Supplementary Information: Computational Design of ACE2-Based Peptide Inhibitors of SARS-CoV-2

Yanxiao Han[1], and Petr Král[1,2]*
[1]*Department of Chemistry, University of Illinois at Chicago,*
Chicago, Illinois 60607, United States and
[2]*Departments of Physics, Biopharmaceutical Sciences,*
and Chemical Engineering, University of Illinois at Chicago,
Chicago, Illinois 60607, United States.

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Table S1: Sequence of one letter code for all the inhibitors

	Sequence
Inhibitor 1	residue 21 to 55 **I EEQA KTFLD KFNHE AEDLF YQSSL ASWNY NTNIT**
Inhibitor 2	residues 21 to 88 and 349 to 357 **(1) I EEQA KTFLD KFNHE AEDLF YQSSL ASWNY NTNIT EENVQ NMNNA GDKWS AFLKE QSTLA QMYPL QEI** **(2) WD LGKGD FR**
Inhibitor 3	residues 21 to 105 and 323 to 362 **(1) I EEQA KTFLD KFNHE AEDLF YQSSL ASWNY NTNIT EENVQ NMNNA GDKWS AFLKE QSTLA QMYPL QEIQA LTVKL QLQAL QQNGS** **(2) MTQ GFWEN SMLTD PGNVQ KAVCH PTAWD LGKGD FRILM CT**
Inhibitor 4	residues 21 to 95 and 335 to 400 **(1) I EEQA KTFLD KFNHE AEDLF YQSSL ASWNY NTNIT EENVQ NMNNA GDKWS AFLKE QSTLA QMYPL QEIQA LTVKL** **(2) D PGNVQ KAVCH PTAWD LGKGD FRILM CTKVT MDDFL TAHHE MGHIQ YDMAY AAQPF LLRNG ANEGF**

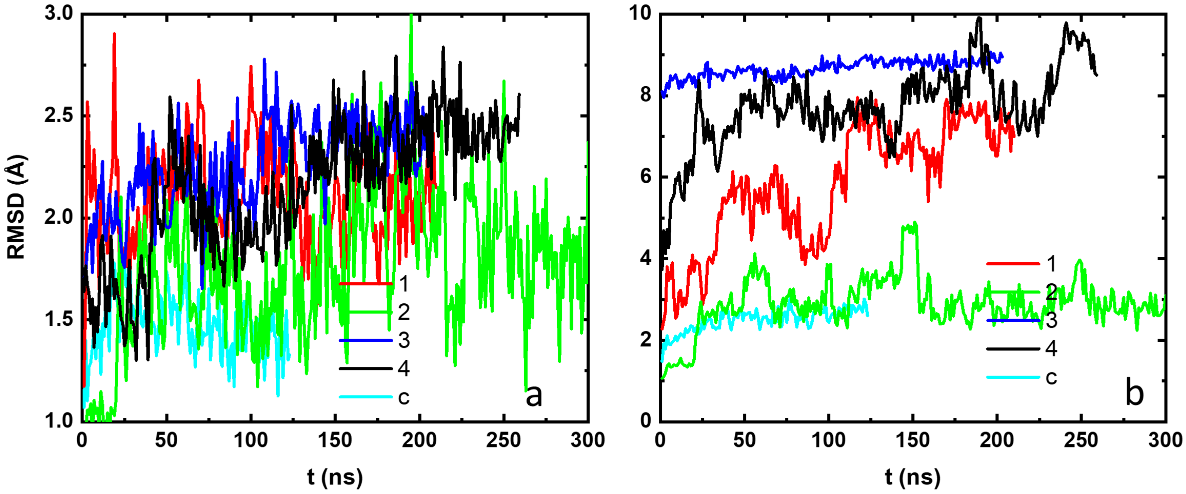

Figure S1: (a) RMSD for the critical amino acids in each inhibitor; (b) RMSD for the whole inhibitors when they bind with the RBD of SARS-CoV-2. Numbering scale: 1-4 - inhibitors 1-4 with RBD; C - control system of PD from ACE2 and the RBD of SARS-CoV-2.

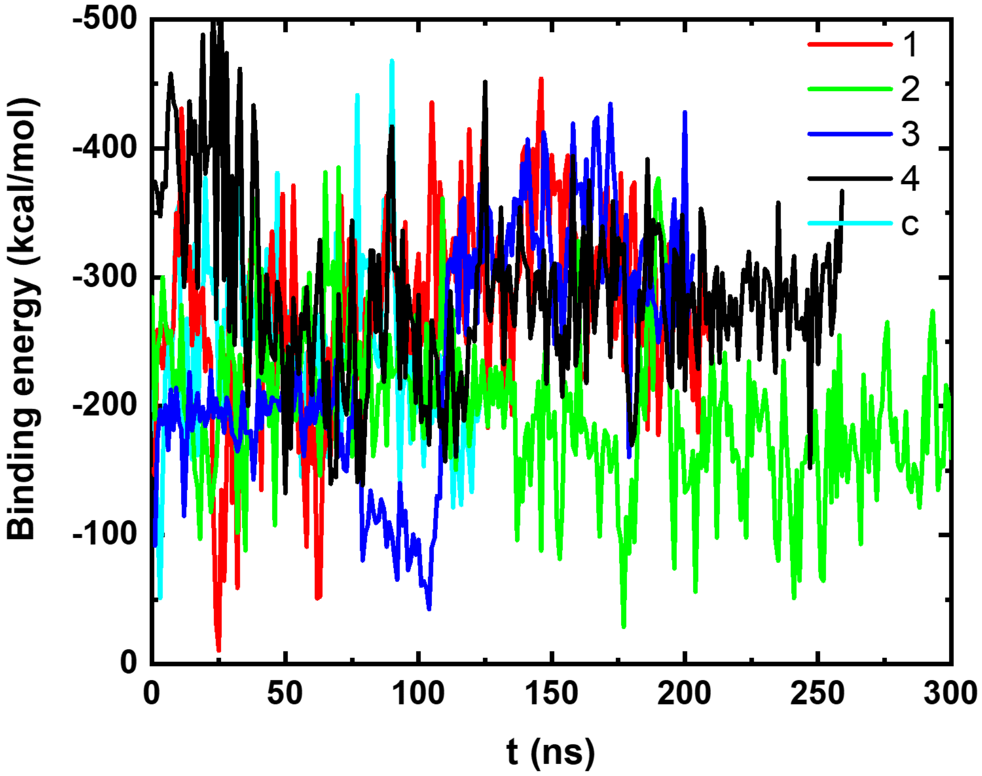

Figure S2: The interaction energies between the contact residues of inhibitors (or ACE2) and SARS-CoV-2. Numbering scale: 1-4 - inhibitors 1-4 with RBD; C - control system of PD from ACE2 and the RBD of SARS-CoV-2.