Supplementary information

Nanotechnology for COVID-19: Therapeutics and Vaccine Research

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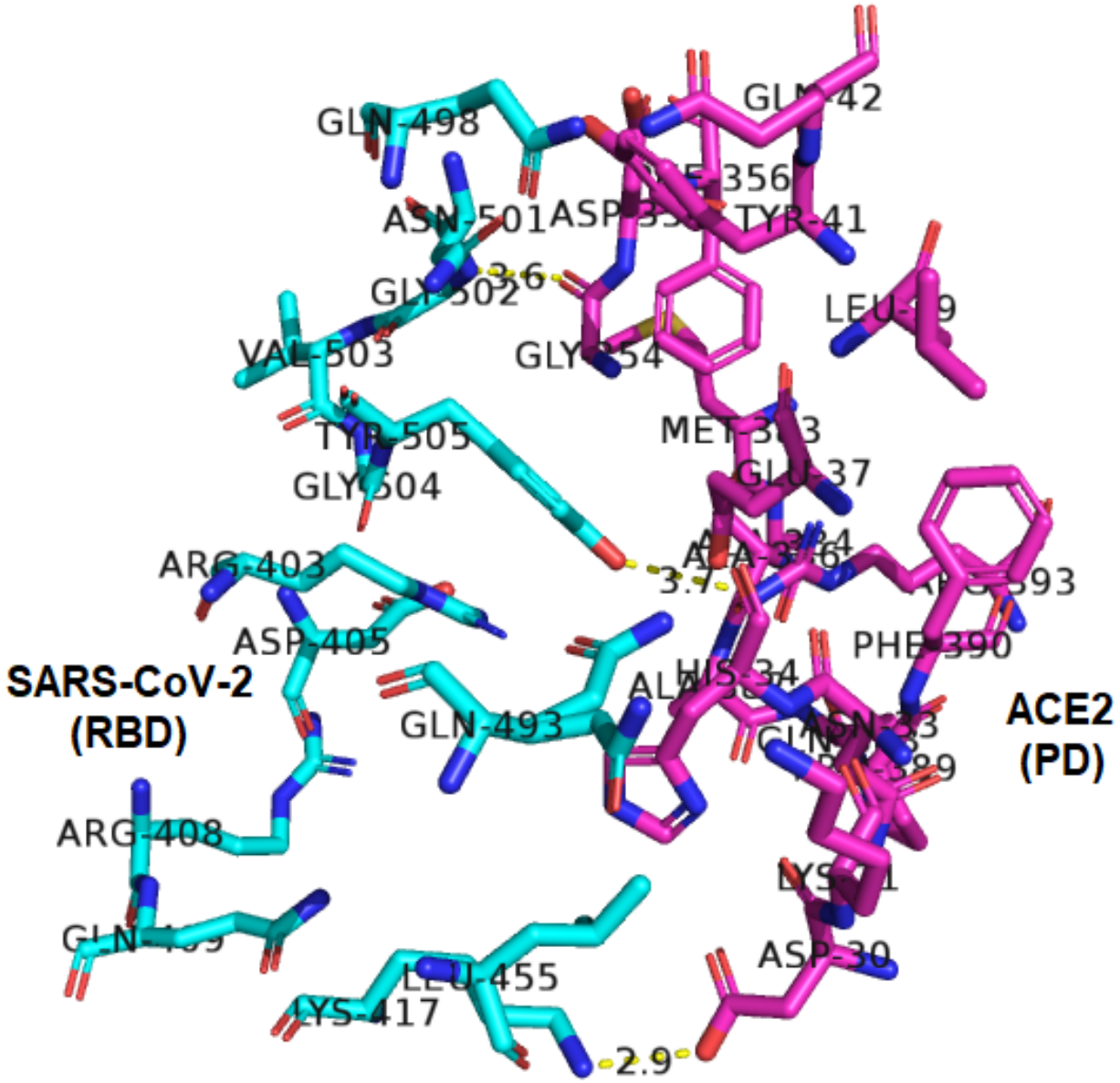

S-Fig. 1 Representation of the residues that are involved in the interaction of RBD domain of the SARS-CoV-2 with peptidase domain of Human ACE 2 (PDB ID: 6M0J)

Table-S1. Side effects/toxicity of existing antiviral molecules under development for COVID-19 therapeutics

Candidate	Side effects/ toxicity
Chloroquine	Visual acuity, insomnia, pruritus, the feeling of "stings" into the skin, and paresthesias.
Hydroxychloroquine	Blistering, peeling, loosening of the skin, blurred vision or other vision changes, chest discomfort, pain, or tightness, cough or hoarseness, dark urine, decreased urination, defective color vision, diarrhea, difficulty breathing, difficulty seeing at night, dizziness or fainting, fast, pounding, uneven heartbeat, fever with or without chills, general feeling of tiredness or weakness, headache, sore throat sores, ulcers, or white spots on the lips or in the mouth.
Tenofovir	Depression, pain, back pain, diarrhea, headache, trouble sleeping, nausea or vomiting, rash, lactic acidosis, liver enlargement, worsening hepatitis B virus infection, decreased bone mineral density, immune reconstitution syndrome, kidney damage and reduced kidney function.
Remdesivir	Nausea, Vomiting.
Favipiravir	Teratogenic and embryotoxic effects on animals.
Galidesivir	NA
EIDD-2801	NA
Ribavirin	Causes ribavirin-induced anemia has been shown to involve reductions in reticulocyte counts and erythrocyte Na-K pump activity, and increases in K-Cl cotransport, membrane bound IgG, and C3, and erythrocyte band 3.
Emtricitabine	Headache, dizziness, weakness; indigestion, stomach pain, nausea, vomiting, diarrhea hepatotoxicity with steatosis, as well as lactic acidosis.
Darunavir	Stuffy or runny nose, liver problems and severe skin reactions or rash, diarrhea, nausea, vomiting, heartburn, stomach pain, weakness, headache, or changes in the shape or location of body fat.
α-Ketomide inhibitor	NA
Lopinavir	Increased serum cholesterol and increased serum triglycerides, blurred vision, chills, constipation, darkened urine, dry mouth, fast heartbeat.
Ritonavir	Hepatotoxicity, pancreatitis, and allergic reactions / hypersensitivity.
Camostat	Dizziness, burning sensation, chest pain, skin rash, hair loss, nausea, vomiting, stomach pain, dry mouth.
Baricitinib	Upper respiratory tract infections (common cold, sinus infections), and shingles.

Ruxolitinib	Anemia, balance impairment, dizziness, headache, labyrinthitis, meniere's disease, neutropenia, thrombocytopenia, vertigo, and orthostatic dizziness. Other side effects include weight gain, and flatulence.
Umifenovir	Side effects in children include sensitization to the drug, allergic reactions are limited to people with hypersensitivity.
Fingolimod	Liver problems, increased risk of infections, macular edema, trouble breathing, increased blood pressure, leukoencephalopathy, cancer (Basal cell carcinoma and melanoma), allergy.
Thalidomide	Drowsiness, sleepiness, dizziness, constipation, muscle weakness, dry skin, anxiety, confusion, tremors or shaking, bone pain, sleep problems (insomnia),nausea, or loss of appetite, May cause possibly severe nerve damage, which may be permanent, can cause severe birth defects or embryofetal death, even with 1 dose, if taken during pregnancy.

Table-S2. Predicted properties of Existing antiviral molecules under development for COVID-19 therapeutics

Drug candidate	Pka (acid) (Predicted)	Pka (basic) (predicted)	Bioavailability	Biodegradation
α-Ketomide inhibitor	NA	NA	NA	NA
Ribavirin	11.88	-1.2	1	0.7406
Favipiravir	9.39	-3.7	1	NA
Galidesivir	12.95	8.46	1	NA
EIDD-2801	8.21	-3.7	1	NA
Thalidomide	11.59	-6.4	1	0.8838
Emtricitabine	14.29	-3.61	1	1 (not ready degradable
Tenofovir	1.35	3.74	1	NA
Baricitinib	13.89	3.91	1	NA
Remdesivir	10.23	0.65	0	NA
Ruxolitinib	13.89	5.51	1	0.9917
Darunavir	13.59	2.39	0	1(not ready degradable
Camostat	19.54	8.54	1	NA

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Hydroxychloroquine	15.59	9.76	1	1(not ready degradable
Chloroquine	NA	10.32	1	1(not ready degradable
Fingolimod	14.41	9.38	1	0.9662(not ready degradable
Umifenovir	6.01	9.87	1	NA
Lopinavir	13.39	-1.5	0	0.9182 not ready degradable
Ritonavir	13.68	2.84	0	0.9633 not ready degradable

pKa (acid), pKa (base) and bioavailibilty is calculated by **ChemAxon**
Biodegradation was calculated **admetSAR**

ChemAxon for pKa (acid) and pKa (basic): Highly-accurate calculation of pKa values along with pH-% of distribution plots of relevant microspecies in water - pKa documentation

Chemaxon for Bioavailibilty:

(mass() <= 500) + (logP() <= 5) + (donorCount() <= 5) + (acceptorCount() <= 10) + (rotatableBondCount() <= 10) + (PSA() <= 200) + (fusedAromaticRingCount() <= 5) >= 6	A bioavailability filter. 6 out of the 7 filters must pass for the whole rule to evaluate to TRUE. In the context of the + operator the value or the individual rules is 0 (fail) or 1 (pass), and so this expression is just adding up the 1's to find out how many individual terms have passed, and then checked whether this total is greater than or equal to 6

admetSAR for Biodegradation:

A large diverse biodegradability database containing 1440 unique compounds was obtained 529 (ready biodegradable) and 911 (not ready biodegradable). QBSR (quantitative biodegradable structure relationship)