

Supplementary Information

Study on cubic-orientation settlement of angiotensin converting enzyme II immobilized on polystyrene by molecular dynamics simulation

Table S1. Number of amino acid residues in ACE2.

Charged residues		Neutral residues	
Amino acid	Number	Amino acid	Number
Positively Charged		ALA	38
ARG	18	ASN	39
HIS	16	GLN	30
LYS	34	GLY	32
Negatively Charged		ILE	22
ASP	33	LEU	60
GLU	47	MET	21
		PHE	27
		PRO	27
		SER	34
		THR	32
		TRP	20
		TYR	28
		VAL	31
		CYS	8

Table S2. Total charge of ACE2 under different conditions.

0.15 M NaCl pH	4.5	6	7	8	9.5
Total charge (e)	-6	-19	-22	-26	-27
pH 7 NaCl (M)	0.01	0.05	0.1	0.2	0.25
Total charge (e)	-19	-20	-22	-23	-21

Table S3. The number of atoms used in MD simulation.

NaCl (M)	pH	PS	ACE2	Na ⁺	Cl ⁻	Water	Total
0.15	4.5	29160	9523	239	233	20.3 w	24.2 w
	6			252	233		
	7			255	233		
	8			259	233		
	9.5			260	233		
0.01	7	29160	9523	35	16	20.4 w	24.3 w
0.05				98	78	20.4 w	24.3 w
0.1				178	156	20.3 w	24.2 w
0.2				334	311	20.2 w	24.2 w
0.25				410	389	20.2 w	24.1 w

Table S4. Parameters of adsorption behavior of ACE2 on PS surface at different pH values of 0.15 M NaCl. Energy and RMSD/Rg were averaged in the last 5 ns.

0.15 M NaCl	pH	begins t (ns)	Adsorption	
			VDW/Electrostatic interac- tion energy (KJ/mol)	RMSD/Rg (nm)
(0, 0, 0)	4.5	34	-244.1/-43.5	0.35/2.45
	6	19	-216.7/-76.6	0.22/2.50
	7	67	-136.4/-61.0	0.21/2.50
	9.5	56	-136.1/-60.2	0.22/2.48
(0, 90, 0)	4.5	95	-20.6/-5.2	0.22/2.49
	6	6	-221.9/-21.6	0.38/2.44
	7	3.5	-119.3/-26.2	0.27/2.48
	8	10.5	-98.0/-46.7	0.20/2.50
	9.5	3	-131.0/-20.8	0.21/2.52
(0, 270, 0)	4.5	52	-244.8/18.3	0.28/2.48
	6	8.5	-292.0/-79.2	0.22/2.49
	7	45	-208.5/-50.0	0.25/2.50
	8	17	-192.4-68.7	0.23/2.47
(90, 0, 0)	4.5	12.5	-216.3/-40.0	0.25/2.51
	6	23	-236.7/-106.2	0.35/2.44
	8	28	-239.9/-15.6	0.27/2.46
	9.5	7	-143.2/-129.2	0.26/2.50
(180, 0, 0)	4.5	52	-237.3/-49.1	0.21/2.49
	6	30.5	-77.0/-17.3	0.19/2.50
	7	15	-350.5/-100.9	0.27/2.50
	8	36.5	-140.5/-87.6	0.24/2.48
	9.5	66	-75.2/-58.2	0.27/2.48
(270, 0, 0)	4.5	85.5	-117.0/9.8	0.36/2.42
	7	49	-167.0/-81.2	0.26/2.48
	9.5	68.5	-116.9/-41.2	0.21/2.49

Table S5. Parameters of adsorption behavior of ACE2 on PS surface with different NaCl concentrations at pH 7. Energy and RMSD/Rg were averaged in the last 5 ns.

pH7	NaCl (M)	begins t (ns)	Adsorption	
			VDW/Electrostatic interac- tion energy (KJ/mol)	RMSD/Rg (nm)
(0, 0, 0)	0.1	1	-178.6/-112.9	0.27/2.47
	0.15	67	-136.4/-61.0	0.21/2.50
(0, 90, 0)	0.05	9	-99.1/-40.7	0.25/2.49
	0.15	3.5	-119.3/-26.2	0.27/2.48
	0.2	5.5	-295.5/-110.5	0.23/2.49
	0.25	10	-101.3/-5.7	0.29/2.48
(0, 270, 0)	0.01	73	-121.9/-15.2	0.21/2.49
	0.05	10	-273.9/-74.7	0.26/2.46
	0.1	78	-57.8/-28.8	0.23/2.49
	0.15	45	-208.5/-50.0	0.25/2.50
	0.25	57	-96.9/-27.8	0.25/2.52
(90, 0, 0)	0.01	69	-67.7/-59.8	0.36/2.44
	0.1	22	-264.4/-70.8	0.26/2.50
	0.2	13	-113.1/-78.4	0.24/2.48
(180, 0, 0)	0.01	93.5	-172.5/-70.5	0.26/2.48
	0.05	35.5	-327.8/-86.3	0.29/2.46
	0.1	84.5	-264.4/-110.0	0.22/2.49
	0.15	15	-350.5/-100.9	0.27/2.50
	0.2	88	-169.9/-64.5	0.24/2.48
(270, 0, 0)	0.05	89	-45.9/-46.1	0.21/2.53
	0.15	49	-167.0/-81.2	0.26/2.48
	0.2	57.5	-147.4/-54.1	0.27/2.46
	0.25	68.5	-67.0/-33.3	0.36/2.45