Electronic Supplementary Material (ESI) for RSC Advances.

Drug Repurposing and Computational Modeling for Discovering of Inhibitors of the Main Protease (M^{pro}) of SARS-CoV-2

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Supplementary Information

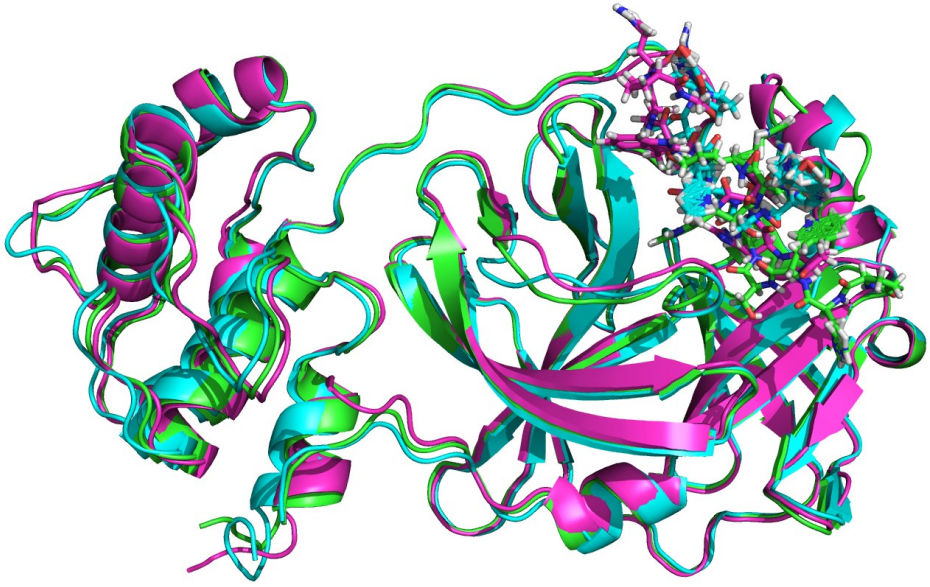

Fig. S1 Overlay of average structures of M^{pro} –triptorelin systems of 3 MD runs performed using random seed with different atomic velocities after 100 ns of MD simulations (RMSD = 0.76 ± 0.20 Å).

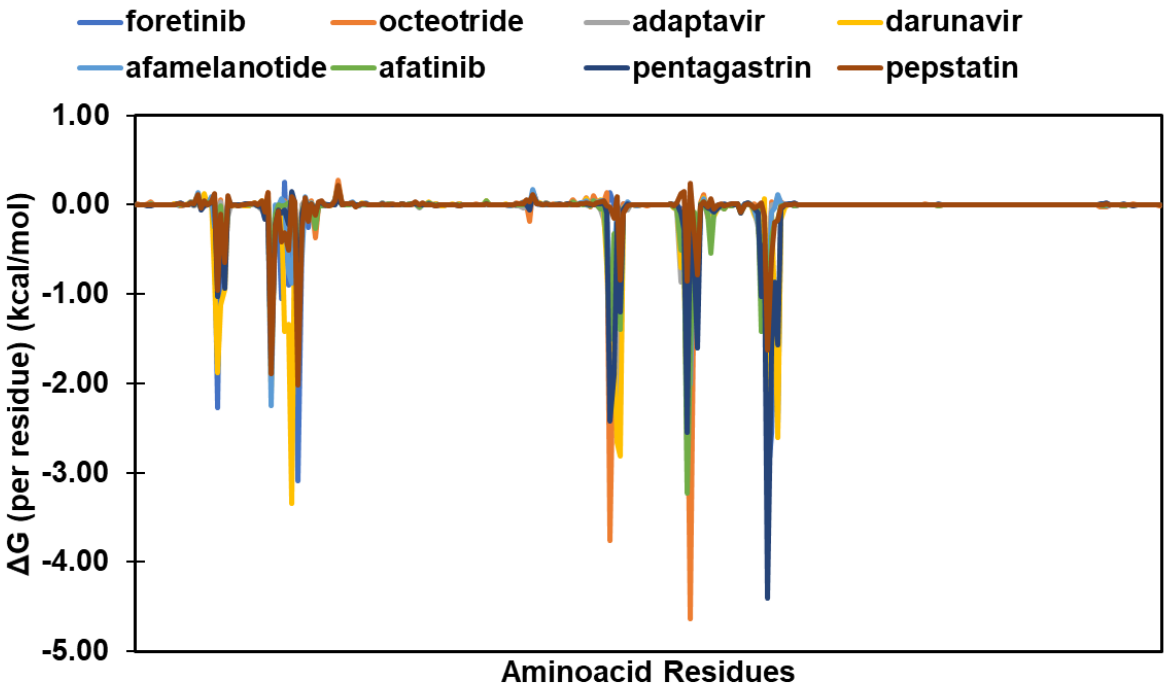

Fig. S2 Per-residue binding free energy decomposition (in kcal/mol) for other M^{pro}-drug systems.