Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Information

Molecular insights into the binding variance of SARS-CoV-2 spike with human, cat and dog ACE2 proteins

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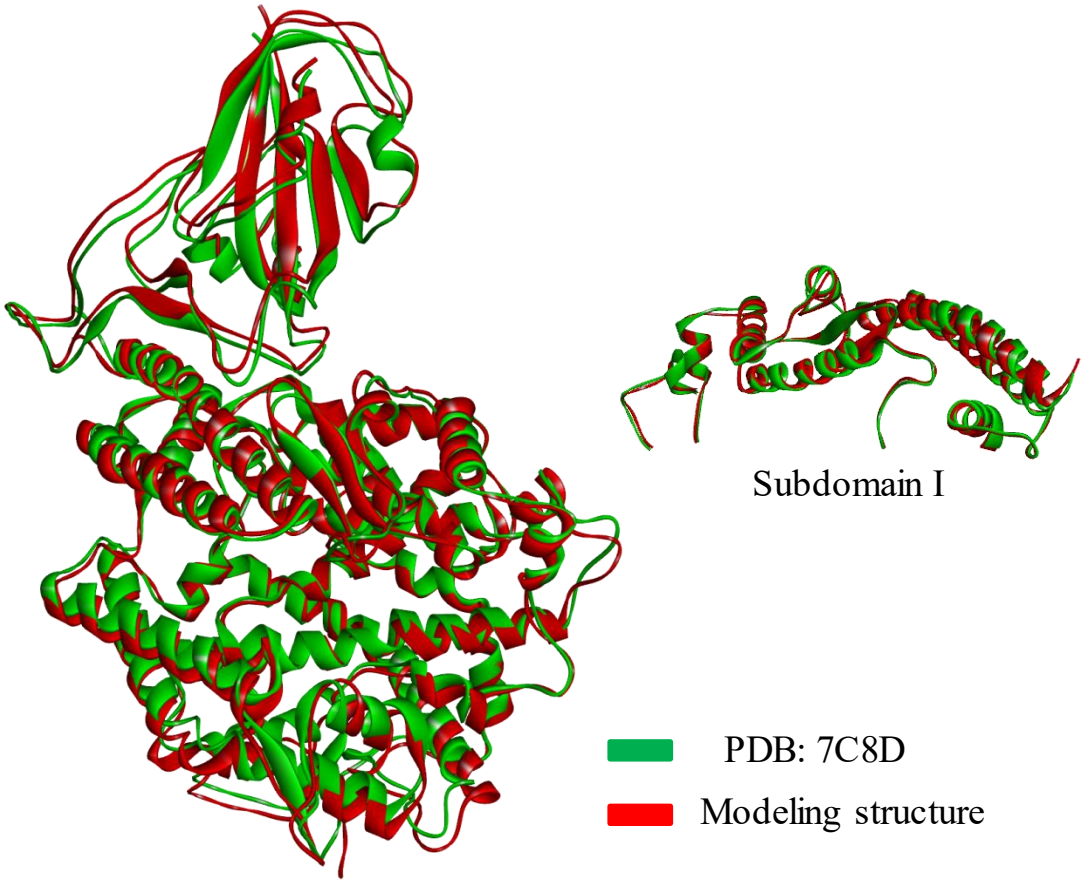

Fig. S1. The structure of Cat ACE2 was conducted by the MODELER module. The cryo-EM structure of cACE2-RBD (PDB: 7C8D) was released during the manuscript preparation. The modeling structure (in red) is almost entirely accord with the cryo-EM structure (in green), especially subdomain I that interacts with spike RBD, with the heavy-atom root mean square deviation (RMSD) of 0.823 Å

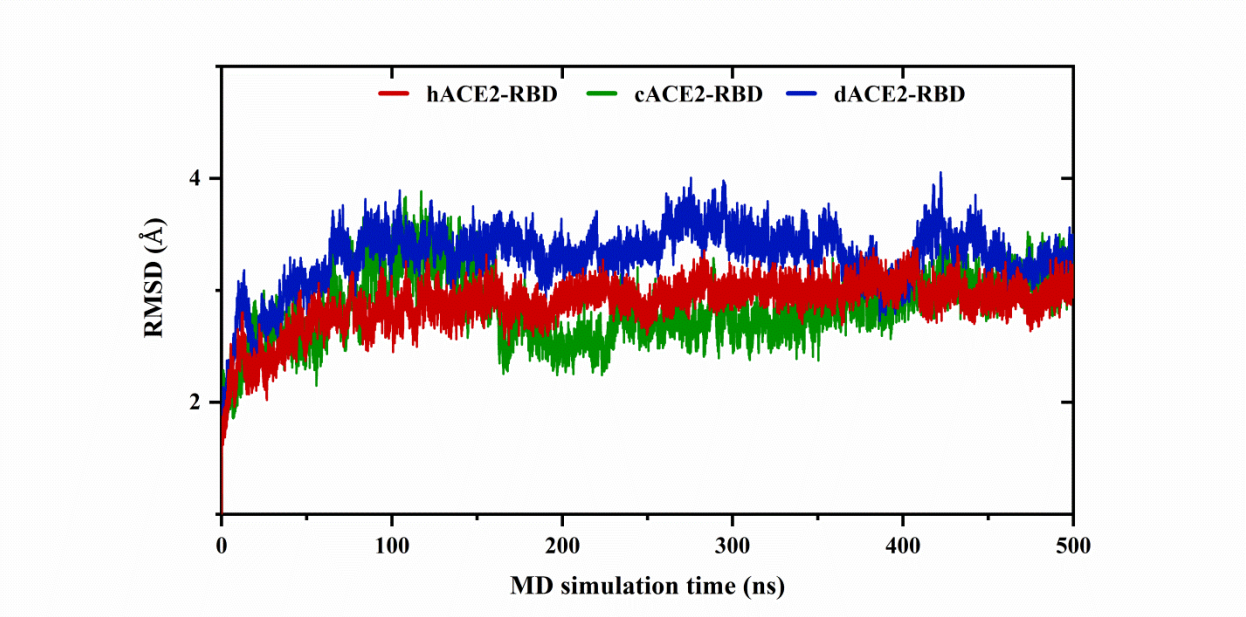

Fig. S2. Variation of the backbone-atom root-mean-square deviations (RMSD) for the h/c/dACE2-RBD complexes during the 500-ns MD simulations.

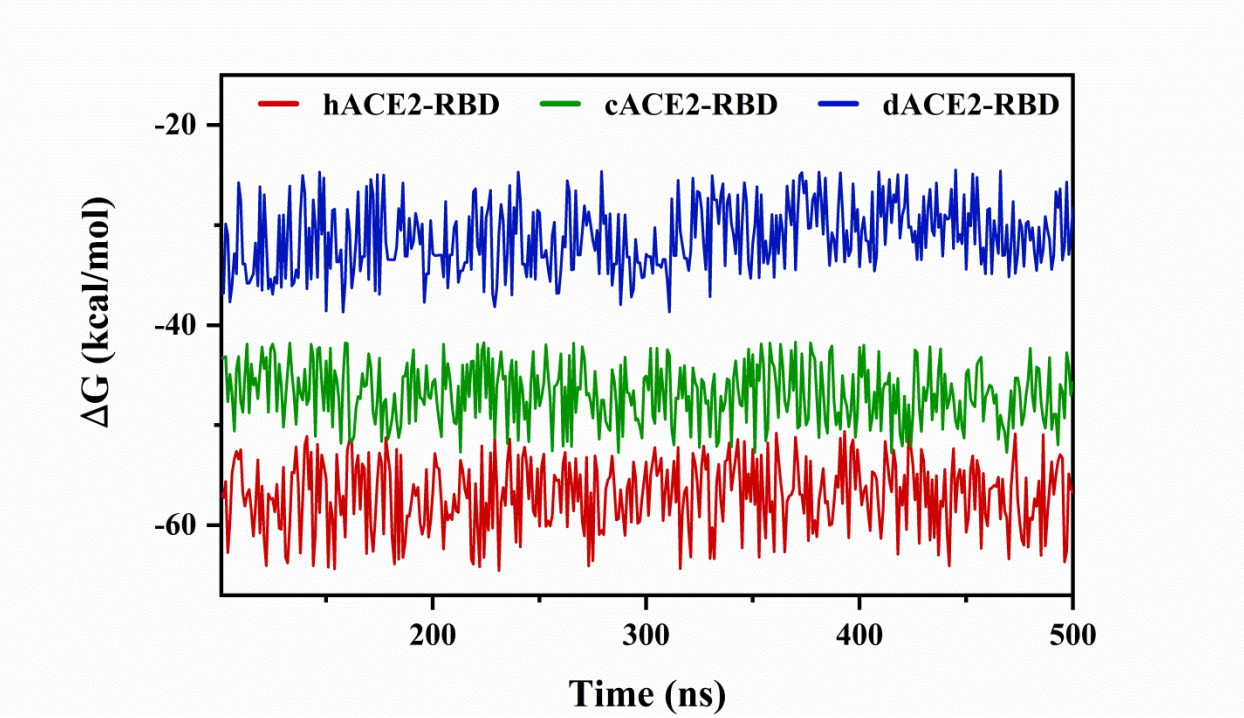

Fig. S3. Variation of the binding free energies (kcal/mol) for h/c/dACE2-RBD complexes over 100-500 ns MD trajectories.

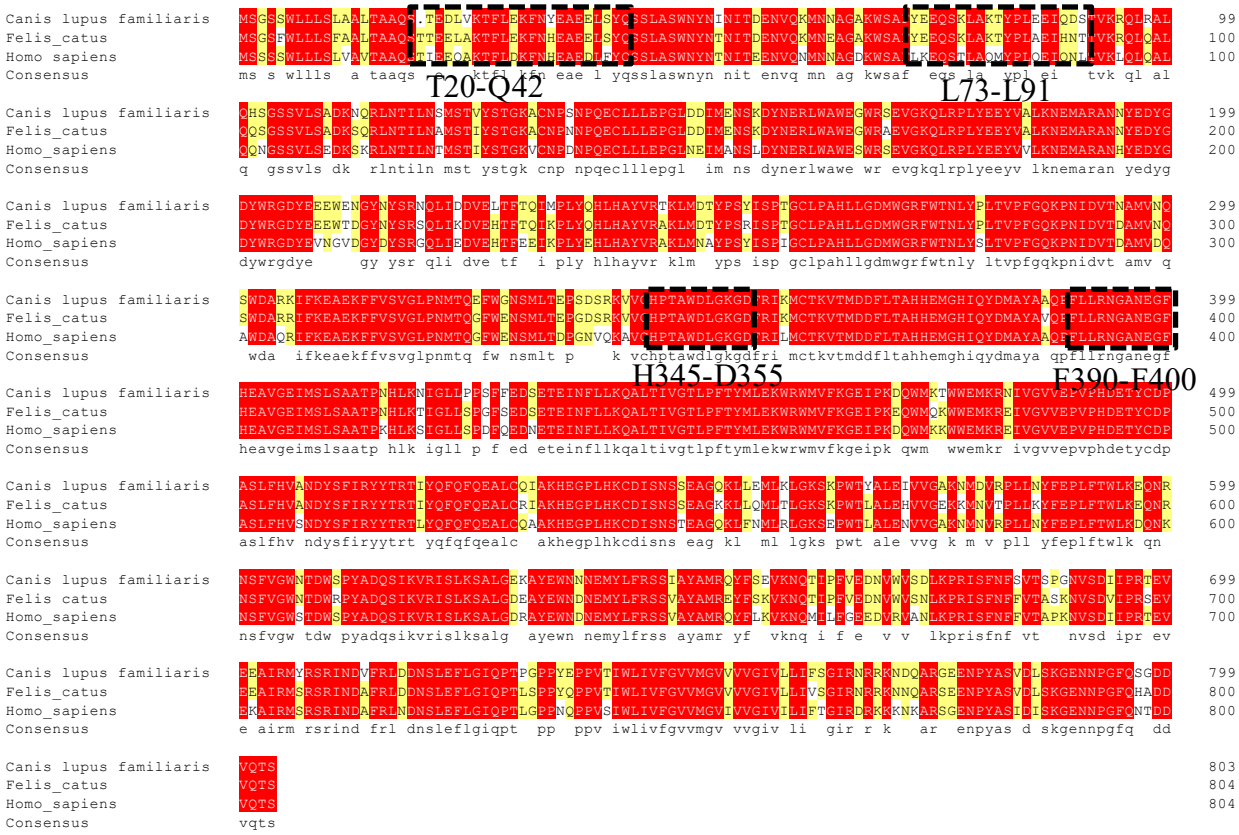

Fig. S4. The multiple sequence alignment for the ACE2 proteins derived from human (Homo sapiens, BAB40370) and cat (Felis catus, AAX59005) and dog (Canis lupus familiaris, NP_001158732). The sequence numbering refers to the human ACE2 sequence. The same amino acids are highlighted by the colored bars. The dotted boxes mark the regions that interact with SARS-CoV-2 RBD.

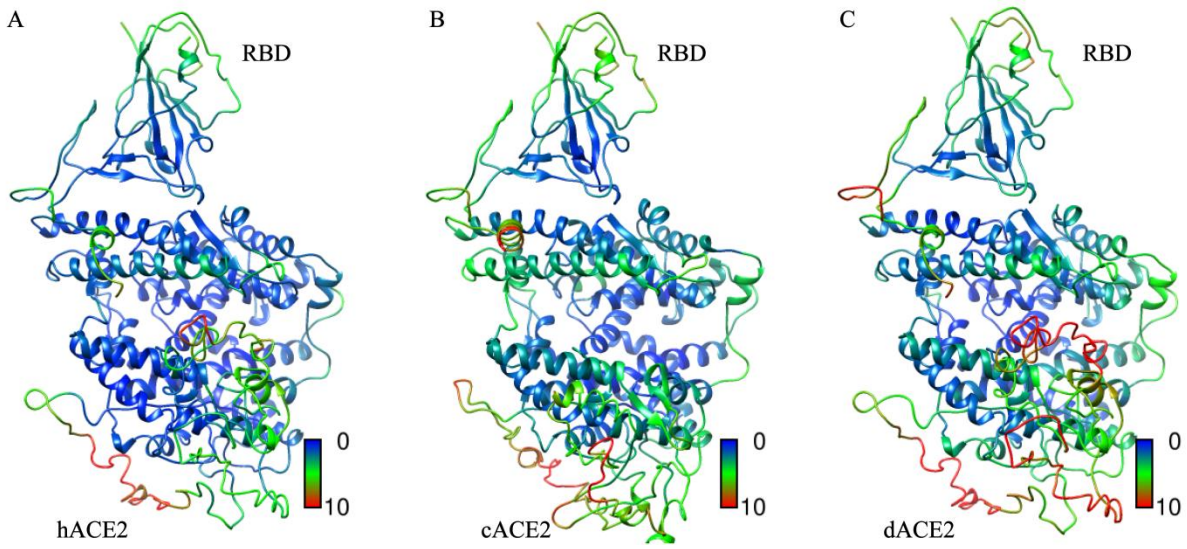

Fig. S5. The root means square fluctuations (RMSF) of Cα atoms of the hACE2-RBD, cACE2-RBD and dACE2-RBD complexes were mapped onto each surface, the colors of residues are according to the RMSF values. (units in Å)

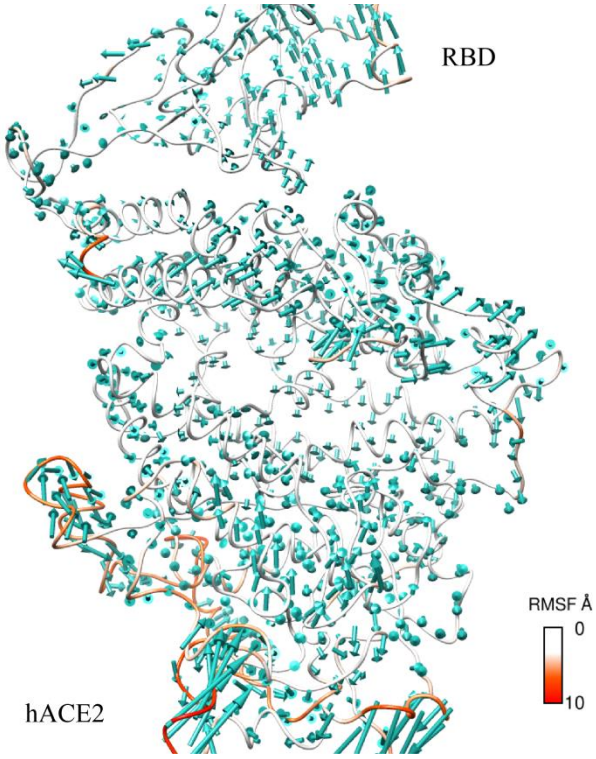

Fig. S6. The large principal component of the hACE2-RBD complex based on the two independent 200-ns MD simulations with the initial structure 7KNB. Light sea green arrows point from one end to the other. The colors of residues are according to the RMSF values. (units in Å)