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Supplementary Information

Discovery of Potent Inhibitors for SARS-CoV-2's Main Protease by Ligand-based/Structure-based Virtual Screening, MD Simulations, and Binding Energy Calculations.

Abd Al-Aziz A. Abu-Saleh[a]*, Ibrahim E. Awad[a], Arpita Yadav[b], Raymond A. Poirier[a]*.

[a]Chemistry Department, Memorial University, St. John's, NL A1B 3X7, Canada

[b]Department of Chemistry, University Institute of Engineering & Technology, Chhatrapati Shahu Ji Maharaj University, Kanpur 208024, India

*Corresponding author

E-Mail: rpoirier@mun.ca; aabusaleh@mun.ca

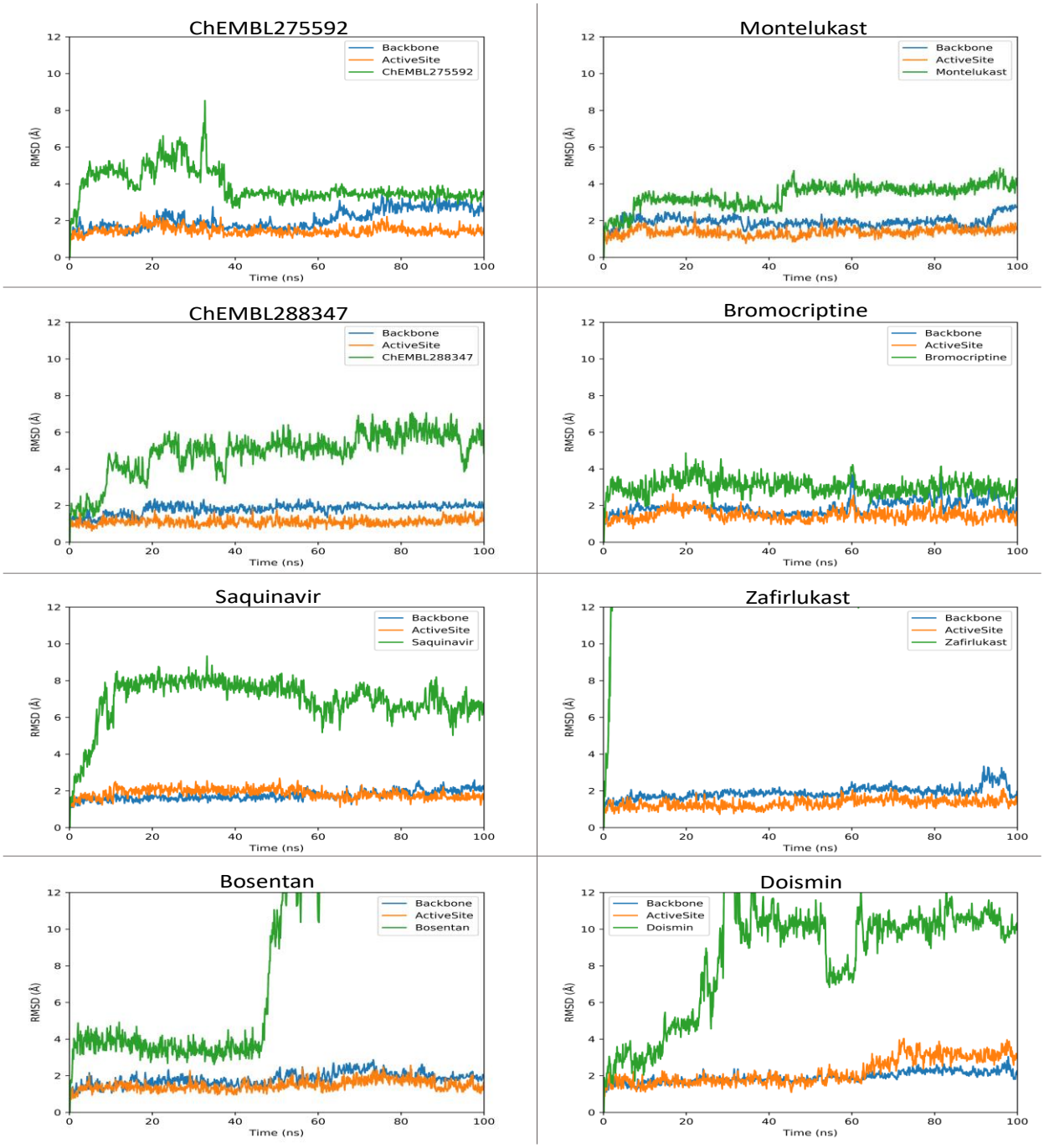

Fig. S1. RMSD analysis of the top docking compounds complexed individually with the M^{pro}.

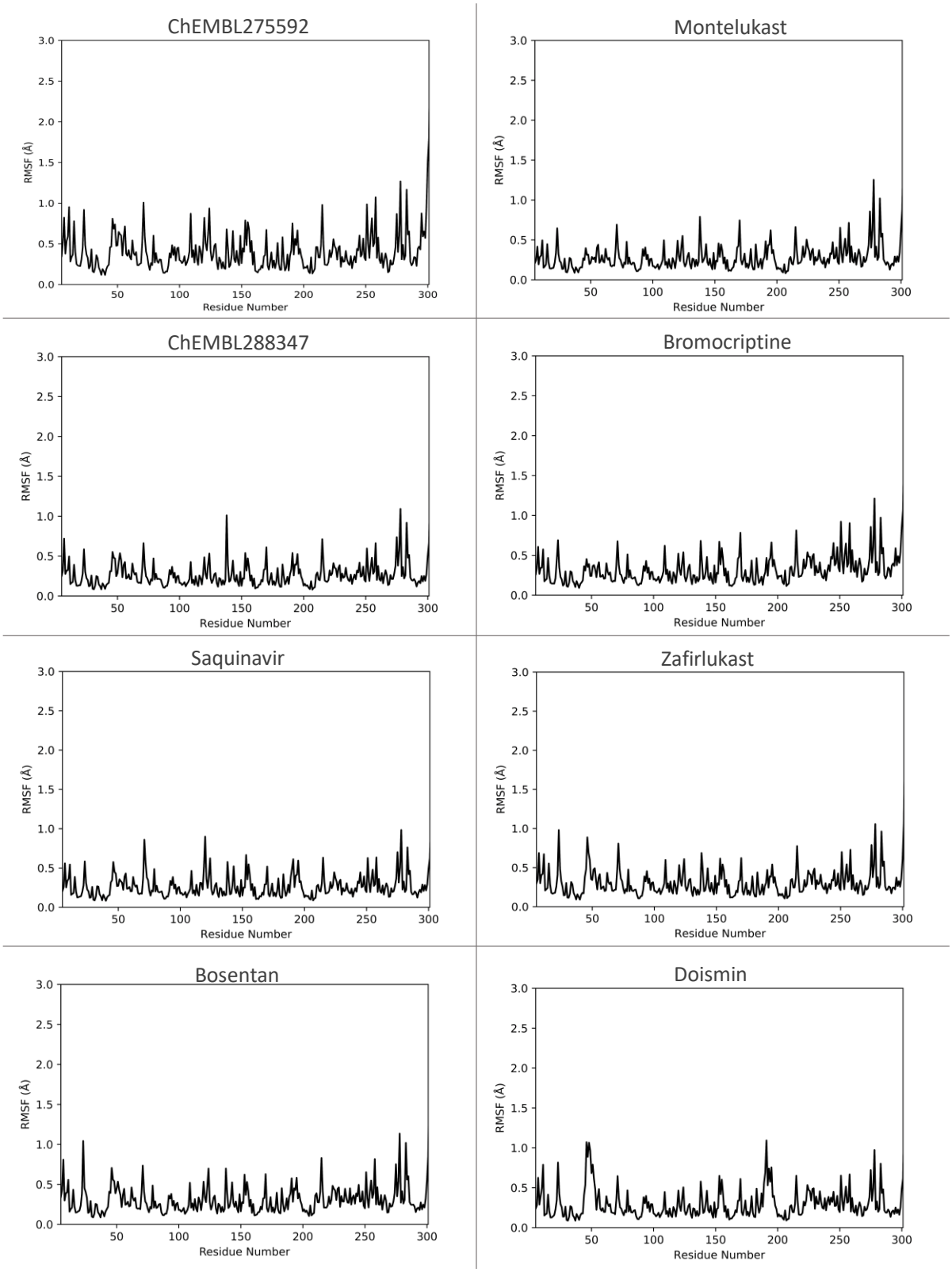

Fig. S2. RMSF analysis of the top docking compounds complexed individually with the M^{pro}.

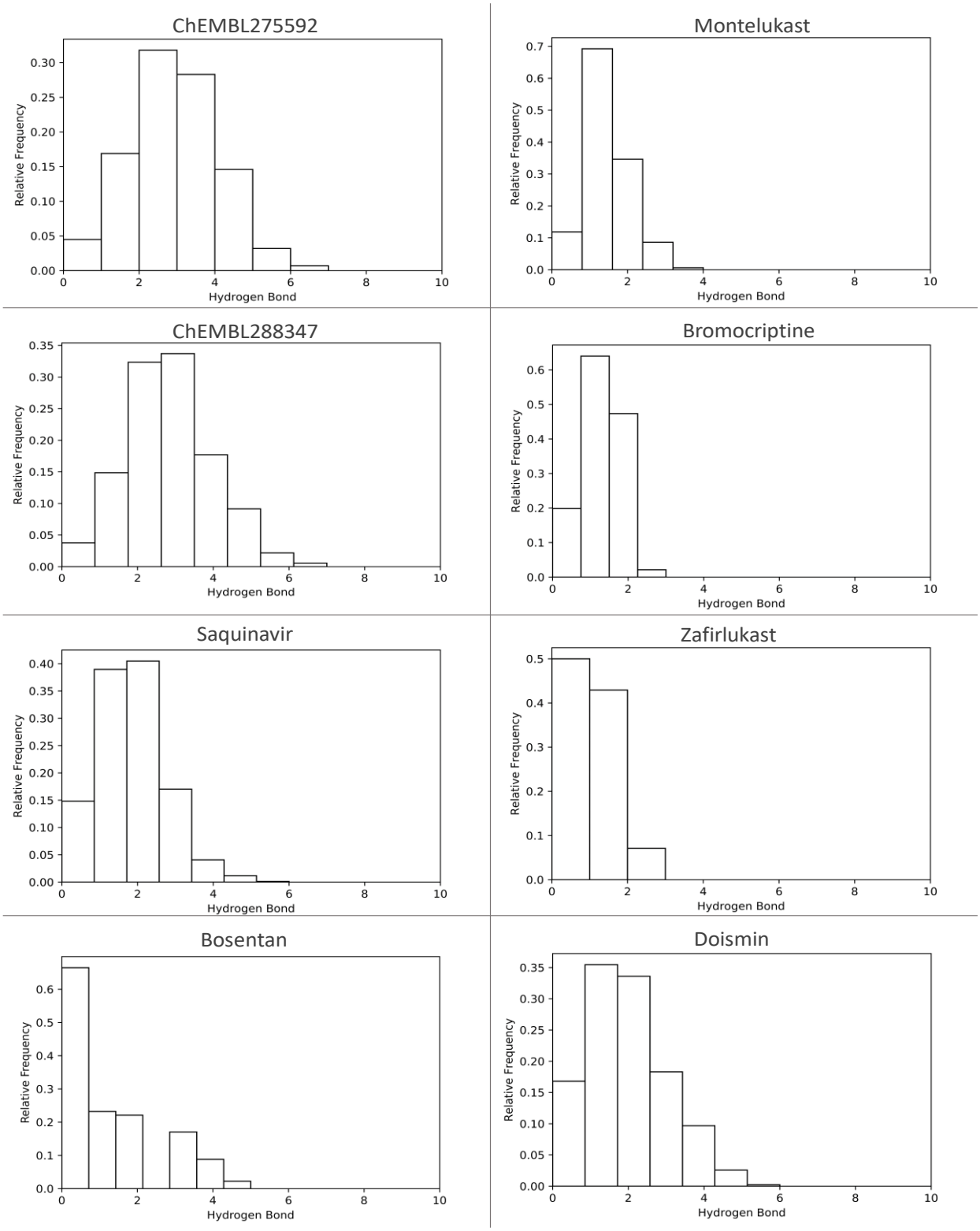

Fig. S3. Averaged hydrogen bond interactions of the top docking compounds complexed individually with the M^{pro} during the 100 ns NPT ensemble.

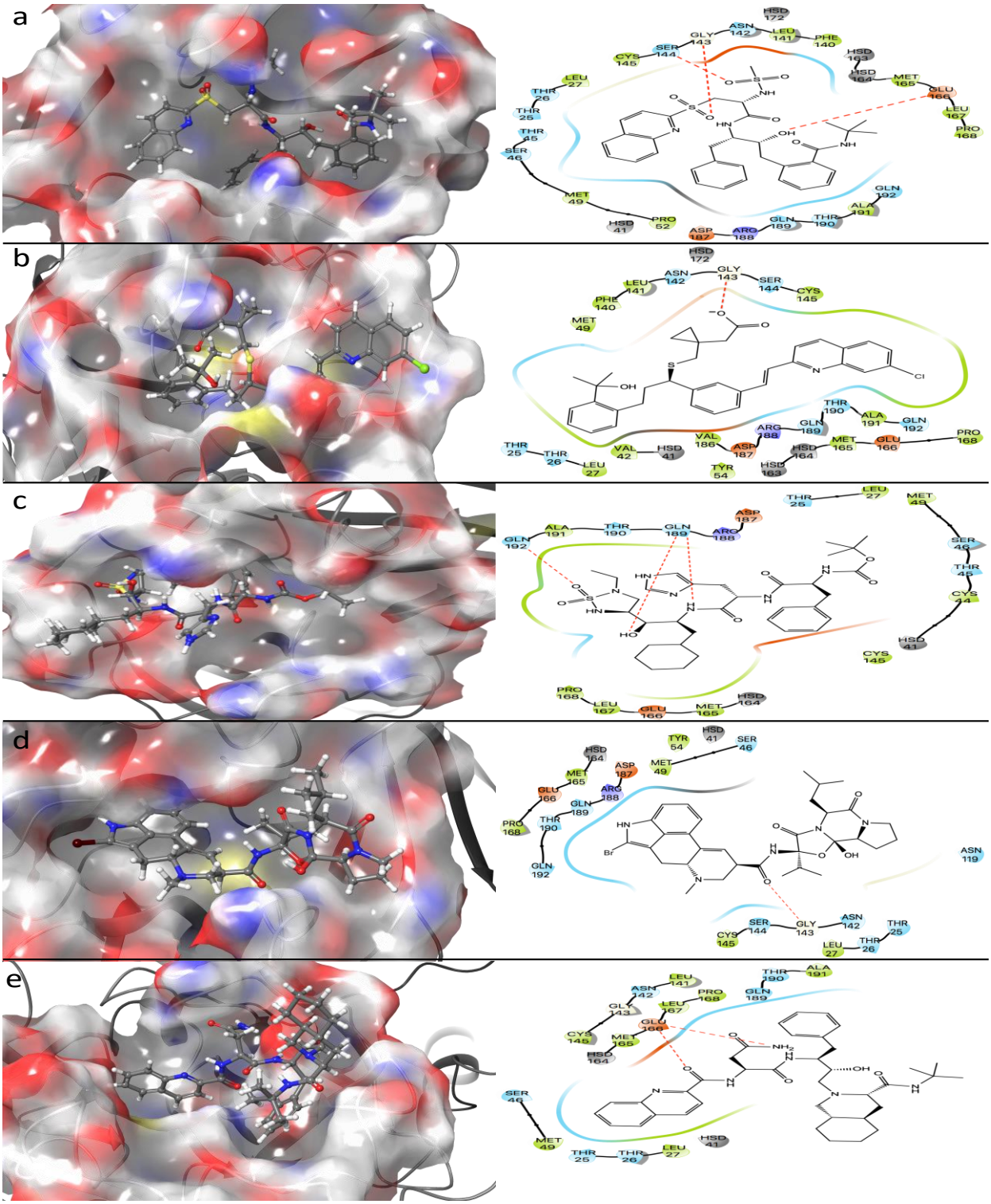

Fig. S4. (a) ChEMBL275592, (b) montelukast, (c) ChEMBL288347, (d) bromocriptine, (e) saquinavir. (Left) representative pose of the stable compounds of the last frame of the 100 ns NPT ensemble, where, the protein surface is colored based on the electrostatic potential. (Right) the red dashed line represents hydrogen bond interactions of the stable compounds in complex with the Mpro.

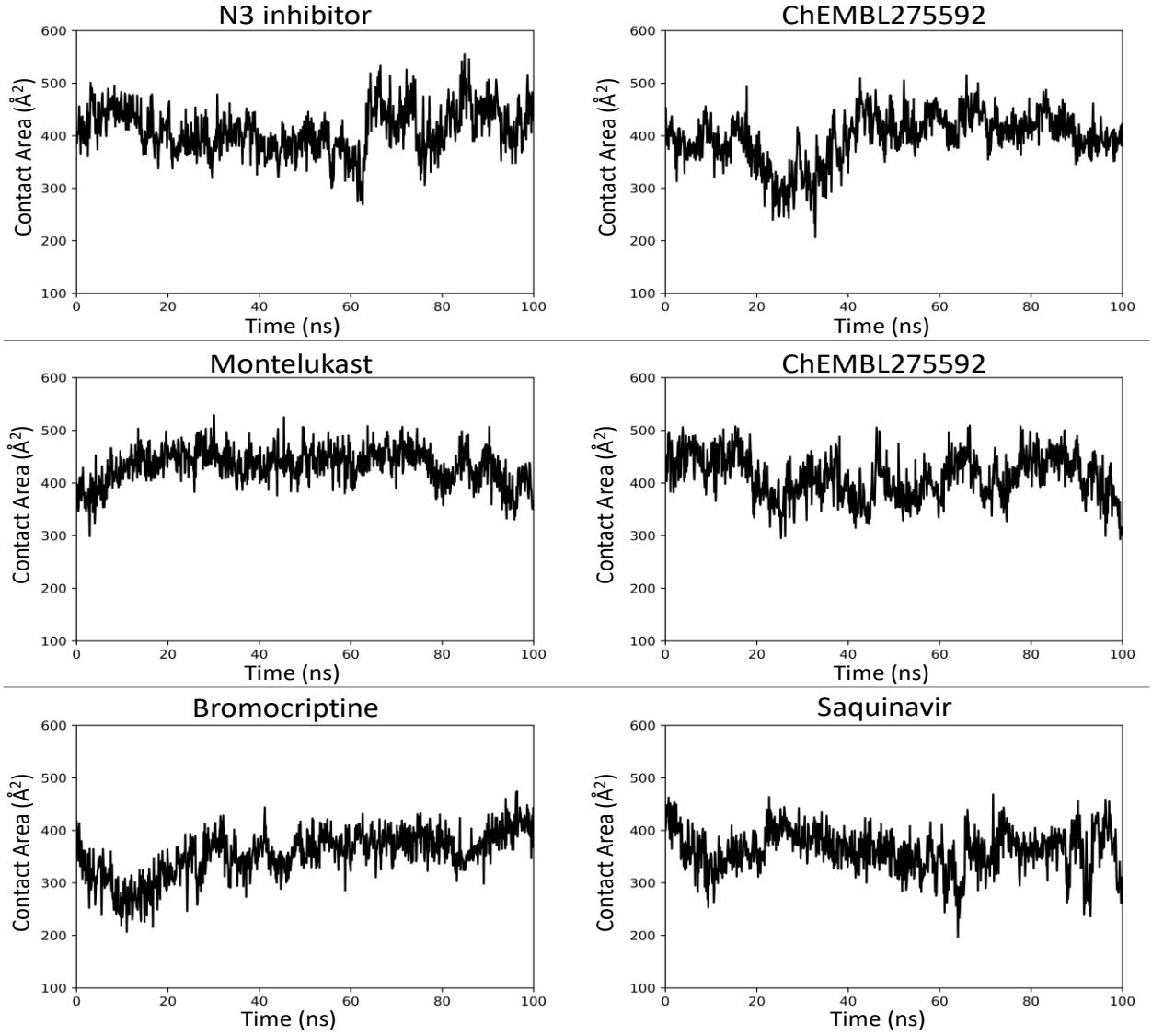

Fig. S5. The time-dependent evolution of the contact surface area during the 100 ns NPT ensemble.

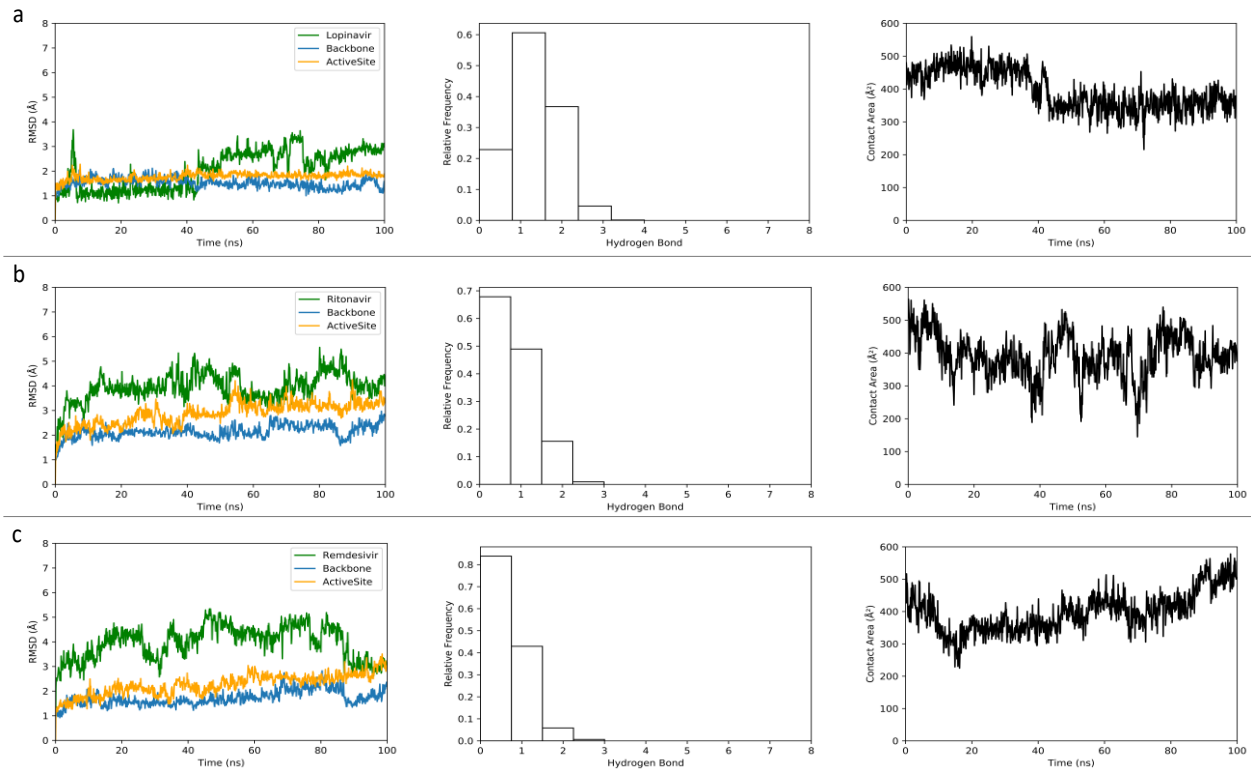

Fig. S6. RMSD, averaged hydrogen bond interaction, and the contact surface area of lopinavir (a), ritonavir (b), and remdesivir (c) complexed individually with the Mpro.

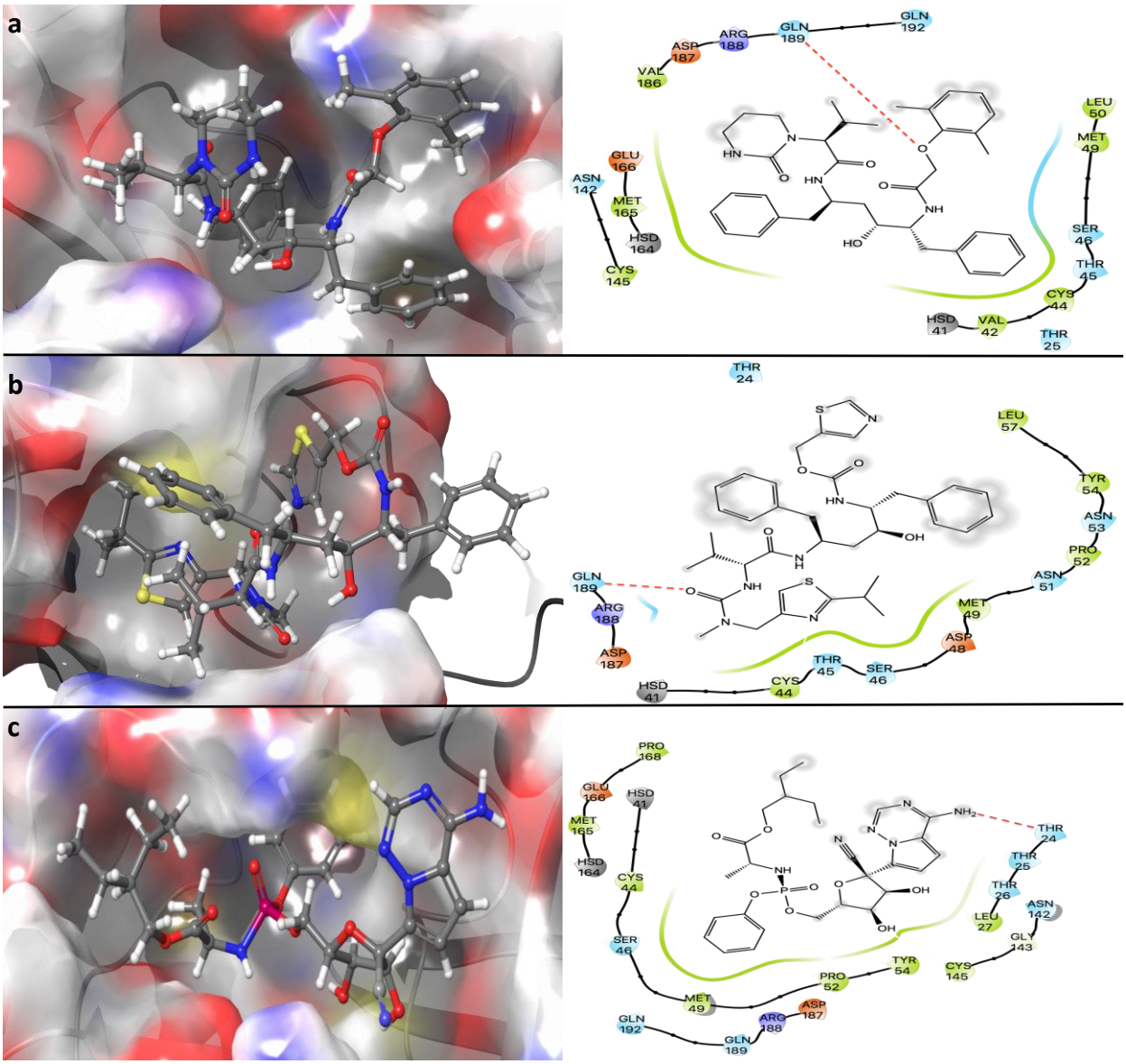

Fig. S7. (a) lopinavir, (b) ritonavir, (c) remdesivir. (Left) representative pose of antiviral drugs of the last frame of the 100 ns NPT ensemble, where, the protein surface is colored based on the electrostatic potential. (Right) the red dashed line represents hydrogen bond interactions of antiviral drugs in complex with the Mpro.