

## Anti-HIV drugs repurposing against SARS-CoV-2

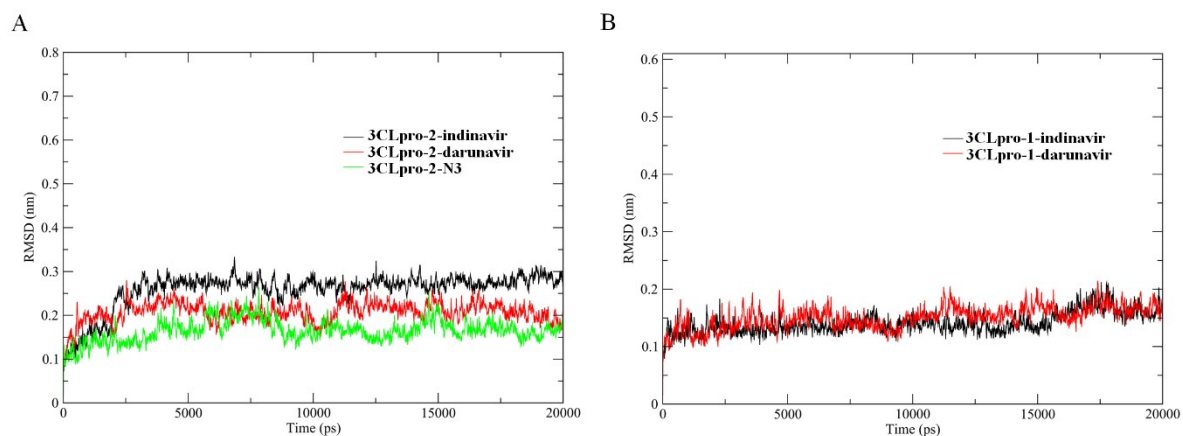


Fig. S1. Time evolution of backbone RMSD values of SARS HCoV 3CLpro with respect to the starting structure during the enzyme-inhibitor complex MD simulations. (A) 3CLpro-2-inhibitors; (B) 3CLpro-1-inhibitors.

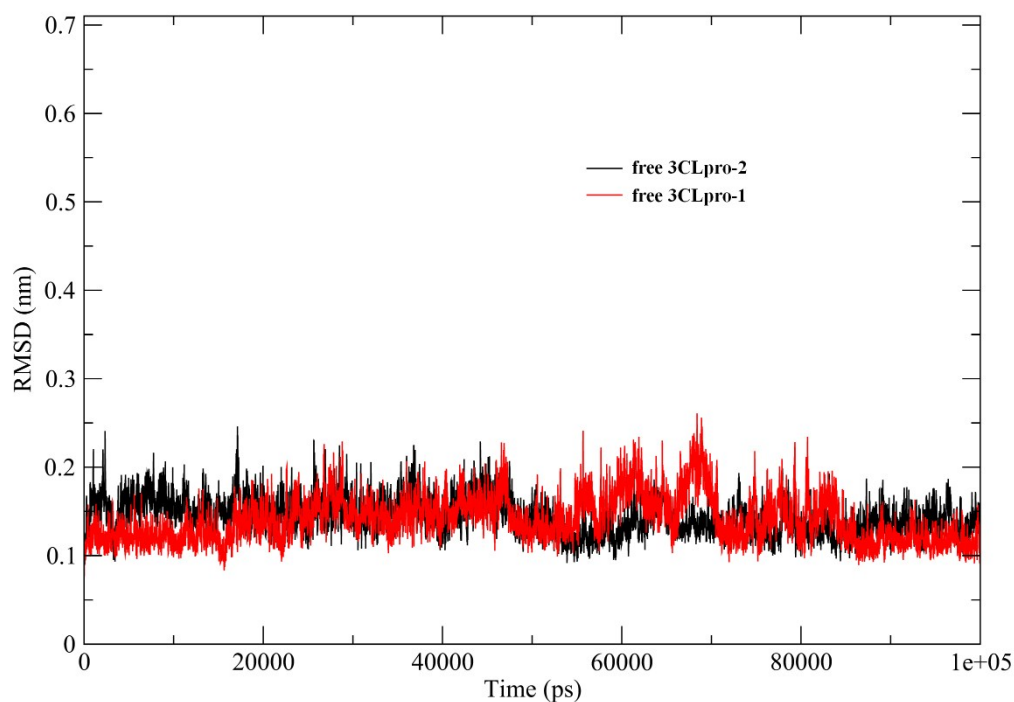


Fig. S2. Time evolution of backbone RMSD values of SARS HCoV 3CLpro with respect to the starting structure during the free enzyme MD simulations.