Supporting Information

Structure-aided ACEI-capping remdesivir loaded novel PLGA nanoparticles: Toward a computational simulation design to anti-SARS-CoV-2 therapy

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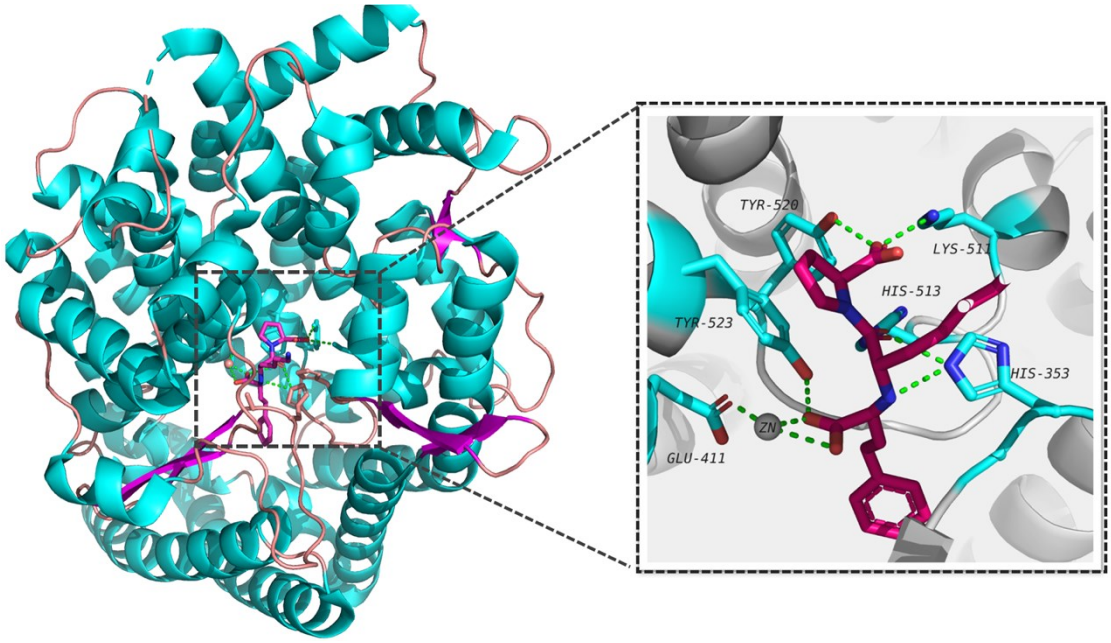

Figure S1. One representative 3D conformation of lisinopril and ACE protein based on molecular docking. Hydrogen bond interactions represented in green dashes.

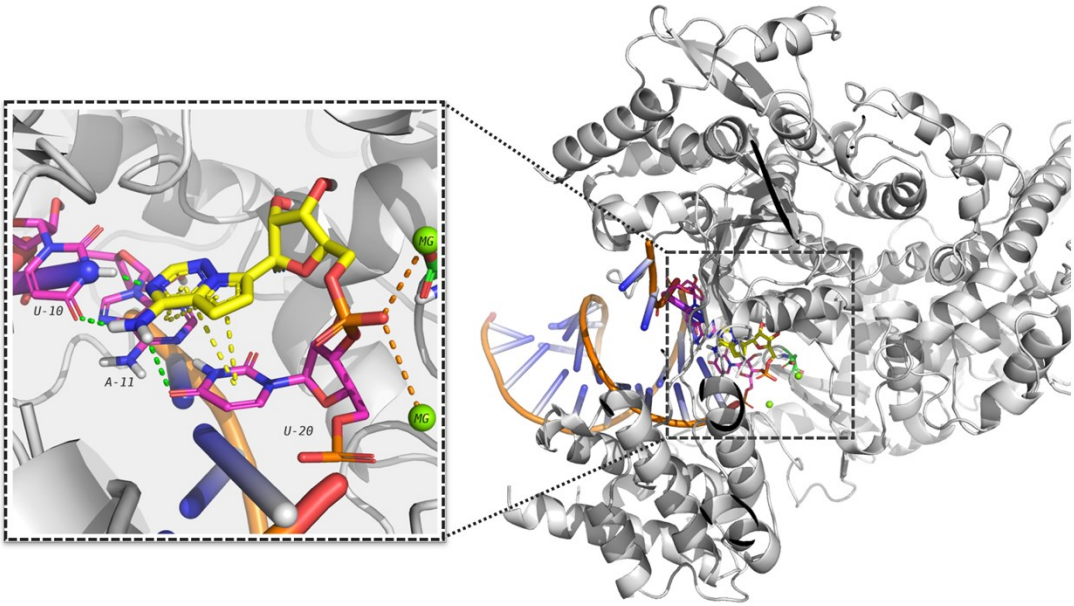

Figure S2. One representative 3D conformation of remdesivir and RdRp protein based on molecular docking. Hydrogen bond interactions represented in green dashes. And the π-π stacking interactions represented in yellow dashes.

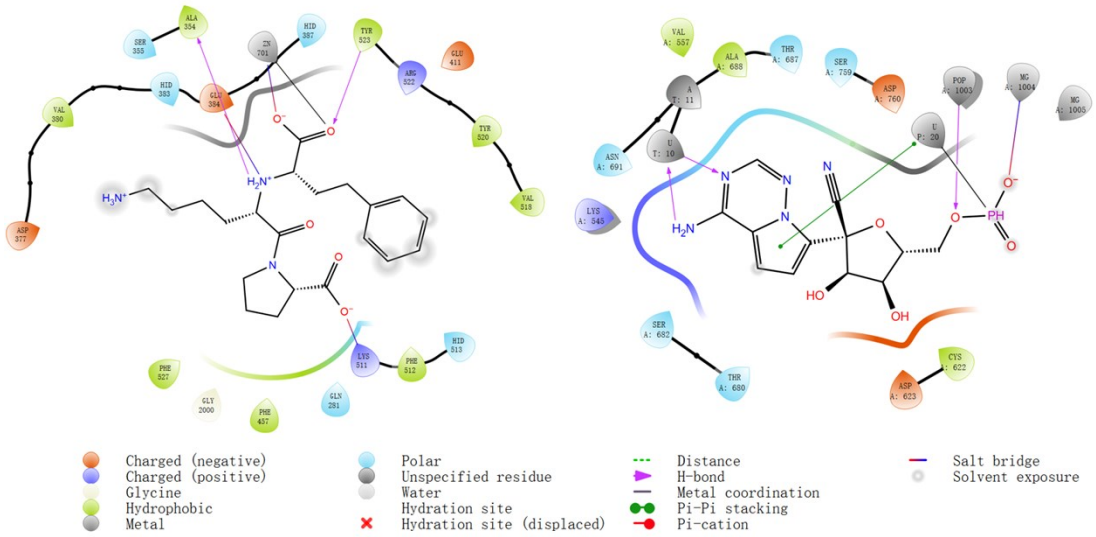

Figure S3. Both representative 2D interactions between lisinopril and ACE protein (Left), as well as remdesivir and RdRp protein (Right) based on molecular docking.

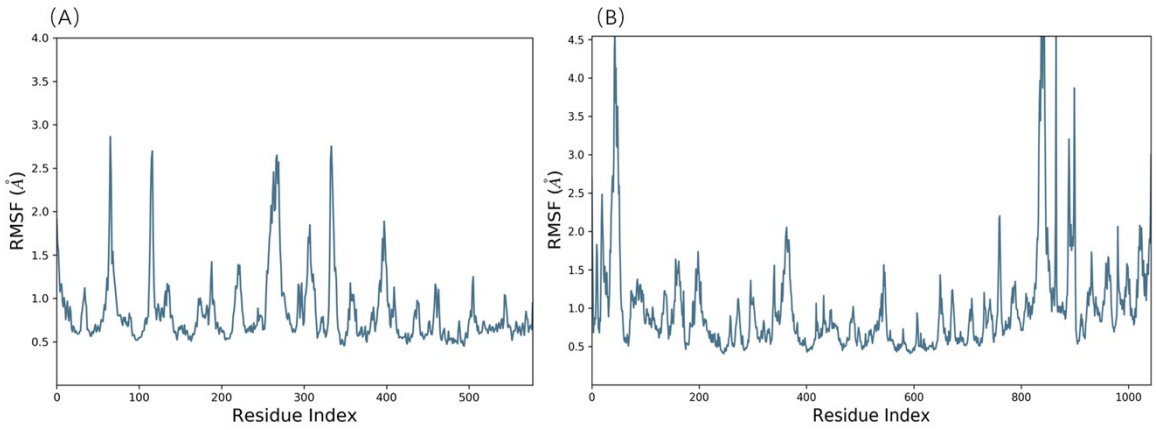

Figure S4. RMSF plots of ACE protein (A) and RdRp protein (B) based on MD simulations.

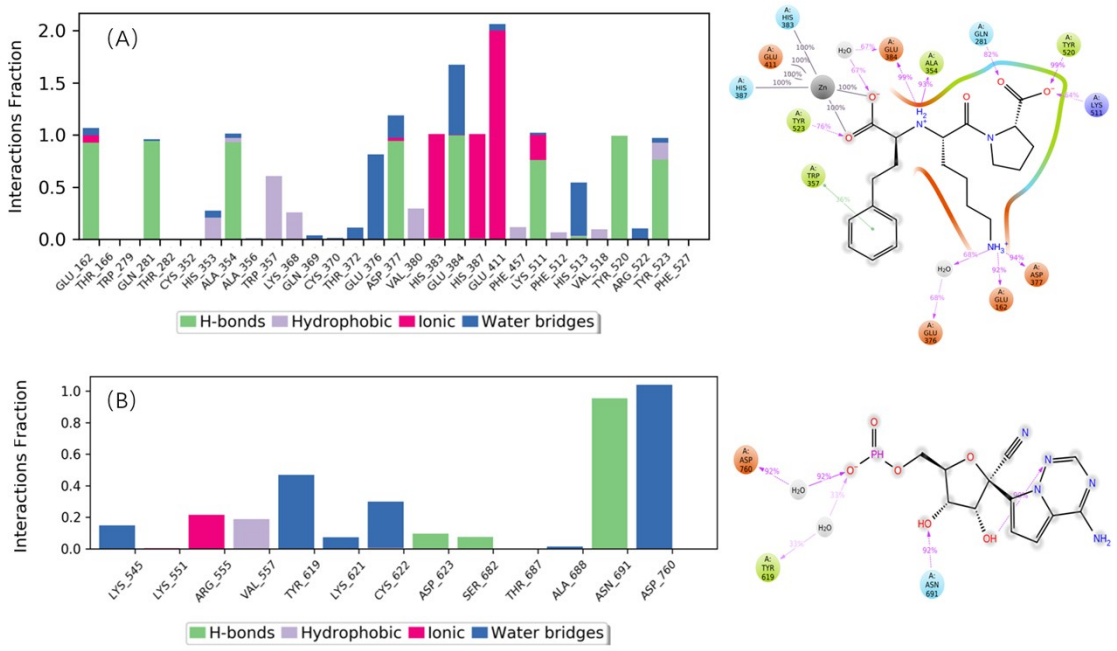

Figure S5. Protein-ligand contacts are monitored during the whole MD simulations. (A) Interaction fraction of lisinopril-ACE complex. (B) Interaction fraction of remdesivir - RdRp complex.

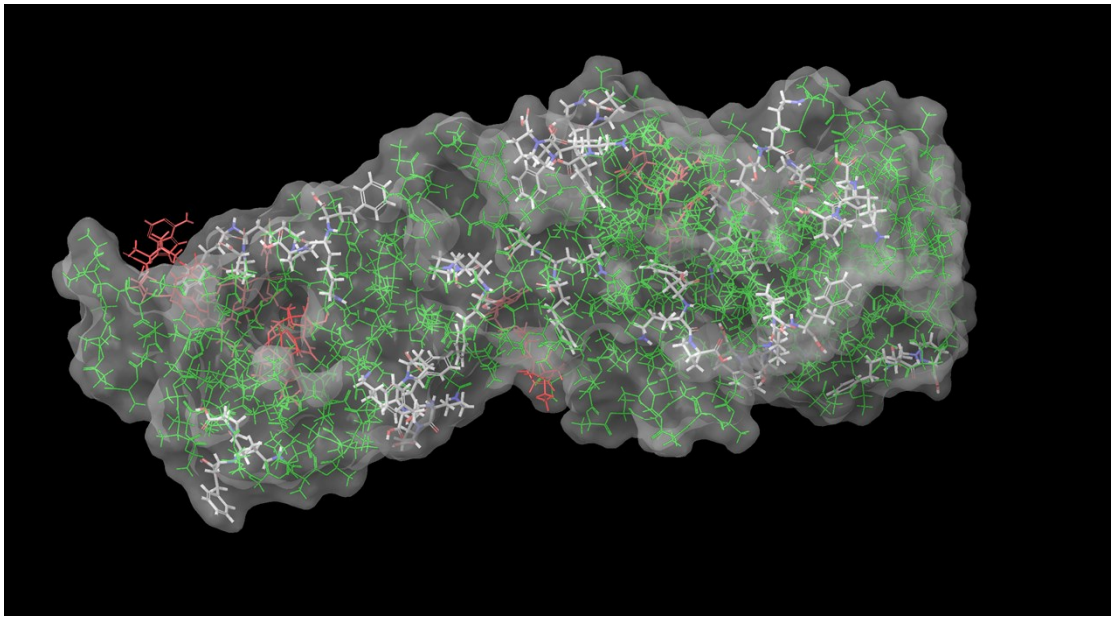

Figure S6. MD simulations of lisinopril-containing PLGA polymers interacting with remdesivir molecules. Red represented remdesivir molecules; white-blue-red represented lisinopril molecules, and green represented PLGA polymer molecule.

Table S1. The interaction parameters between different kinds of beads.

	W	L	P	R
W	25	27	100	100
L		25	100	100
P			25	27
R				25

Table S2. The Molar Mass and the Volume Fraction of the Four Types of CG Beads.

Bead type	W	R	L	P
M(g/mol)	18	602.58	405.49	996.78
(g/cm^3)	1	1.47	1.251	1.2295