Supplementary Information

High Throughput Virtual Screening of Drug Databanks for Potential Inhibitors of SARS-CoV-2 Spike Glycoprotein

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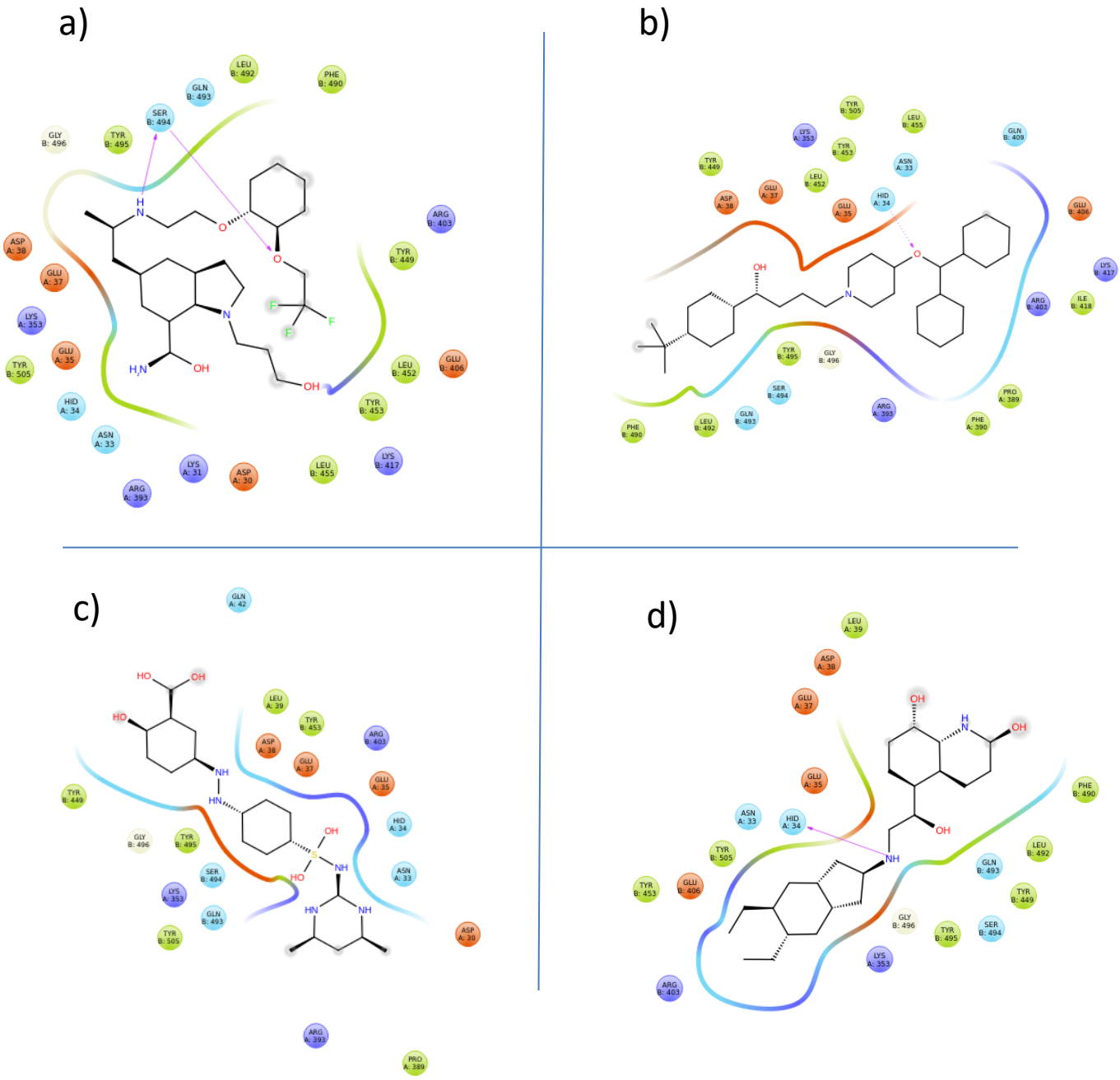

Figure S1. Ligand interaction 2D maps for a) silodosin b) ebastine, c) salazosulfadimidine, and d) indacaterol obtained using best docking configurations. Residues with A indicates ACE2 and residues with B indicates SARS-Cov-2 spike RBD.

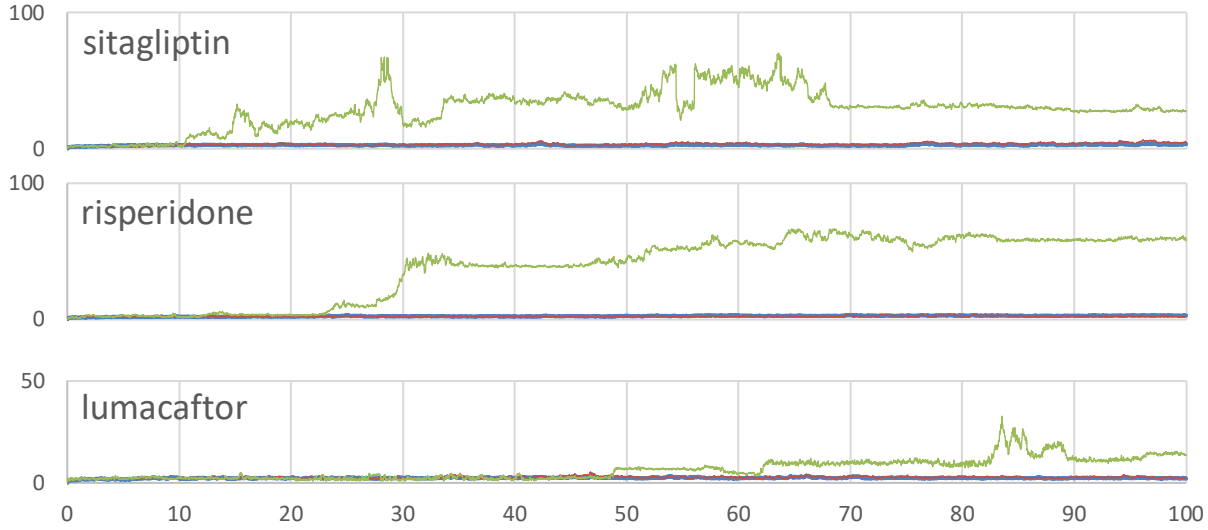

Figure S2. RMSD analysis for a) sitagliptin, b) risperidone, and c) lumacaftor. The light green represents the ligand, blue color represents ACE2, and red color represents the SARS-CoV-2 Spike RBD.

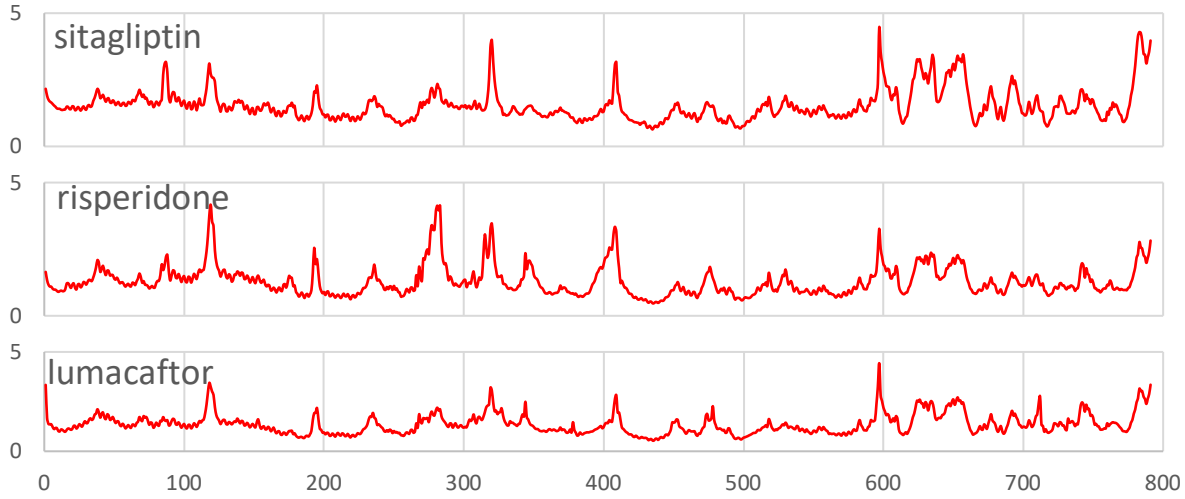

Figure S3. RMSF analysis for a) sitagliptin, b) risperidone, and c) lumacaftor.

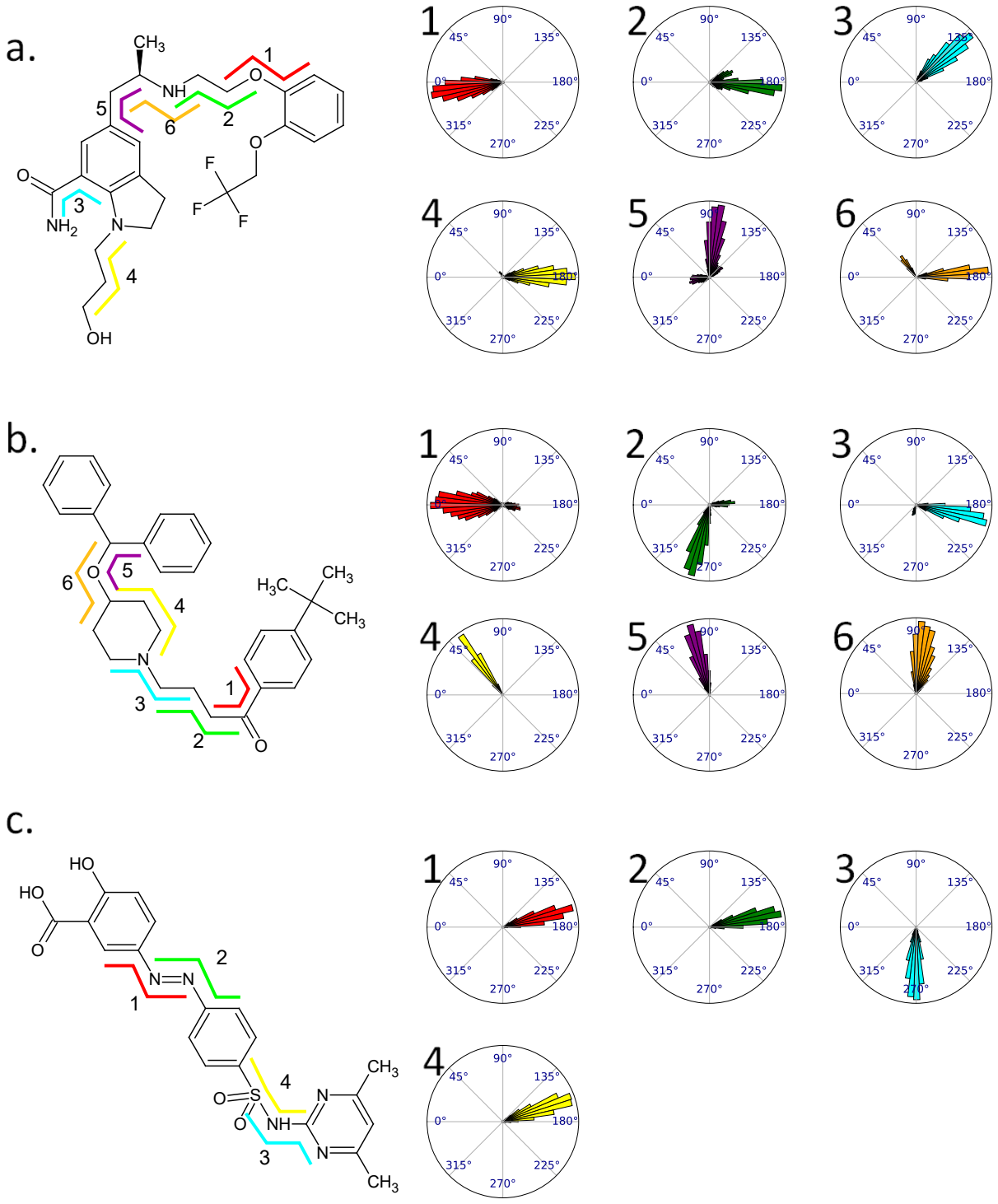

Figure S4. Polar histograms for selected torsion angles during 100ns MD simulations for the top three compounds based on the relative binding energies; a) silodosin b) ebastine, and c) salazosulfadimidine.