

Supplementary Tables

Table S1. Clinical peptide drugs with potential ability to inhibit ACE2-spike protein interactions

Name	CAS	Reported target/function	Binding energy (kcal/mol)
Terlipressin	14636-12-5	V1 receptors	-89.82
Desmopressin	16679-58-6	V1/2/3 receptors	-82.64
Octreotide acetate	79517-01-4	Hormone somatostatin	-82.61
DAPTA	106362-34-9	CCR5	-75.49
Colistin sulfate	1264-72-8	Anti-infection	-74.68
Dalbavancin	171500-79-1	Anti-infection	-68.78
Pralmorelin	158861-67-7	Growth hormone-releasing	-66.96
Thymopentin	69558-55-0	Immunology & HIV	-55.08
Oxiglutatione	27025-41-8	Detoxification	-55.07
Polymyxin B sulfate	1405-20-5	Anti-infection	-51.36

Table S2. Routine blood test results in rhesus macaques inoculated with SARS-CoV-2 with or without dalbavancin treatment.

Parameter		0 dpi	1 dpi	3 dpi	5 dpi	7 dpi
Saline	White blood cell count	8.900 ± 2.905	8.500 ± 1.305	6.333 ± 0.8192	7.967 ± 0.4333	8.200 ± 0.1000
	Lymphocyte count	1.900 ± 0.7638	2.967 ± 1.419	2.867 ± 0.7219	2.800 ± 0.7767	3.333 ± 0.4333
	Monocyte count	0.6333 ± 0.1453	0.7333 ± 0.1202	0.5667 ± 0.1453	0.7667 ± 0.1764	0.6000 ± 0.05774
	Neutrophil count	6.367 ± 3.299	4.800 ± 1.747	2.900 ± 0.4000	4.400 ± 0.7371	4.267 ± 0.5044
	Lymphocyte ratio	28.30 ± 13.78	35.10 ± 14.96	44.37 ± 6.471	34.53 ± 8.028	40.47 ± 5.725
	Monocyte ratio	7.733 ± 0.9025	8.567 ± 0.4702	8.800 ± 1.069	9.367 ± 1.761	7.600 ± 0.6807
	Neutrophil ratio	63.97 ± 14.68	56.33 ± 15.43	46.83 ± 6.919	56.10 ± 9.782	51.93 ± 5.948
	Red blood cell count	7.080 ± 0.04726	6.873 ± 0.3221	5.777 ± 0.2270	5.657 ± 0.3832	5.950 ± 0.1358
	Hemoglobin	170.3 ± 2.667	163.0 ± 2.517	142.7 ± 1.764	137.0 ± 7.550	141.0 ± 3.606
	Hematocrit	53.97 ± 1.757	51.93 ± 0.4333	42.67 ± 0.4096	41.60 ± 2.163	43.40 ± 1.124
	Mean corpuscular volume	76.37 ± 2.990	75.90 ± 2.804	74.13 ± 2.339	73.93 ± 2.697	73.10 ± 2.200
	Mean corpuscular hemoglobin	24.03 ± 0.5175	23.77 ± 0.8413	24.70 ± 0.6658	24.20 ± 0.7211	23.67 ± 0.7333
	Mean corpuscular hemoglobin concentration	315.3 ± 5.608	313.3 ± 4.055	334.0 ± 1.732	329.0 ± 2.517	324.3 ± 0.3333
	Red blood cell distribution width	13.53 ± 0.3283	13.97 ± 0.4910	12.10 ± 0.4041	12.07 ± 0.6173	12.17 ± 0.6119
	Platelet	550.7 ± 16.68	462.0 ± 31.58	353.0 ± 54.78	392.0 ± 75.74	446.7 ± 66.96
	Mean platelet volume	8.533 ± 0.3756	8.233 ± 0.3383	8.233 ± 0.3528	8.167 ± 0.3180	8.200 ± 0.3512

	Platelet	16.40 ±	16.27 ±	16.57 ±	16.30 ±	16.47 ±
	distribution width	0.2082	0.1202	0.1202	0.1528	0.2186
		0.4707 ±	0.3820 ±	0.2940 ±	0.3237 ±	0.3670 ±
	Thrombocytocrit	0.03451	0.04204	0.05903	0.07435	0.06285
Dalba	White blood cell	9.300 ±	8.433 ±	7.167 ±	9.167 ±	8.233 ±
vancin	count	0.4933	1.203	0.4842	2.338	1.033
	Lymphocyte	2.667 ±	3.067 ±	3.467 ±	3.333 ±	3.500 ±
	count	0.7881	0.7219	0.3180	0.5364	0.2517
		0.8000 ±	0.9333 ±	0.7333 ±	0.7333 ±	0.9000 ±
	Monocyte count	0.1528	0.2848	0.03333	0.2333	0.2646
		5.833 ±	4.433 ±	2.967 ±	5.100 ±	3.833 ±
	Neutrophil count	0.9770	1.486	0.7424	1.960	0.5364
		28.90 ±	38.93 ±	49.57 ±	39.53 ±	43.03 ±
	Lymphocyte ratio	8.883	11.37	8.137	8.589	2.298
		8.500 ±	10.83 ±	10.20 ±	7.567 ±	10.83 ±
	Monocyte ratio	1.234	1.991	0.7638	0.7126	2.025
		62.60 ±	50.23 ±	40.23 ±	52.90 ±	46.13 ±
	Neutrophil ratio	9.655	9.672	8.500	7.881	0.7446
	Red blood cell	6.847 ±	7.180 ±	6.047 ±	5.953 ±	6.007 ±
	count	0.2375	0.1387	0.1625	0.1239	0.3055
		166.3 ±	170.3 ±	149.0 ±	142.7 ±	141.3 ±
	Hemoglobin	10.04	9.955	7.024	4.410	11.35
		50.77 ±	53.23 ±	44.10 ±	43.17 ±	43.93 ±
	Hematocrit	3.230	2.910	1.637	1.317	3.483
	Mean corpuscular	74.20 ±	74.20 ±	73.17 ±	72.73 ±	73.13 ±
	volume	3.620	3.747	3.430	3.524	3.710
	Mean corpuscular	24.23 ±	23.67 ±	24.63 ±	23.97 ±	23.47 ±
	hemoglobin	1.135	1.260	1.302	1.132	1.132
	Mean corpuscular	327.3 ±	319.3 ±	337.0 ±	330.3 ±	321.3 ±
	hemoglobin	1.202	1.333	3.786	3.667	1.764
	concentration					
	Red blood cell	13.73 ±	13.80 ±	13.93 ±	13.43 ±	13.97 ±
	distribution width	0.8667	0.8185	0.8007	0.7753	0.8950
		650.0 ±	534.0 ±	480.7 ±	452.0 ±	545.3 ±
	Platelet	42.00	49.90	10.59	24.58	41.91
	Mean platelet	7.567 ±	7.467 ±	7.333 ±	7.267 ±	7.633 ±
	volume	0.2906	0.2848	0.08819	0.2028	0.5207
	Platelet	16.30 ±	16.37 ±	16.27 ±	16.23 ±	16.27 ±

distribution width	0.1528	0.06667	0.1333	0.1333	0.1333
	0.4887 ±	0.3957 ±	0.3520 ±	0.3273 ±	0.4187 ±
Thrombocytocrit	0.01338	0.02281	0.004726	0.008969	0.05795

Data are mean ± SD.

Table S3. Blood biochemistry results in rhesus macaques inoculated with SARS-CoV-2 with or without dalbavancin treatment.

Parameter	0 dpi	1 dpi	3 dpi	5 dpi	7 dpi
Saline Blood sugar	144.7 ±	89.00 ±	50.33 ±	52.67 ±	56.33 ±
mg/dL	40.88	13.43	5.239	6.766	13.54
Creatinine	0.7667 ±	0.7000 ±	0.5000 ±	0.5333 ±	0.5333 ±
(CREA) mg/dL	0.1764	0.1528	0.05774	0.03333	0.03333
Blood urea nitrogen (BUN)	40.00 ±	34.33 ±	25.00 ±	19.67 ±	18.00 ±
mg/dL	8.185	4.842	1.155	0.6667	1.155
BUN/CREA	52.67 ±	51.33 ±	49.00 ±	37.00 ±	34.00 ±
	6.064	4.096	3.606	3.055	4.000
Total protein g/dL	8.300 ±	8.033 ±	7.300 ±	7.233 ±	6.967 ±
	0.1000	0.1333	0.1528	0.06667	0.2603
Albumin (ALB)	4.033 ±	3.733 ±	3.267 ±	3.300 ±	3.167 ±
g/dL	0.06667	0.1202	0.1202	0.05774	0.08819
Globulin (GLOB)	4.233 ±	4.367 ±	4.033 ±	3.967 ±	3.833 ±
g/dL	0.03333	0.1856	0.1453	0.08819	0.2028
ALB/GLOB	0.9333 ±	0.8667 ±	0.8000 ±	0.8333 ±	0.8667 ±
	0.03333	0.06667	0.05774	0.03333	0.03333
Alanine aminotransferase	29.67 ±	31.67 ±	53.67 ±	99.67 ±	59.00 ±
U/L	12.20	7.126	18.49	42.48	24.11
Aspartate aminotransferase	22.33 ±	45.33 ±	51.00 ±	52.33 ±	45.00 ±
U/L	11.61	7.219	7.550	11.41	10.58
Cholesterol	155.7 ±	109.0 ±	70.67 ±	84.00 ±	83.67 ±
mg/dL	15.86	18.88	2.728	3.786	1.667
Triglyceride	57.33 ±	54.00 ±	31.33 ±	48.67 ±	52.00 ±
mg/dL	9.838	6.506	19.13	0.8819	5.132
Creatine kinase	83.67 ±	349.7 ±	69.67 ±	92.67 ±	96.00 ±
U/L	22.30	122.5	6.489	13.48	28.01
Lactate dehydrogenase	792.7 ±	864.7 ±	1634 ± 532.9	1279 ±	1286 ±
U/L	316.5	154.7		541.7	301.0
Lactate mmol/L	8.060 ±	8.907 ±	5.497 ±	4.683 ±	6.517 ±

		0.9829	1.583	1.066	0.8274	1.353
Dalba	Blood sugar	117.7 ±	72.33 ±	52.67 ±	53.00 ±	42.67 ±
vancin	mg/dL	23.31	8.007	4.842	4.583	4.667
	Creatinine	0.6000 ±	0.6333 ±	0.5333 ±	0.5667 ±	0.7000 ±
	(CREA) mg/dL	0.05774	0.1453	0.06667	0.03333	0.1528
	Blood urea					
	nitrogen (BUN)	50.67 ±	39.00 ±	27.67 ±	25.67 ±	24.33 ±
	mg/dL	15.38	8.083	4.667	4.702	4.910
		94.67 ±	70.33 ±	55.33 ±	46.33 ±	41.33 ±
	BUN/CREA	38.52	26.27	9.735	5.548	12.99
		8.067 ±	8.667 ±	7.700 ±	7.633 ±	7.833 ±
	Total protein g/dL	0.1667	0.1764	0.2082	0.3844	0.3756
	Albumin (ALB)	3.633 ±	4.033 ±	3.467 ±	3.400 ±	3.933 ±
	g/dL	0.2028	0.3528	0.2333	0.1528	0.6888
	Globulin (GLOB)	4.400 ±	4.600 ±	4.233 ±	4.200 ±	3.900 ±
	g/dL	0.3786	0.4933	0.4333	0.4359	0.3786
		0.8000 ±	0.9000 ±	0.8333 ±	0.8000 ±	1.067 ±
	ALB/GLOB	0.1155	0.1732	0.1453	0.1000	0.2728
	Alanine					
	aminotransferase	31.00 ±	39.67 ±	25.67 ±	44.67 ±	50.67 ±
	U/L	6.658	16.33	9.563	13.87	26.34
	Aspartate					
	aminotransferase	16.00 ±	91.33 ±	40.33 ±	50.67 ±	55.50 ±
	U/L	8.000	58.34	8.413	11.68	21.50
	Cholesterol	171.0 ±	153.0 ±	89.33 ±	88.67 ±	107.0 ±
	mg/dL	16.20	15.95	9.333	8.212	16.07
	Triglyceride	38.67 ±	82.00 ±	60.33 ±	48.67 ±	75.33 ±
	mg/dL	8.293	42.00	14.81	0.8819	38.40
	Creatine kinase	189.3 ±	573.0 ±	141.0 ±	275.7 ±	552.7 ±
	U/L	63.94	370.5	47.04	47.68	337.8
	Lactate					
	dehydrogenase	1544 ± 271.6	1771 ±	2249 ± 372.7	1650 ±	1932 ±
	U/L		122.0		195.2	63.50
		6.787 ±	7.463 ±	6.500 ±	3.193 ±	6.110 ±
	Lactate mmol/L	2.322	2.455	2.757	0.5154	2.954

Data are mean ± SD.