

Supplementary Files

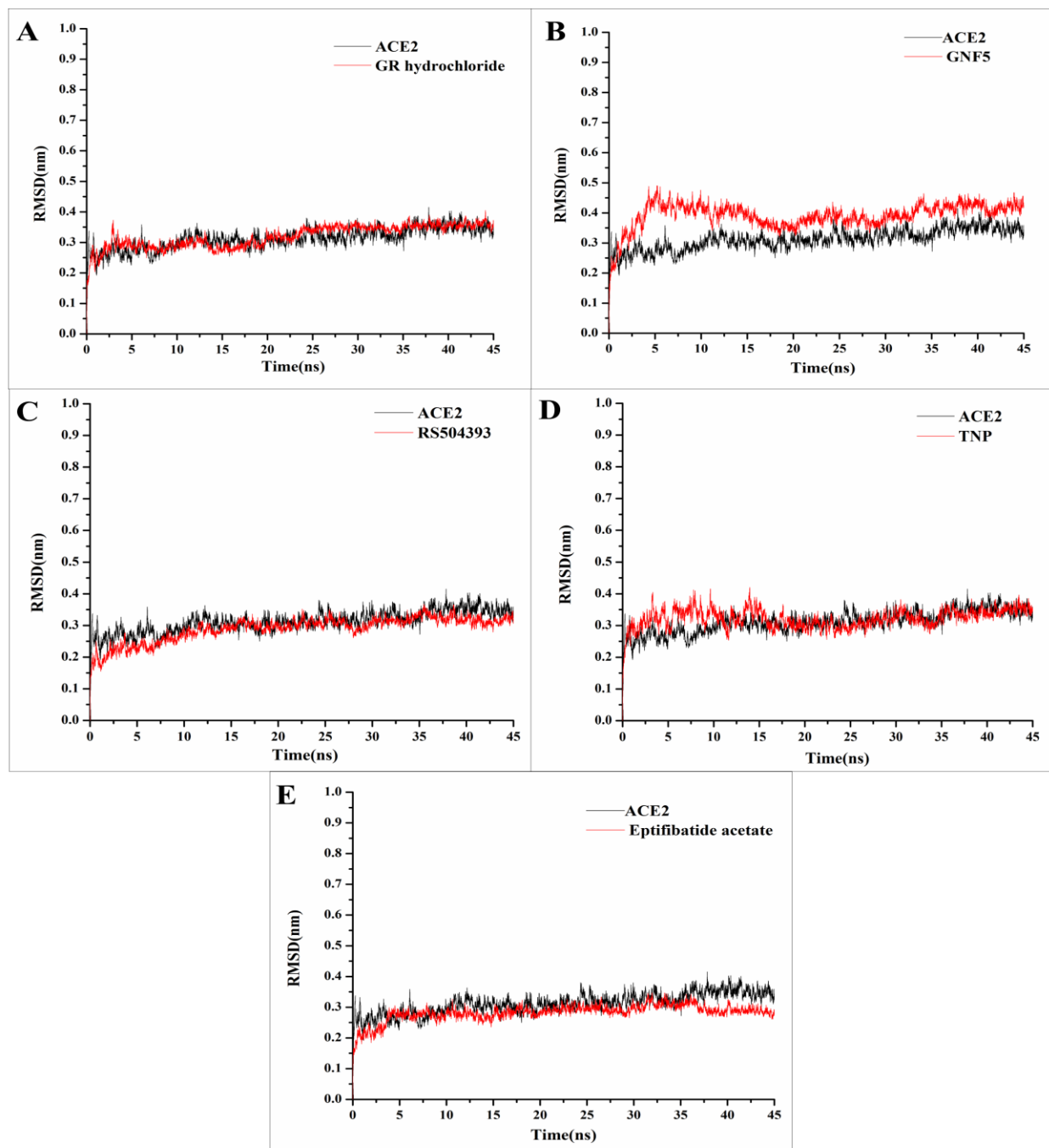


Figure S1 | RMSD values for native ACE2 protein and protein-ligand complexes. The RMSD plot for 45ns simulation run for protein-inhibitor complexes (A) ACE2-GR hydrochloride complex (B) GNF-5 (C) RS504393 (D) TNP and (E) Eptifibatide acetate. RMSD plot for ACE2 is depicted in Black color, and ACE2-inhibitor complexes are represented in Red color.

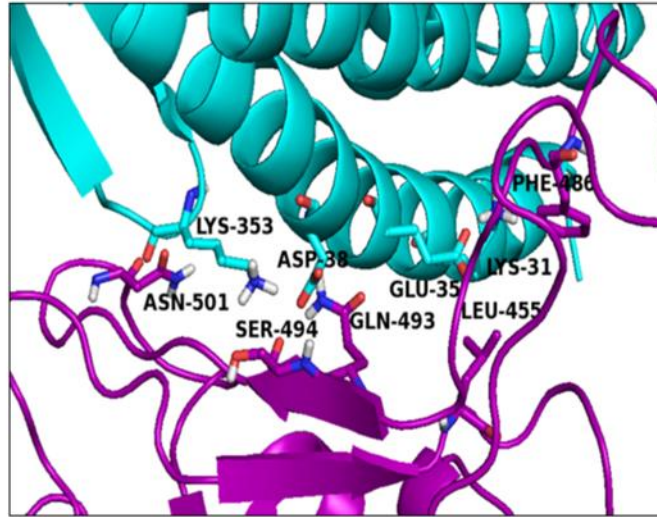


Figure S2 | The S-RBD of S-protein and ACE2 receptor interface showing molecular interactions of residues involved in binding of SARS-CoV-2 virus to the receptor

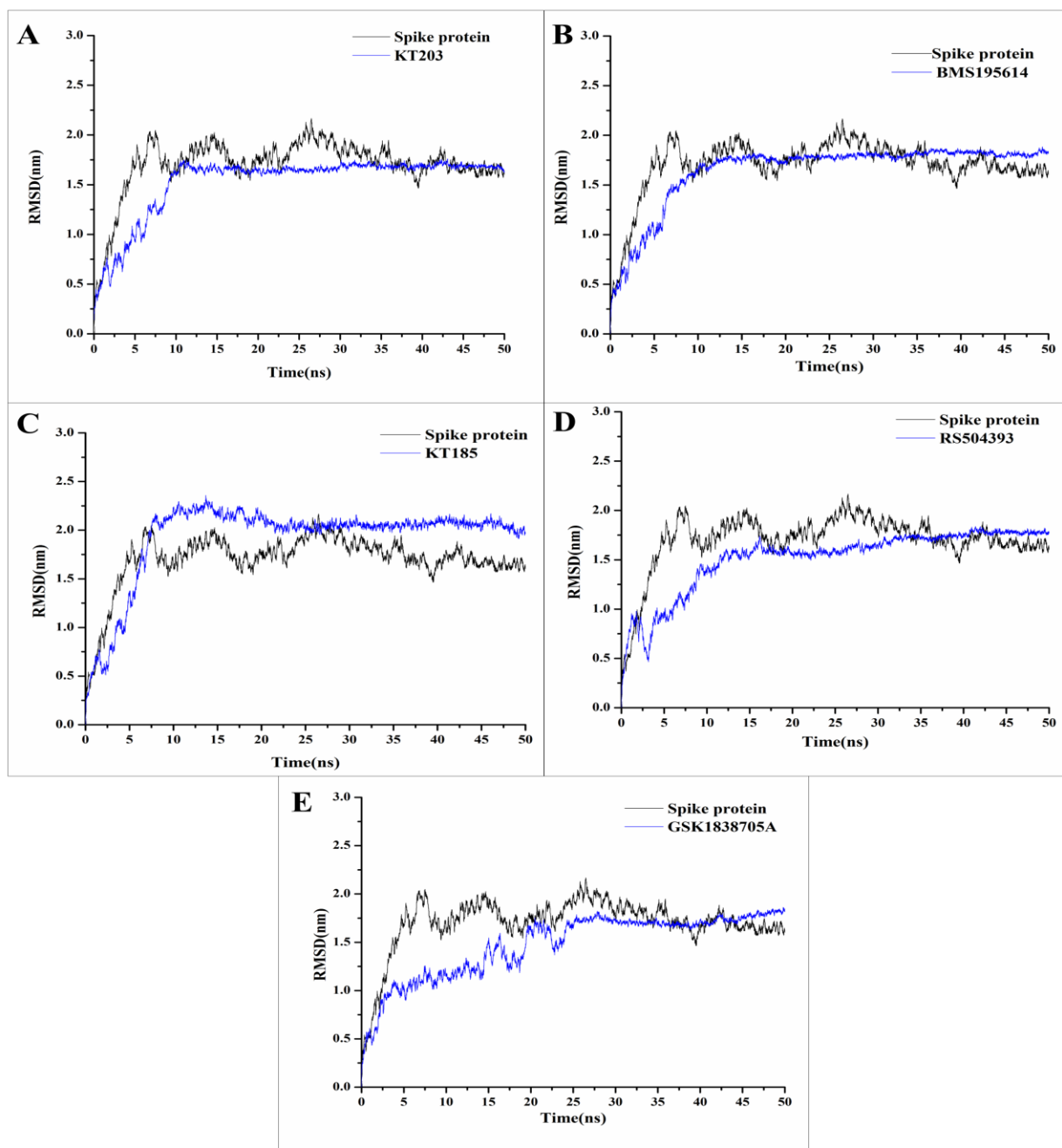


Figure S3 | RMSD values for native S1 subunit of S-protein and protein-ligand complexes. The RMSD plot for 50ns simulation run for protein-inhibitor complexes (A) KT203 (B) BMS195614(C) KT185 (D) RS504393 and (E) GSK1838705A. RMSD plot for S-protein is depicted in black color, and protein-inhibitor complexes are represented in blue color.