

Supplementary File

Title:- Molecular prediction of SARS-CoV-2 transmission in domesticated livestock

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Table S1. Percent Identity matrix of ACE2 alignment

	<i>Bos</i>	<i>Capra</i>	<i>Ovis</i>	<i>Camelus</i>	<i>Sus</i>	<i>Mus</i>	<i>Oryctolagus</i>	<i>Human</i>	<i>Felis</i>	<i>Canis</i>
<i>Bos</i>	100.00	97.51	97.26	88.56	88.04	80.47	83.23	81.09	83.33	82.32
<i>Capra</i>	97.51	100.00	99.25	88.31	88.43	80.22	83.10	81.72	83.33	81.94
<i>Ovis</i>	97.26	99.25	100.00	88.43	88.17	80.10	82.98	81.72	83.46	81.94
<i>Camalus</i>	88.56	88.31	88.43	100.00	90.26	80.99	84.76	83.23	85.71	83.96
<i>Sus</i>	88.04	88.43	88.17	90.26	100.00	81.56	83.27	82.34	84.94	82.70
<i>Mus</i>	80.47	80.22	80.10	80.99	81.56	100.00	83.63	82.11	81.74	81.22
<i>Oryctolagus</i>	83.23	83.10	82.98	84.76	83.27	83.63	100.00	85.14	84.51	83.23
<i>Human</i>	81.09	81.72	81.72	83.23	82.34	82.11	85.14	100.00	85.22	83.46
<i>Felis</i>	83.33	83.33	83.46	85.71	84.94	81.74	84.51	85.22	100.00	90.67
<i>Canis</i>	82.32	81.94	81.94	83.96	82.70	81.22	83.23	83.46	90.67	100.00

Table S2. Details interaction of RBD of SARA-CoV-2 to ACE2 of human and pets

Pet name	Total interactive residue		No of H-bond	H-bond participating residues	Bond length (angstrom)	No of hydrophobic bond	Hydrophobic bond participating residues	Bond length							
	RBD	ACEII													
Human	E484,E493, Y453,S494, Y489, G496, Q498,T500, F486,E35, L79, Y449, F456,	K74, K31, Q76,N103, Q81,E75, E35,D38, M82,S106, Q81,Y495, F456,L39,	13	K31:Y453	2.07893	4	L79:F456 L39:Y449 M82:F456 M82:Y489	3.76981 5.24567 4.81581 4.64581							
				K31:E493	2.43061										
				Q76:S494	2.56837										
				Q76:Q493	1.94333										
				N103:E484	2.53706										
				Q81:Y489	3.00816										
				E75:S494	1.70466										
				E35:G496	1.73167										
				E35:Q498	2.14841										
				D38:T500	1.74691										
				M82:Y489	3.21622										
				S106:E484	3.50956										
				Q81:F486	3.24016										
Felis	R403,Y453, Q493,S494, Y505,T500, Q498,Y449, F490,Y486, Y489,P499,	E35,K31, Q76,T82, Y83,T27, E38,E75, R357,D355, Y41,L24, L79	11	K31:Y453	1.64697	3	Y41:Y489 L24:P499 L79:Y505	5.26629 5.28358 4.61434							
				K31:Q493	2.73763										
				K31:S494	1.9146										
				Q76:Y505	2.56855										
				T82:T500	2.17479										
				Y83:Q498	2.16915										
				T27:Y449	2.48163										
				E35:Y453	2.85273										
				E38:F490	1.87742										
				Y83:T500	1.77501										
				E75:Y505	1.81851										
				Camalus	E484,Y449, S494,G496, Q498,G446 F490,D493, T500,N501, Y495,F486, L455,				K353,K76, T79,T82, Y83,D38, E35,E75, E31,D355, L39,K68	13	K76:Y449	1.83198	2	L39:L455 K68:L455	5.10204 5.36218
											K76:S494	1.99363			
T79:G496	3.07895														
T82:Q498	1.78184														
Y83:G446	2.79722														
D38:F490	1.95654														
E35:D493	3.06868														
E35:S494	1.72128														
E35:S494	1.84234														
E75:G496	1.7826														
Y83:Q498	2.32092														
T82:T500	1.73597														
E75:N501	2.49411														

<i>Sus</i>	E484,R403 S494,L455, F490,S494, N501,R403, F456,Y489, A475	K353,E75, K31,K68, D38,E35, E35,R78, E75,K68, D64,Y41, Q42,L39, K68,L45	9	K353:E484 E75:R403 K31:S494 K68:L455 D38:F490 E35:S494 E35:S494 R78:N501 E75:R403	1.63633 1.7528 2.10218 2.51225 2.19472 2.67943 1.63722 2.73512 3.25278	5	Y41:Y489 Q42:Y489 L39:L455 K68:L455 L45:A475	5.14687 4.49325 5.29132 4.18373 5.01999		
	<i>Oryctolagus</i>	R403,E484, K417,F486, S494,Y453, Q493,Y489, Y449,N487, Q498,Y489, L455,F456 Y505	D53,K342, E45,Y30, Q31,K57, R346,E64, N319,Q31, A60,D53, L34,A35, A56	12	D53:R403 Y30:F486 Q31:S494 K57:Y453 K57:Q493 R346:Y489 E64:Y449 N319:N487 Q31:Q493 A60:Q498 D53:R403 D53:R403	1.81053 2.20789 1.98302 2.67933 2.55242 2.6192 1.83101 2.25737 2.60283 3.0088 3.49754 3.58093	4	L34:Y489 A35:L455 L34:F456 A56:Y505	3.56129 4.28194 4.05195 4.28932	
		<i>Mus</i>	R403,K417, T500, Q498,S494, Y505,Y453, Q493,F486, Y495,F456, Y489,Y505, R403	E35,E75, N24,T27, N31,T79 S82,H353, D38, 28, H353	13	E35:R403 E75:K417 E75:K417 N24:T500 T27:Q498 N31:S494 T79:Y505 E35:Y453 E35:Q493 N31:Q493 S82:T500 H353:F486 N31:Y495	2.35102 1.72271 2.62513 2.09536 1.77793 2.31401 2.92863 1.88647 1.78842 2.36633 3.61035 3.267 3.13858	2	F28:Y505 H353:Y489	5.01386 5.35673

Table S3. Contact residues between ACE2 and RBD-Spike. The alterations of amino acids are shown in bold as present in the pet animals.

ACE2	RBD-Spike
Q24L	K417
T27	G446
F28	Y449
D30E	Y453
K31	L455
H34Y	F456
E35	A475
E37	F486
D38E	N487
Y41	Y489
Q42	Q493
M82T	Y495
Y83	G496

N330	Q498
K353	T500
G354	N501
D355	G502
R357	Y505

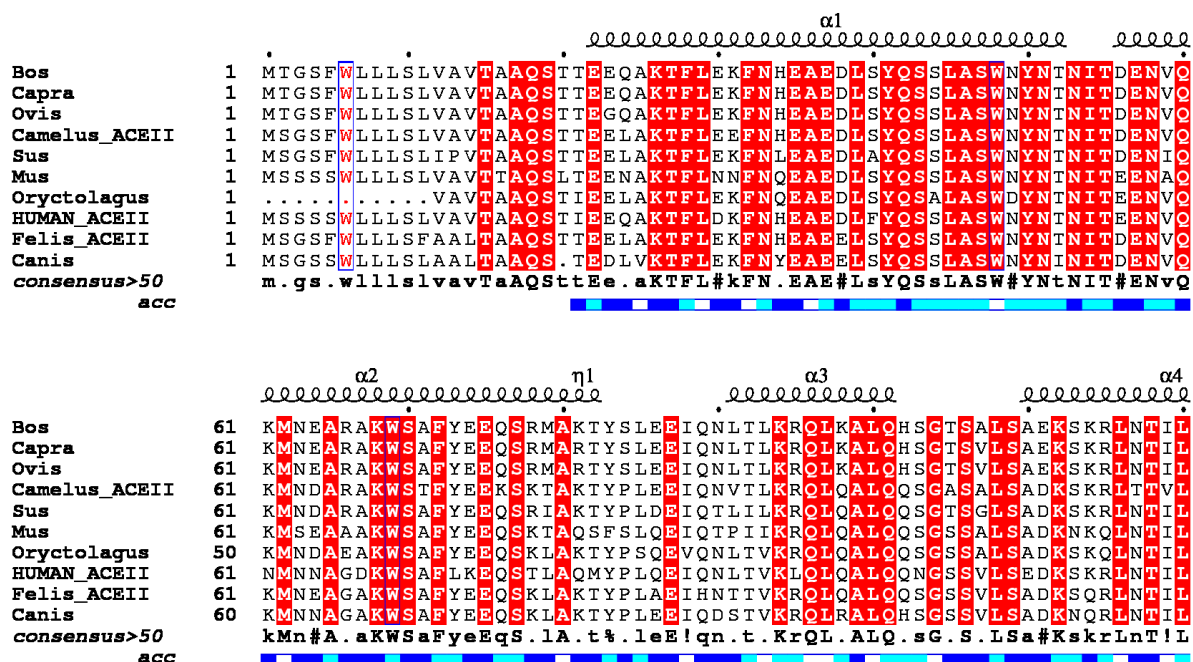


Fig. S1. MSA among the ten different mammalian pet including human ACE2 were performed by Clustal omega web server and visualized by Esprit 3 software. The secondary structure for the ACE2 spike model is displayed at the top of the MSA, and residual surfACE accessibility is present at the bottom. Alpha helices are shown by helix on the top of MSA. The residues that are surfACE accessible are in blue, while buried residues are in white at the bottom of the MSA. Identical residues are highlighted in red and others are in white. Multiple sequence alignment of ACE2 of pets and human. The red highlighted residues are conserved among the ten ACE2. SurfACE accessible regions (dark blue) and buried regions (whitish) are shown schematically at the bottom. Alpha helix are shown at the top.

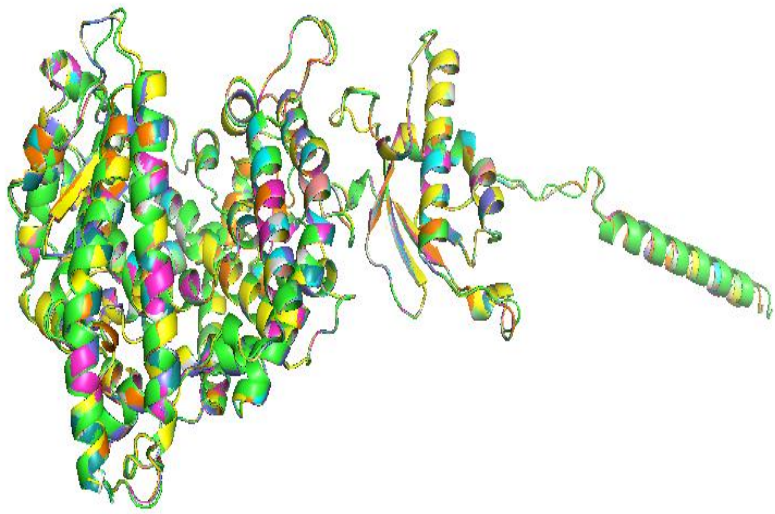


Fig. S2. Superimpose of ACE2 of nine pet animals and human

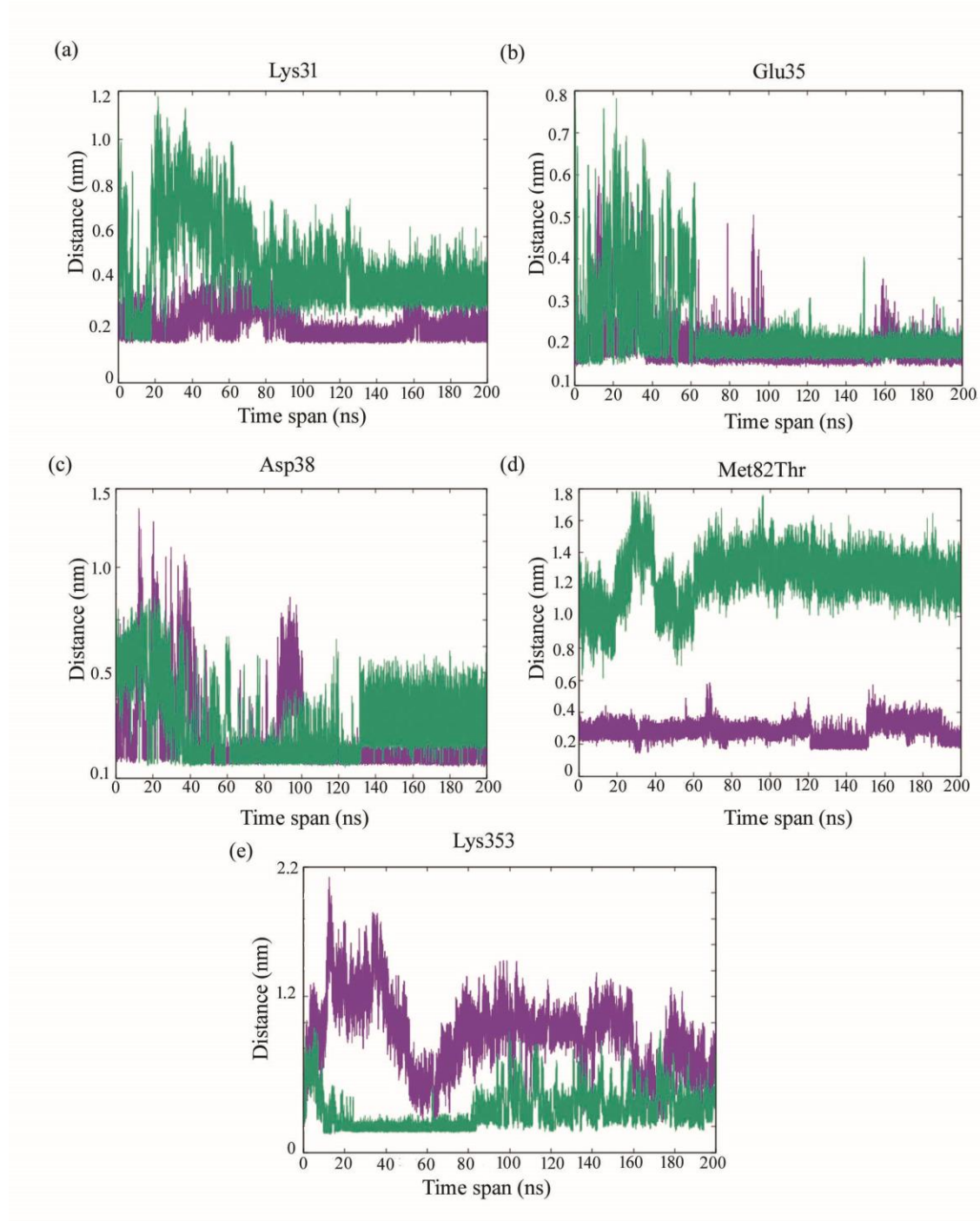


Fig. S3. Minimum distances at (a) Lys31, (b) Glu85, (c) Asp38, (d) Met82Thr and (e) Lys353 of hACE2 (purple) and oACE2 (green) binding with RBD spike glycoprotein of SARS-CoV-2.

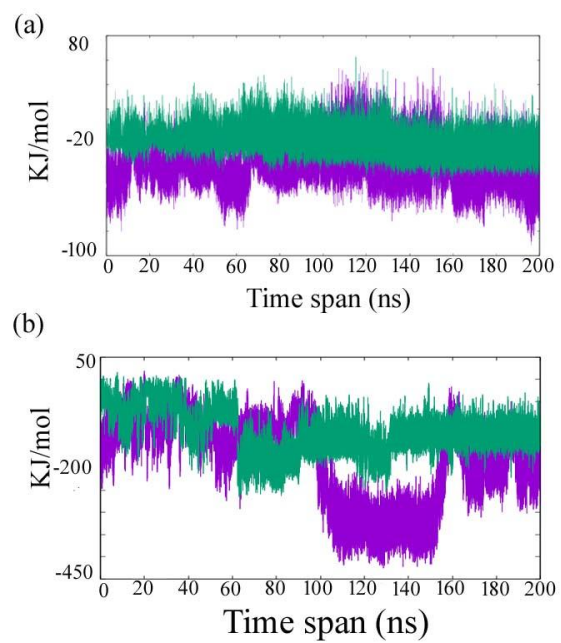


Fig. S4. Energy of interaction at the binding site. (a) LJ-SR (b) Coul-SR

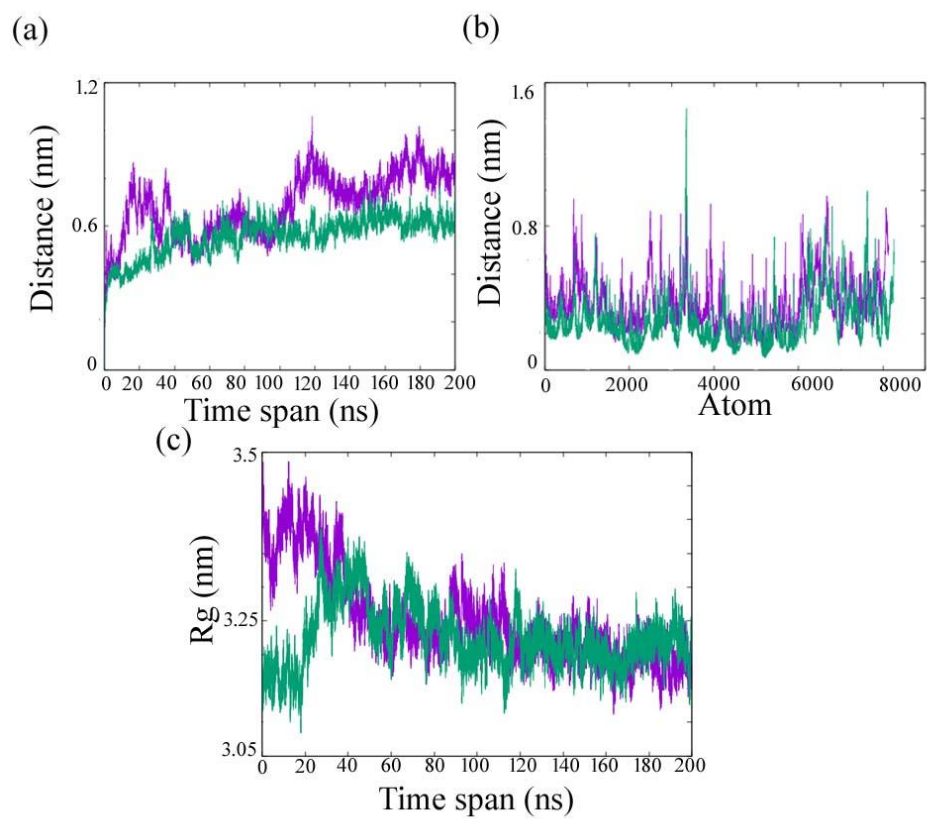


Fig. S5. Comparative analysis of simulated trajectory of hACE2-RBD (purple) and oACE2-RBD for 200 ns (green). (a) RMSD (b) RMSF (c) Rg