A	MISSING	N/A	
Quinine	antimalarial	OrganicChemical	30.175	0.091	0.648	8.351	treats	prevents	neg treats	neg prevent	d.2020.101873	PROVEN	Primary	
Quinolone Antibacterial Agents	antimalarial	OrganicChemical	30.588	0.093	0.654	8.530	prevents	treats	part of	neg treats	2020.00420	UNCLEAR	N/A	
quinoline	antimalarial	OrganicChemical	31.022	0.094	0.667	8.855	part of	neg treats	treats	prevents	N/A	MISSING	N/A	
Sulfonamides	antimalarial	OrganicChemical	31.433	0.095	0.634	8.328	treats	prevents	neg treats	part of	N/A	MISSING	N/A	
Antiviral Therapy	antiviral agent	TherapeuticOrPreventiveProcedure	22.254	0.086	0.561	6.886	treats	neg treats	prevents	N/A	10.1136/thorax	PROVEN	Primary	
prevention of disorder	antiviral agent	TherapeuticOrPreventiveProcedure	23.438	0.091	0.614	8.266	N/A	N/A	N/A	N/A	N/A	MISSING	N/A	
Adoptive Transfer	antiviral agent	TherapeuticOrPreventiveProcedure	24.425	0.095	0.620	8.624	prevents	treats	neg treats	N/A	N/A	N/A	MISSING	N/A
Antiretroviral Therapy, Highly Active	antiviral agent	TherapeuticOrPreventiveProcedure	25.461	0.099	0.606	8.605	neg treats	treats	prevents	N/A	https://pubmed	UNCLEAR	N/A	
Influenza vaccination	antiviral agent	TherapeuticOrPreventiveProcedure	25.746	0.100	0.606	8.674	prevents	treats	neg treats	N/A	N/A	N/A	MISSING	N/A
Clinical Treatment	antiviral agent	TherapeuticOrPreventiveProcedure	25.859	0.100	0.606	8.711	N/A	N/A	N/A	N/A	N/A	N/A	MISSING	N/A
Therapeutic immunosuppression	antiviral agent	TherapeuticOrPreventiveProcedure	26.364	0.102	0.539	7.470	prevents	neg treats	treats	N/A	https://doi.org/1	UNCLEAR	N/A	
Hematopoietic Stem Cell Transplantation	antiviral agent	TherapeuticOrPreventiveProcedure	26.404	0.102	0.581	8.334	treats	neg treats	prevents	N/A	DOI: 10.1038/s4139	UNCLEAR	N/A	
Vaccination	antiviral agent	TherapeuticOrPreventiveProcedure	26.233	0.102	0.405	4.697	treats	prevents	neg treats	N/A	2-020-00286-5	UNCLEAR	N/A	
Empirical therapy	antiviral agent	TherapeuticOrPreventiveProcedure	26.556	0.103	0.614	9.051	treats	prevents	neg treats	N/A	N/A	N/A	MISSING	N/A

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HIV therapy	antiviral agent	TherapeuticOrPreventiveProcedure	26.527	0.103	0.635	9.469	neg treats	treats	prevents	N/A	DOI: 10.1586/14	UNCLEAR	N/A
early identification	antiviral agent	TherapeuticOrPreventiveProcedure	26.904	0.104	0.583	8.498	treats	prevents	neg treats	N/A	N/A	MISSING	N/A
interferon therapy	antiviral agent	TherapeuticOrPreventiveProcedure	27.117	0.105	0.615	9.221	prevents	treats	neg treats	N/A	DOI: 10.1517/14	PROVEN	Primary
Immunotherapy	antiviral agent	TherapeuticOrPreventiveProcedure	27.345	0.106	0.488	6.677	treats	prevents	neg treats	N/A	DOI: 10.1016/j.ir	UNCLEAR	N/A
Cytomegalovirus prophylaxis	antiviral agent	TherapeuticOrPreventiveProcedure	27.210	0.105	0.645	9.847	N/A	N/A	N/A	N/A	N/A	MISSING	N/A
Post-exposure prophylaxis	antiviral agent	TherapeuticOrPreventiveProcedure	27.420	0.106	0.607	9.123	prevents	treats	neg treats	N/A	N/A	MISSING	N/A
The science and art of healing	antiviral agent	TherapeuticOrPreventiveProcedure	27.920	0.108	0.544	7.954	N/A	N/A	N/A	N/A	N/A	MISSING	N/A
Therapeutic Intervention	antiviral agent	TherapeuticOrPreventiveProcedure	28.210	0.109	0.509	7.308	treats	neg treats	prevents	N/A	N/A	MISSING	N/A
Biological Response Modifier Therapy	antiviral agent	TherapeuticOrPreventiveProcedure	28.245	0.109	0.591	9.000	treats	prevents	neg treats	N/A	N/A	MISSING	N/A
Bone Marrow Transplantation	antiviral agent	TherapeuticOrPreventiveProcedure	27.609	0.107	0.549	7.976	treats	prevents	neg treats	N/A	doi: 10.1089/scd	PROVEN	Adjuactive
Capsid Proteins	envelope protein	AminoAcidPeptid eOrProtein	6.355	0.079	0.612	6.742	part of	neg part of	treats	prevents	10.1016/j.anndi	PROVEN	Other
Viral Proteins	envelope protein	AminoAcidPeptid eOrProtein	6.266	0.078	0.599	6.399	neg part of	part of	treats	prevents	N/A	MISSING	N/A
Flagellin	envelope protein	AminoAcidPeptid eOrProtein	7.146	0.089	0.688	8.931	treats	neg part of	part of	prevents	10.1016/j.ebio	UNCLEAR	N/A
Gene Products, env	envelope protein	AminoAcidPeptid eOrProtein	6.994	0.087	0.673	8.493	neg part of	part of	treats	compared w/N/A	N/A	MISSING	N/A
Structural protein	envelope protein	AminoAcidPeptid eOrProtein	7.312	0.091	0.627	7.719	N/A	N/A	N/A	N/A	N/A	MISSING	N/A
Neuraminidase	envelope protein	AminoAcidPeptid eOrProtein	7.707	0.096	0.634	8.144	neg part of	treats	part of	prevents	0353	PROVEN	Other
Nucleocapsid	envelope protein	AminoAcidPeptid eOrProtein	7.731	0.097	0.642	8.322	part of	neg part of	compared w/treats	10.1016/j.imb	2	PROVEN	Other
Chemokine (C-C Motif) Receptor 5 CCR5	envelope protein	Receptor	8.312	0.104	0.652	8.941	treats	neg part of	part of	prevents	10.1016/j.antivir	DISPROVEN	Other
Viral Core Proteins	envelope protein	AminoAcidPeptid eOrProtein	8.154	0.102	0.634	8.436	neg part of	part of	treats	prevents	N/A	MISSING	N/A
Polymerase ERVK-9 ERVK-19 ERVK-11	envelope protein	AminoAcidPeptid eOrProtein	8.238	0.103	0.603	7.826	N/A	N/A	N/A	N/A	N/A	MISSING	N/A

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Gene Products, gag	envelope protein	AminoAcidPeptid eOrProtein	8.373	0.105	0.650	8.938	part of	neg part of	treats	compared w/N/A	MISSING	N/A		
Virus-neutralizing Antibody	envelope protein	ImmunologicFact or	8.491	0.106	0.650	9.017	prevents	part of	treats	neg part of es8030404	10.3390/vaccin UNCLEAR	N/A		
Membrane Fusion Proteins	envelope protein	AminoAcidPeptid eOrProtein	9.376	0.117	0.531	7.040	part of	neg part of	treats	neg treats	10.1016/i.antivi	DISPROVEN	Other	
synthetic peptide	envelope protein	AminoAcidPeptid eOrProtein	8.768	0.110	0.591	7.925	part of	treats	prevents	neg part of id.2020.104474	10.1016/i.meeg UNCLEAR	N/A		
Interferon Alpha, Human IFNA1	envelope protein	ImmunologicFact or	8.770	0.110	0.625	8.655	N/A	N/A	N/A	N/A	MISSING	N/A		
Bacterial Proteins	envelope protein	AminoAcidPeptid eOrProtein	9.488	0.119	0.634	9.353	part of	treats	neg part of	prevents	N/A	MISSING	N/A	
HIV Envelope Protein gp160 (gp160 ENPEP)	envelope protein	AminoAcidPeptid eOrProtein	9.188	0.115	0.647	9.425	part of	neg part of	treats	prevents	10.1128/JVI.78. 19.10328- 10.1007/s1093	UNCLEAR	N/A	
Polyclonal antibody	envelope protein	ImmunologicFact or	9.271	0.116	0.578	7.988	treats	part of	prevents	neg part of	0-020-09921-0 10.1007/s1056	UNCLEAR	N/A	
Receptors, Virus	envelope protein	Receptor	8.788	0.110	0.688	10.050	part of	neg part of	prevents	treats	1-020-09869-6	PROVEN	Other	
Ubiquitin	envelope protein	AminoAcidPeptid eOrProtein	9.449	0.118	0.559	7.695	part of	neg part of	treats	prevents	10.3389/fmolb.	UNCLEAR	N/A	
small molecule	glycoproteins big	OrganicChemical	31.411	0.056	0.733	9.705	prevents	treats	part of	neg treats	N/A	MISSING	N/A	
Chloroquine	glycoproteins big	OrganicChemical	40.646	0.073	0.709	10.306	treats	prevents	neg treats	neg prevent 2020.08.011	10.1016/i.virol. PROVEN	Primary		
RABBIT SERUM	glycoproteins big	OrganicChemical	33.844	0.061	0.756	10.575	N/A	N/A	N/A	N/A	MISSING	N/A		
Edetic Acid	glycoproteins big	OrganicChemical	40.971	0.074	0.701	10.141	treats	prevents	neg treats	part of	N/A	MISSING	N/A	
Biotin	glycoproteins big	OrganicChemical	42.352	0.076	0.695	10.169	prevents	part of	treats	N/A	N/A	MISSING	N/A	
Fluoroquinolones	glycoproteins big	OrganicChemical	46.814	0.084	0.716	11.245	treats	prevents	neg treats	part of	10.1016/i.ctim. 2020.102473	PROVEN	Adjunctive	
Methotrexate	glycoproteins big	OrganicChemical	48.234	0.087	0.658	10.030	treats	prevents	neg treats	part of	DOI: 10.1111/dt	UNCLEAR	N/A	
Vitamin A	glycoproteins big	OrganicChemical	48.329	0.087	0.667	10.248	prevents	treats	neg treats	part of	10.3888	UNCLEAR	N/A	
Sulphydryl Compounds	glycoproteins big	OrganicChemical	45.896	0.083	0.665	9.889	treats	prevents	part of	neg treats	N/A	MISSING	N/A	
Pentetic Acid	glycoproteins big	OrganicChemical	46.035	0.083	0.723	11.328	treats	prevents	neg treats	part of	N/A	MISSING	N/A	
Esters	glycoproteins big	OrganicChemical	46.060	0.083	0.678	10.240	N/A	N/A	N/A	N/A	N/A	MISSING	N/A	
Adriamycin	glycoproteins big	OrganicChemical	49.257	0.089	0.680	10.678	treats	prevents	part of	neg treats	10.1016/j.compl	UNCLEAR	N/A	
Ethylene	glycoproteins big	OrganicChemical	46.668	0.084	0.714	11.183	treats	prevents	part of	neg treats	N/A	MISSING	N/A	
2,5-dichloro-4-bromophenol	glycoproteins big	OrganicChemical	46.752	0.084	0.726	11.501	prevents	part of	treats	neg prevent N/A	N/A	MISSING	N/A	
Daunorubicin	glycoproteins big	OrganicChemical	47.436	0.085	0.707	11.125	treats	part of	neg treats	interacts with N/A	N/A	MISSING	N/A	
favor	glycoproteins big	OrganicChemical	48.312	0.087	0.660	10.085	prevents	treats	part of	neg treats	N/A	MISSING	N/A	
poly(2-acrylamido-2-methyl-1-propanesulfonic acid)	glycoproteins big	OrganicChemical	48.656	0.088	0.718	11.548	N/A	N/A	N/A	N/A	N/A	MISSING	N/A	
fucoidan	glycoproteins big	OrganicChemical	48.601	0.087	0.709	11.301	treats	prevents	neg prevent: neg treats	DOI: 10.1039/d0	PROVEN	Primary		
Tretinoin	glycoproteins big	OrganicChemical	49.687	0.089	0.635	9.633	treats	prevents	neg treats	part of	N/A	MISSING	N/A	
Cytembena	glycoproteins big	OrganicChemical	50.128	0.090	0.710	11.533	N/A	N/A	N/A	N/A	N/A	MISSING	N/A	
small molecule	immunomodulators	OrganicChemical	39.124	0.069	0.662	8.825	prevents	treats	part of	neg treats	https://pubmed	UNCLEAR	N/A	
Chloroquine	immunomodulators	OrganicChemical	47.007	0.083	0.626	9.114	treats	prevents	neg treats	neg prevent https://www.ncbi	PROVEN	Primary		
Fluoroquinolones	immunomodulators	OrganicChemical	44.706	0.079	0.674	9.840	treats	prevents	neg treats	part of	N/A	MISSING	N/A	
Ciprofloxacin	immunomodulators	OrganicChemical	48.003	0.085	0.641	9.581	treats	prevents	neg treats	part of	10.1136/bmija st-2020-000434	PROVEN	Side-Effect	

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fucoidan	immunomodulators	OrganicChemical	46.633	0.082	0.670	10.024	treats	prevents	neg prevent:neg treats	N/A	MISSING	N/A			
Biotin	immunomodulators	OrganicChemical	49.327	0.087	0.612	9.117	prevents	part of	treats	neg treats	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3390712/	UNCLEAR	N/A		
Vitamin A	immunomodulators	OrganicChemical	50.576	0.089	0.598	8.984	prevents	treats	neg treats	part of	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3390712/	UNCLEAR	N/A		
artemisinine	immunomodulators	OrganicChemical	49.243	0.087	0.656	10.078	treats	prevents	neg treats	part of	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3390712/	PROVEN	Primary		
Flavonoids	immunomodulators	OrganicChemical	50.729	0.090	0.625	9.585	prevents	treats	part of	neg treats	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3390712/	UNCLEAR	N/A		
docetaxel	immunomodulators	OrganicChemical	49.562	0.088	0.649	9.968	treats	prevents	part of	neg prevent:N/A	N/A	MISSING	N/A		
Neifinavir	immunomodulators	OrganicChemical	51.126	0.090	0.657	10.342	treats	prevents	neg treats	part of	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3390712/	UNCLEAR	N/A		
temozolomide	immunomodulators	OrganicChemical	51.265	0.091	0.651	10.240	treats	prevents	neg prevent:part of	https://pubmed.ncbi.nlm.nih.gov/16583006/	UNCLEAR	N/A			
polyphenols	immunomodulators	OrganicChemical	51.447	0.091	0.634	9.891	treats	prevents	part of	neg treats	https://pubmed.ncbi.nlm.nih.gov/16583006/	UNCLEAR	N/A		
Ginseng Preparation	immunomodulators	OrganicChemical	51.939	0.092	0.650	10.293	prevents	treats	part of	neg treats	https://pubmed.ncbi.nlm.nih.gov/16583006/	UNCLEAR	N/A		
Tretinoin	immunomodulators	OrganicChemical	50.727	0.090	0.575	8.511	treats	prevents	neg treats	part of	N/A	MISSING	N/A		
sphingosine 1-phosphate	immunomodulators	OrganicChemical	51.373	0.091	0.634	9.873	prevents	treats	neg treats	part of	N/A	MISSING	N/A		
Paclitaxel	immunomodulators	OrganicChemical	51.438	0.091	0.611	9.382	treats	prevents	neg treats	part of	N/A	MISSING	N/A		
Hydroxymethylglutaryl-CoA Reductase Inhibitors	immunomodulators	OrganicChemical	51.537	0.091	0.610	9.371	prevents	treats	neg treats	part of	N/A	MISSING	N/A		
Mistletoe preparation	immunomodulators	OrganicChemical	51.853	0.092	0.660	10.506	N/A	N/A	N/A	N/A	N/A	MISSING	N/A		
bryostatin 1	immunomodulators	OrganicChemical	52.082	0.092	0.657	10.463	treats	prevents	neg prevent:neg treats	N/A	N/A	MISSING	N/A		
Neuraminidase inhibitors	neuraminidase	AminoAcidPeptid eOrProtein	6.300	0.085	0.624	4.738	neg part of	treats	part of	prevents	N/A	MISSING	N/A		
Complement System Proteins	neuraminidase inhibitors	ImmunologicFact or	7.469	0.101	0.549	4.595	prevents	part of	treats	neg part of	https://pubmed.ncbi.nlm.nih.gov/16583006/	DISPROVEN	Other		
Dopamine Receptor	neuraminidase inhibitors	Receptor	7.603	0.103	0.580	4.990	treats	neg part of	part of	prevents	https://pubmed.ncbi.nlm.nih.gov/16583006/	DISPROVEN	Other		
human leukocyte interferon IFNA1	neuraminidase inhibitors	ImmunologicFact or	7.032	0.095	0.583	4.716	treats	prevents	neg part of	part of	https://pubmed.ncbi.nlm.nih.gov/16583006/	PROVEN	Primary		
Sialyltransferases	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	7.243	0.098	0.603	5.036	part of	neg part of	treats	administere	N/A	UNCLEAR	N/A		
Glycoside Hydrolases	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	7.302	0.099	0.598	5.010	treats	part of	neg treats	neg part of	https://pubmed.ncbi.nlm.nih.gov/16583006/	UNCLEAR	Primary		
neuraminidases	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	7.152	0.097	0.605	5.001	part of	neg part of	treats	prevents	N/A	MISSING	N/A		
Polymerase ERVK-9 ERVK-19 ERVK-11	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	7.178	0.097	0.598	4.944	N/A	N/A	N/A	N/A	N/A	MISSING	N/A		
Polymerase	neuraminidase inhibitors	eOrProtein	7.191	0.097	0.602	4.994	part of	neg part of	treats	compared wN/A	N/A	MISSING	N/A		
Ion Channel	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	7.272	0.098	0.591	4.921	part of	neg part of	prevents	treats	N/A	MISSING	N/A		
Brain-Derived Neurotrophic Factor	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	7.536	0.102	0.570	4.851	part of	treats	prevents	stimulates	https://pubmed.ncbi.nlm.nih.gov/16583006/	UNCLEAR	N/A		
PER2 protein, mammalian	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	7.437	0.100	0.585	4.953	neg part of	part of	treats	stimulates	N/A	MISSING	N/A		
Mannose Binding Lectin	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	7.321	0.099	0.582	4.864	treats	part of	prevents	neg part of	https://pubmed.ncbi.nlm.nih.gov/16583006/	PROVEN	Primary		
Recombinant Interferon-gamma	neuraminidase inhibitors	ImmunologicFact or	7.534	0.102	0.558	4.734	treats	prevents	part of	neg part of	https://pubmed.ncbi.nlm.nih.gov/16583006/	PROVEN	Primary		
Cyclosporine	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	7.658	0.103	0.553	4.746	treats	prevents	neg part of	part of	https://pubmed.ncbi.nlm.nih.gov/16583006/	PROVEN	Primary		

Table S1. Top Ranked Link Prediction Nodes for Potential COVID-19 Treatment. Predicted nodes are primarily based on analyzing connections in the knowledge graph from older coronavirus literature on SARS and MERS. Lower hetesim score is better. Standardize hetesim score used for comparison. Predicted link shows predicted relationship type. DOI, validation label, pharmacokinetic label determined by human in the loop validation using multiple trained human reviewers with quality control examining existing COVID-19 specific data sets.

node	Drug Class	node type	standardized hetesim score										validation	pharmacokinetics
			novelty score	count score	predicted link 1	predicted link 2	predicted link 3	predicted link 4	DOI(s)					
Nerve Growth Factors	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	7.647	0.103	0.560	4.807	treats	part of	prevents	neg part of https://pubmed.ncbi.nlm.nih.gov/32144000/	UNCLEAR	N/A		
	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	7.805	0.105	0.580	5.100	part of	neg part of	compared w treats	N/A	MISSING	N/A		
Amino Acids	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	7.873	0.106	0.524	4.567	treats	prevents	part of	neg part of N/A	MISSING	N/A		
	neuraminidase inhibitors	AminoAcidPeptid eOrProtein	8.013	0.108	0.569	5.107	treats	neg part of	part of	neg prevent N/A	MISSING	N/A		
sialic acid receptor	neuraminidase inhibitors	Receptor	7.914	0.107	0.571	5.076	neg part of	part of	prevents	compared w https://pubmed.ncbi.nlm.nih.gov/32144000/	PROVEN	Other		
Antiviral Therapy	nucleoside analogs	TherapeuticOrPre ventiveProcedure	14.801	0.093	0.572	10.781	treats	neg treats	prevents	neg prevent DOI: 10.1080/17443224.2019.1590003	PROVEN	Primary		
	nucleoside analogs	TherapeuticOrPre ventiveProcedure	14.942	0.093	0.565	10.707	neg treats	treats	prevents	neg prevent N/A	MISSING	N/A		
Nucleoside Analogs	nucleoside analogs	PharmacologicSu bstance	15.776	0.099	0.554	10.897	treats	neg treats	prevents	part OF	N/A	UNCLEAR	N/A	
	nucleoside analogs	TherapeuticOrPre ventiveProcedure	16.262	0.102	0.522	10.369	prevents	neg treats	treats	neg prevent https://doi.org/10.1080/17443224.2019.1590003	UNCLEAR	N/A		
interferon therapy	nucleoside analogs	TherapeuticOrPre ventiveProcedure	15.689	0.098	0.569	11.250	prevents	treats	neg treats	neg prevent DOI: 10.1517/143203	PROVEN	Primary		
	nucleoside analogs	TherapeuticOrPre ventiveProcedure	17.182	0.107	0.577	12.352	neg treats	prevents	treats	neg prevent DOI: 10.1080/17443224.2019.1590003	DISPROVEN	Primary		
gene therapy	nucleoside analogs	TherapeuticOrPre ventiveProcedure	16.409	0.103	0.515	10.258	treats	neg treats	prevents	neg prevent DOI: 10.3390/bioRxiv.2020.02.10.201000	UNCLEAR	N/A		
	nucleoside analogs	TherapeuticOrPre ventiveProcedure	16.319	0.102	0.499	9.809	N/A	N/A	N/A	N/A	MISSING	N/A		
Combination Drug Therapy	nucleoside analogs	TherapeuticOrPre ventiveProcedure	16.492	0.103	0.524	10.564	treats	prevents	neg treats	neg prevent DOI: 10.1371/journal.pone.0253703	MISSING	N/A		
	nucleoside analogs	TherapeuticOrPre ventiveProcedure	16.946	0.106	0.584	12.405	neg treats	treats	prevents	neg prevent DOI: 10.1586/143203	UNCLEAR	N/A		
Cytotoxic Chemotherapy	nucleoside analogs	TherapeuticOrPre ventiveProcedure	16.513	0.103	0.556	11.396	treats	prevents	neg treats	neg prevent N/A	MISSING	N/A		
	nucleoside analogs	TherapeuticOrPre ventiveProcedure	16.607	0.104	0.519	10.497	treats	prevents	neg treats	neg prevent N/A	MISSING	N/A		
Lamivudine	nucleoside analogs	PharmacologicSu bstance	16.726	0.105	0.493	9.889	treats	prevents	neg treats	part OF	N/A	MISSING	N/A	
	nucleoside analogs	TherapeuticOrPre ventiveProcedure	16.751	0.105	0.540	11.122	treats	neg treats	prevents	neg prevent N/A	MISSING	N/A		
Salvage Therapy	nucleoside analogs													

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node	Drug Class	node type	hetesim score	standardized hetesim score	novelty score	count score	predicted link 1	predicted link 2	predicted link 3	predicted link 4	DOI(s)	validation	pharmacokinetics
Psychotherapy, Multiple	nucleoside analogs	TherapeuticOrPreventiveProcedure	16.825	0.105	0.506	10.275	treats	prevents	neg treats	neg prevent	N/A	MISSING	N/A
Clinical Treatment	nucleoside analogs	TherapeuticOrPreventiveProcedure	16.990	0.106	0.544	11.390	N/A	N/A	N/A	N/A	N/A	MISSING	N/A
Zidovudine	nucleoside analogs	PharmacologicSubstance	16.881	0.106	0.474	9.482	neg treats	treats	prevents	part OF	DOI: 10.1016/j.aids	PROVEN	Primary
Cancer Treatment	nucleoside analogs	TherapeuticOrPreventiveProcedure	17.125	0.107	0.499	10.270	N/A	N/A	N/A	N/A	N/A	MISSING	N/A
Retreatments	nucleoside analogs	TherapeuticOrPreventiveProcedure	17.172	0.107	0.539	11.357	treats	neg treats	prevents	neg prevent	N/A	MISSING	N/A
Plasmapheresis	nucleoside analogs	TherapeuticOrPreventiveProcedure	17.115	0.107	0.554	11.709	prevents	neg treats	treats	neg prevent	DOI: 10.1016/j.biotec	UNCLEAR	N/A
small molecule	protease inhibitors	OrganicChemical	28.070	0.075	0.622	8.770	N/A	N/A	N/A	N/A	N/A	MISSING	N/A
Chloroquine	protease inhibitors	OrganicChemical	31.185	0.084	0.613	9.249	treats	prevents	neg treats	neg prevent	DOI: 10.1016/j.virol	PROVEN	Primary
Eddet Acid	protease inhibitors	OrganicChemical	31.726	0.085	0.604	9.158	treats	prevents	neg treats	part of	DOI: 10.1016/j.virol	MISSING	N/A
Ethylene	protease inhibitors	OrganicChemical	33.955	0.091	0.629	10.201	treats	prevents	part of	neg treats	N/A	MISSING	N/A
Pentetic Acid	protease inhibitors	OrganicChemical	33.993	0.091	0.633	10.298	treats	prevents	neg treats	part of	N/A	MISSING	N/A
Sulphydryl Compounds	protease inhibitors	OrganicChemical	34.020	0.091	0.574	8.973	treats	prevents	part of	neg treats	N/A	MISSING	N/A
Vitamin A	protease inhibitors	OrganicChemical	34.314	0.092	0.582	9.231	prevents	treats	neg treats	part of	DOI: 10.18632/aging	UNCLEAR	N/A
Esters	protease inhibitors	OrganicChemical	34.115	0.092	0.586	9.272	N/A	N/A	N/A	N/A	N/A	MISSING	N/A
Adriamycin	protease inhibitors	OrganicChemical	34.633	0.093	0.598	9.649	treats	prevents	part of	neg treats	DOI: 10.1016/j.comb	UNCLEAR	N/A
favor	protease inhibitors	OrganicChemical	34.893	0.094	0.575	9.184	prevents	treats	part of	neg treats	N/A	MISSING	N/A
Amprenavir	protease inhibitors	OrganicChemical	35.924	0.097	0.632	10.685	treats	prevents	part of	neg treats	DOI: 00658-20	PROVEN	Primary
Nelfinavir	protease inhibitors	OrganicChemical	36.656	0.099	0.620	10.583	treats	prevents	neg treats	part of	DOI: 11128/mBio.0	UNCLEAR	N/A
Dimethyl Sulfoxide	protease inhibitors	OrganicChemical	35.013	0.094	0.586	9.459	treats	prevents	neg treats	part of	N/A	MISSING	N/A
Salicylic Acid	protease inhibitors	OrganicChemical	36.658	0.099	0.601	10.140	prevents	treats	part of	neg treats	DOI: 10.1016/j.jaccas	UNCLEAR	N/A
Tretinoin	protease inhibitors	OrganicChemical	35.355	0.095	0.549	8.702	treats	prevents	neg treats	part of	N/A	MISSING	N/A
Curcumin	protease inhibitors	OrganicChemical	36.873	0.099	0.561	9.311	treats	prevents	part of	neg treats	DOI: 10.1007/s1333	UNCLEAR	N/A
Paclitaxel	protease inhibitors	OrganicChemical	35.554	0.096	0.588	9.615	treats	prevents	neg treats	part of	N/A	MISSING	N/A
2-Mercaptoethanol	protease inhibitors	OrganicChemical	35.756	0.096	0.595	9.815	treats	part of	neg treats	prevents	N/A	MISSING	N/A
Suramin	protease inhibitors	OrganicChemical	36.563	0.098	0.599	10.082	prevents	treats	neg treats	part of	DOI: 0900-20	PROVEN	Primary
Hydroxymethylglutaryl-CoA Reductase Inhibitors	protease inhibitors	OrganicChemical	36.703	0.099	0.578	9.650	prevents	treats	neg treats	part of	DOI: 10.1002/phar.2	PROVEN	Side-Effect