

Qualitative and quantitative analysis of anti-viral compounds against SAR-CoV-2 protease enzyme by molecular dynamics simulation and MM/PBSA method

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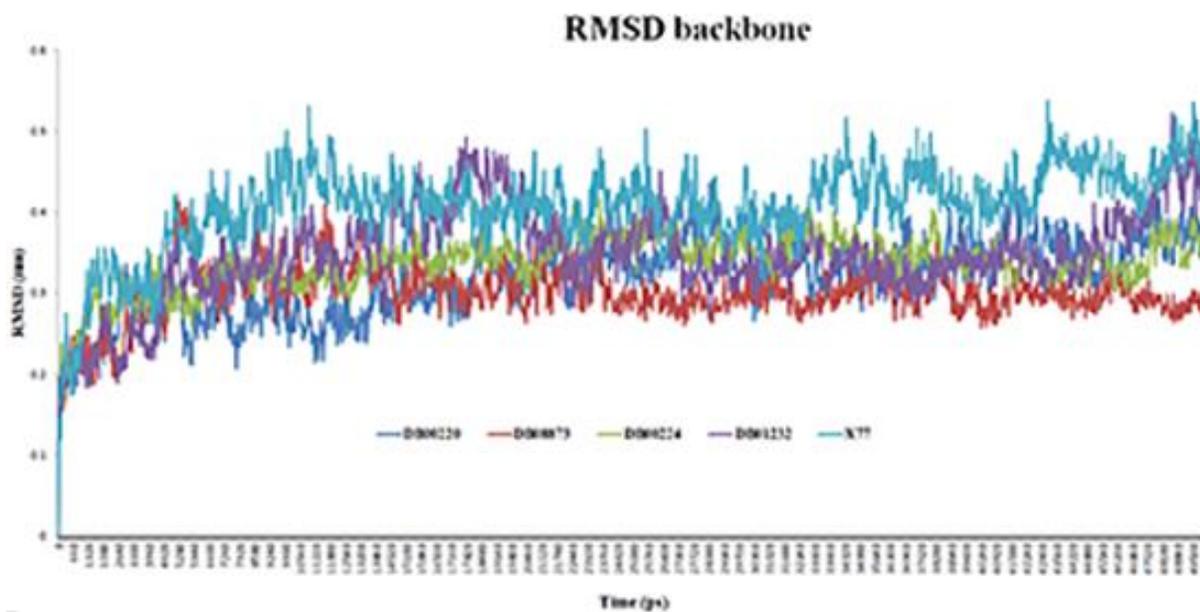


Figure S1. Superimposed RMSD of the backbone atoms of COVID-19 M<[pro] in complex with **DB00220** (Dark Blue), **DB08873** (Red), **DB00224** (Green), **DB01232** (Purple) and **X77** (Light Blue)

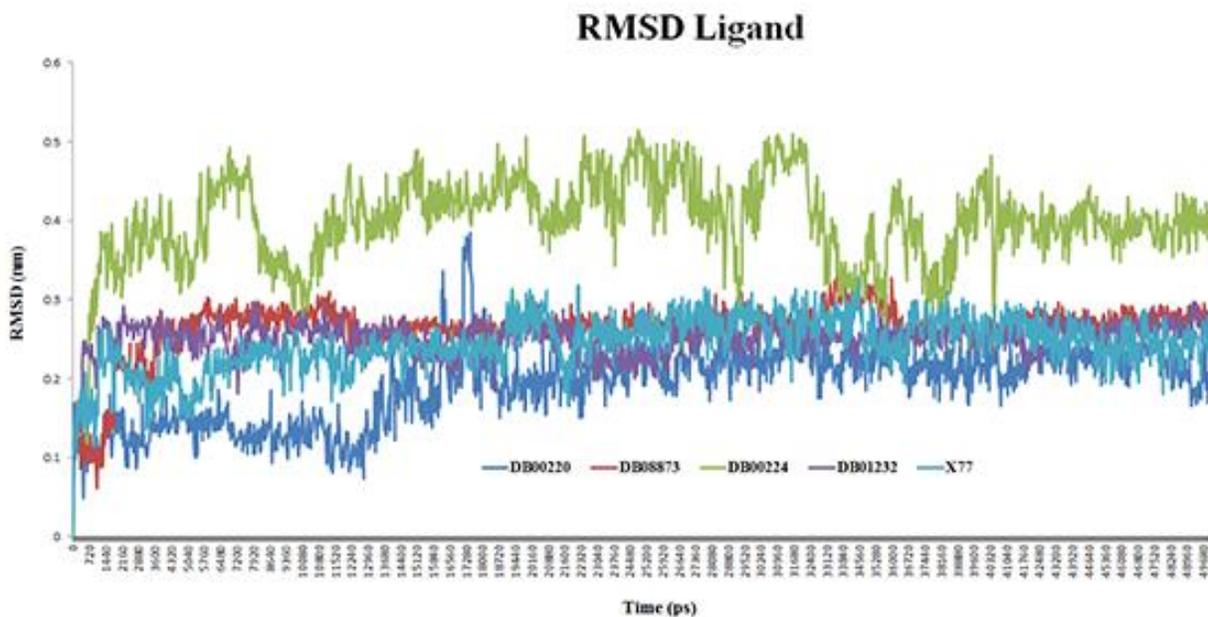


Figure S2. Superimposed RMSD of the ligands **DB00220** (Dark Blue), **DB08873** (Red), **DB00224** (Green), **DB01232** (Purple) and **X77** (Light Blue) in complex with COVID-19 M<[pro]

RMSF backbone

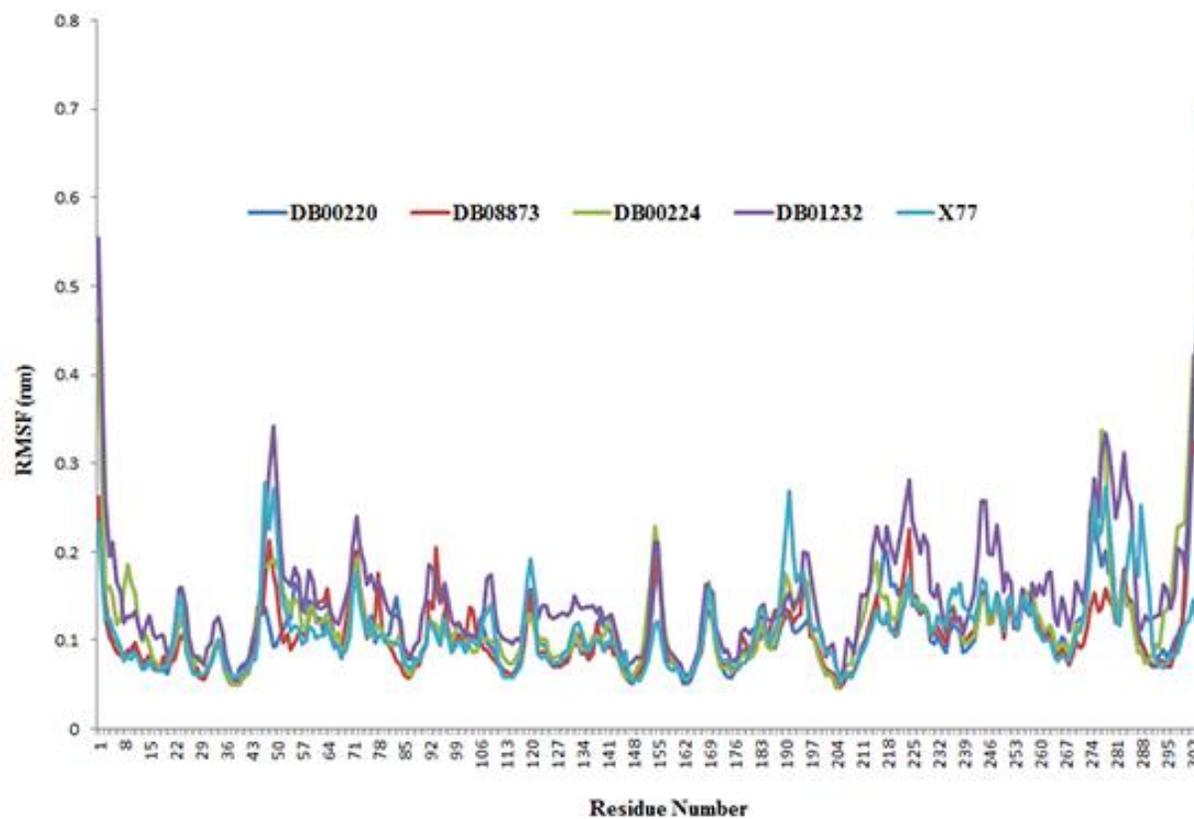


Figure S3. Superimposed RMSF graph for with **DB00220** (Dark Blue), **DB08873** (Red), **DB00224** (Green), **DB01232** (Purple) and **X77** (Light Blue) in complex with COVID-19 M<[pro]

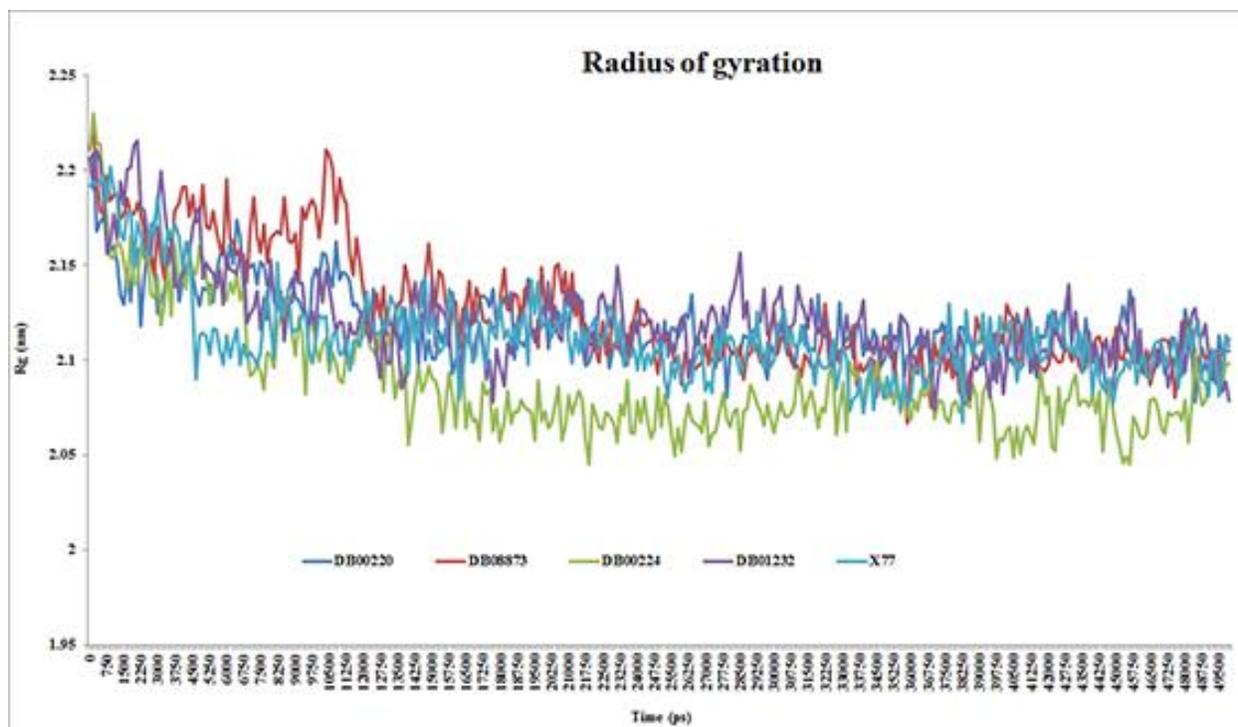


Figure S4. Time dependence of the radius of gyration (Rg) graph of **DB00220** (Dark Blue), **DB08873** (Red), **DB00224** (Green), **DB01232** (Purple) and **X77** (Light Blue) in complex with COVID-19 M<[pro] at different time scale (0-50 ns)

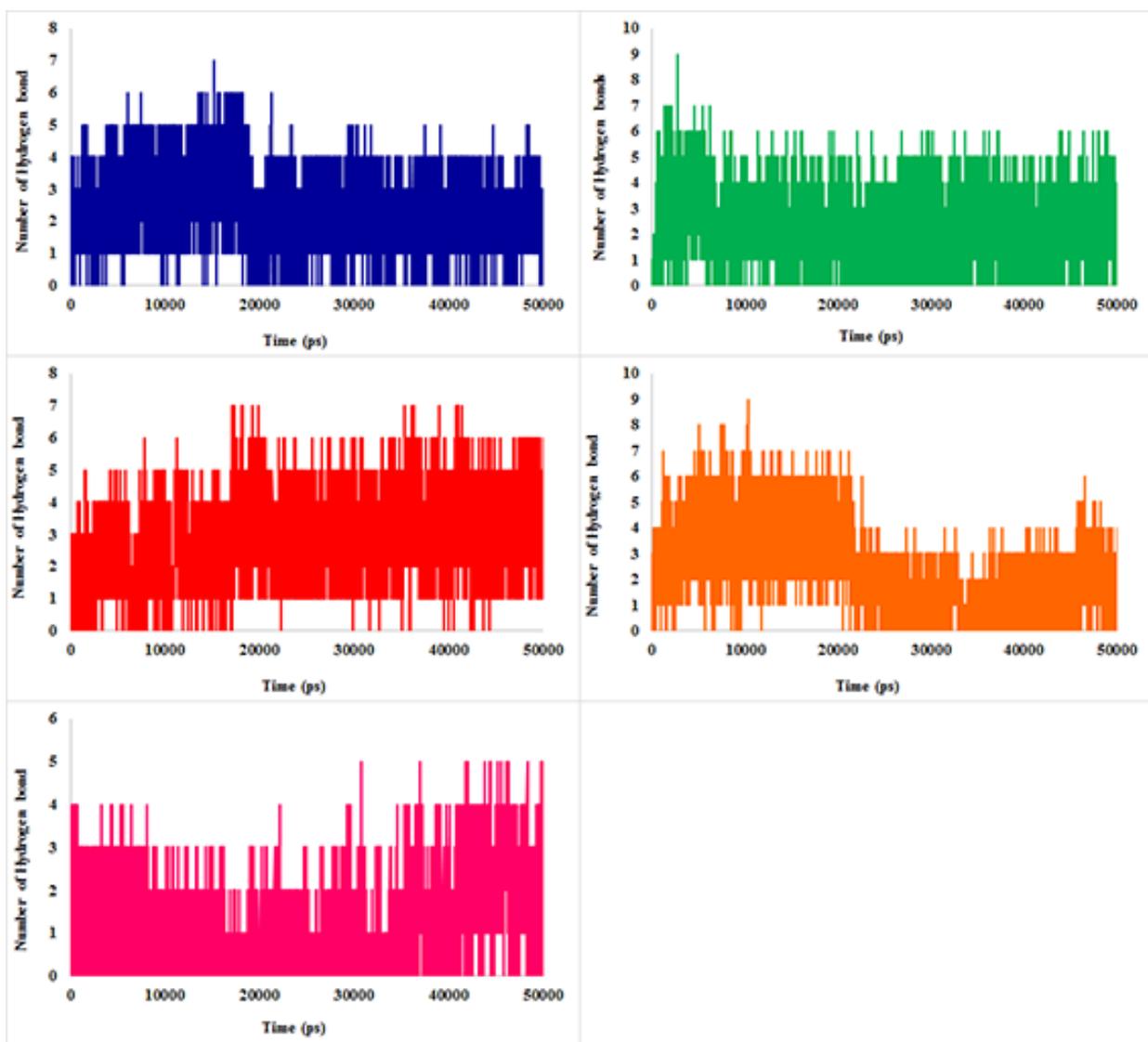


Figure S5. Number of hydrogen bonds formed a between protein-protein (intramolecular) along the trajectory of MD simulation for COVID-19 M<[pro] enzyme with compounds **DB00220** (Red), **DB08873** (Orange), **DB00224** (Purple), **DB01232** (Green) and **X77** (Blue)

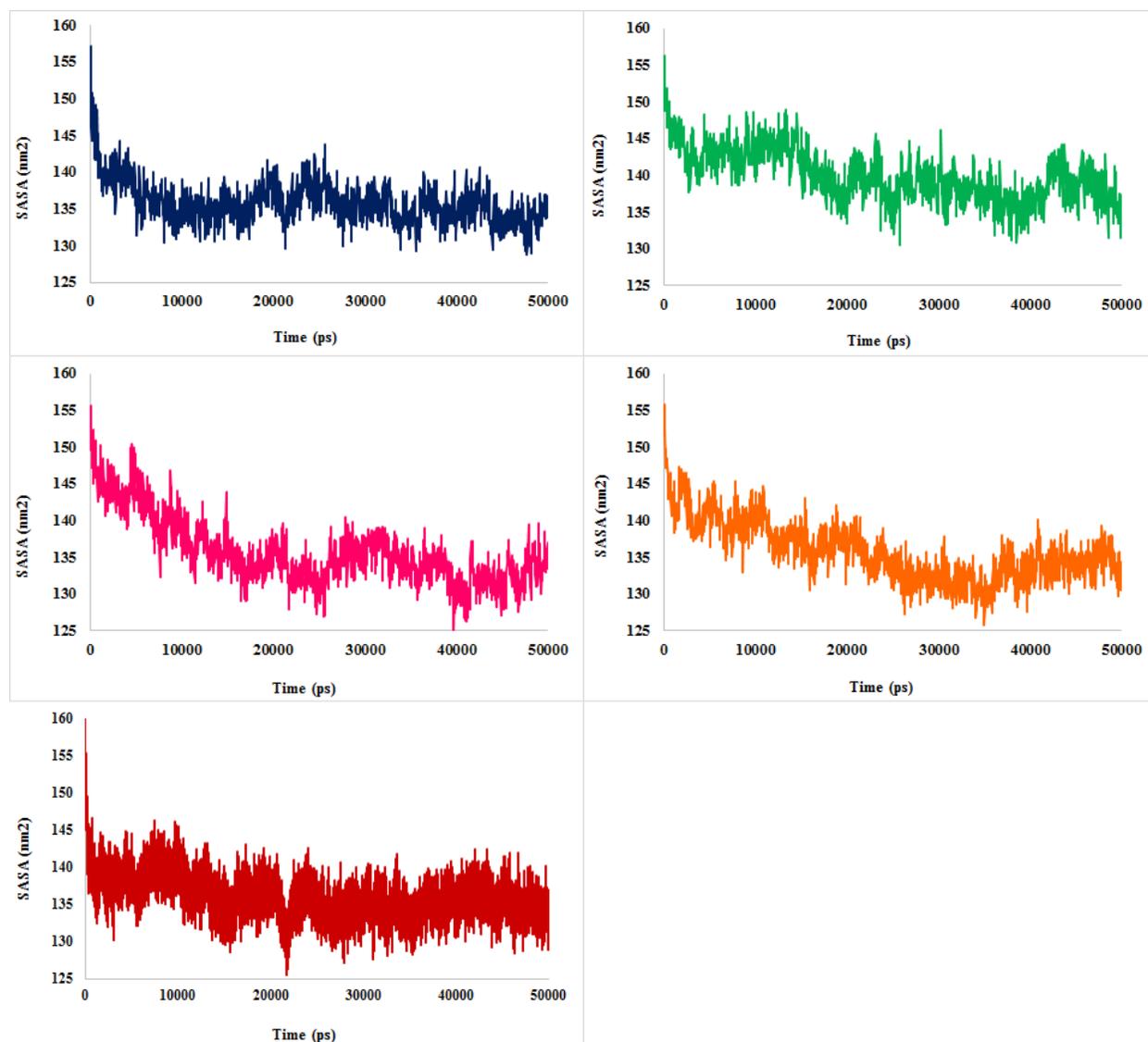


Figure S6. Solvent accessible surface area (SASA) plot of **DB00220** (Red), **DB08873** (Orange), **DB00224** (Purple), **DB01232** (Green) and **X77** (Blue) in complex with COVID-19 M<[pro]

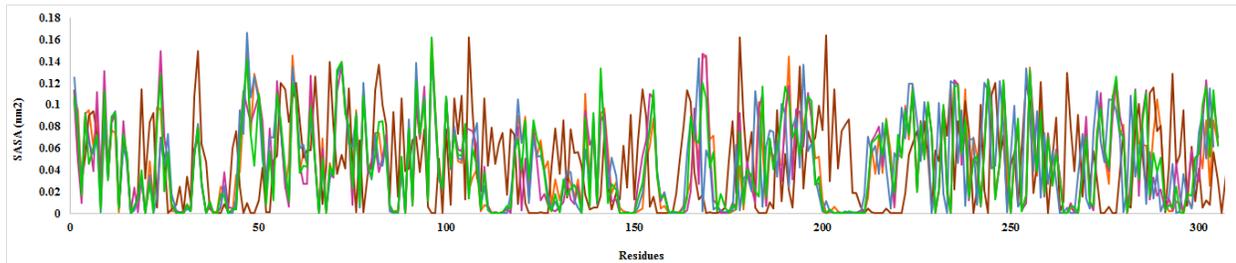


Figure S7. Graphical representation of the SASA of the residues of **DB00220** (Green), **DB08873** (Blue), **DB00224** (Purple), **DB01232** (Brown) and **X77** (Orange) in complex with COVID-19 M<[pro]

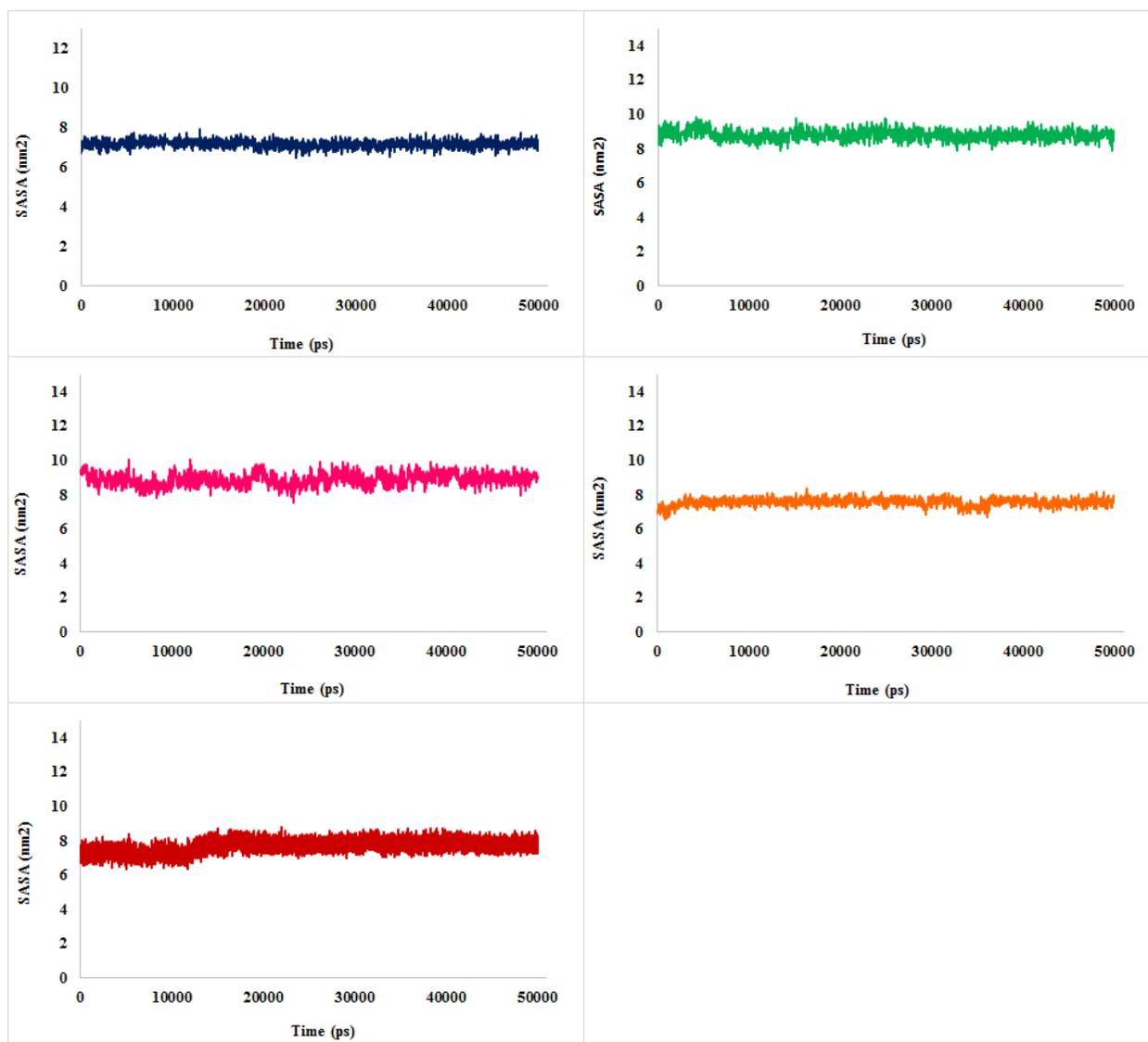


Figure S8. Ligand SASA plot of **DB00220** (Red), **DB08873** (Orange), **DB00224** (Purple), **DB01232** (Green) and **X77** (Blue) in complex with COVID-19 M<[pro]