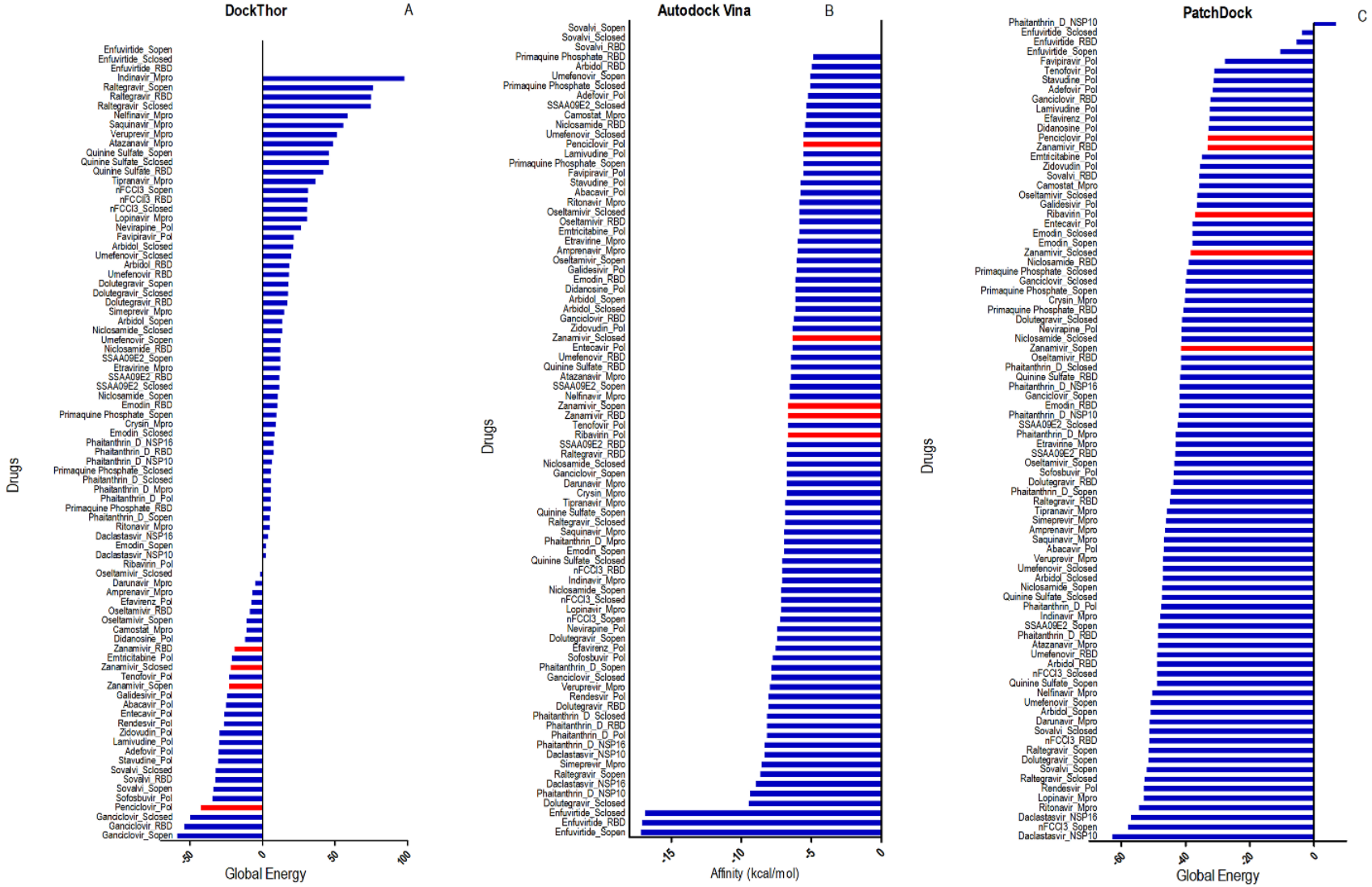
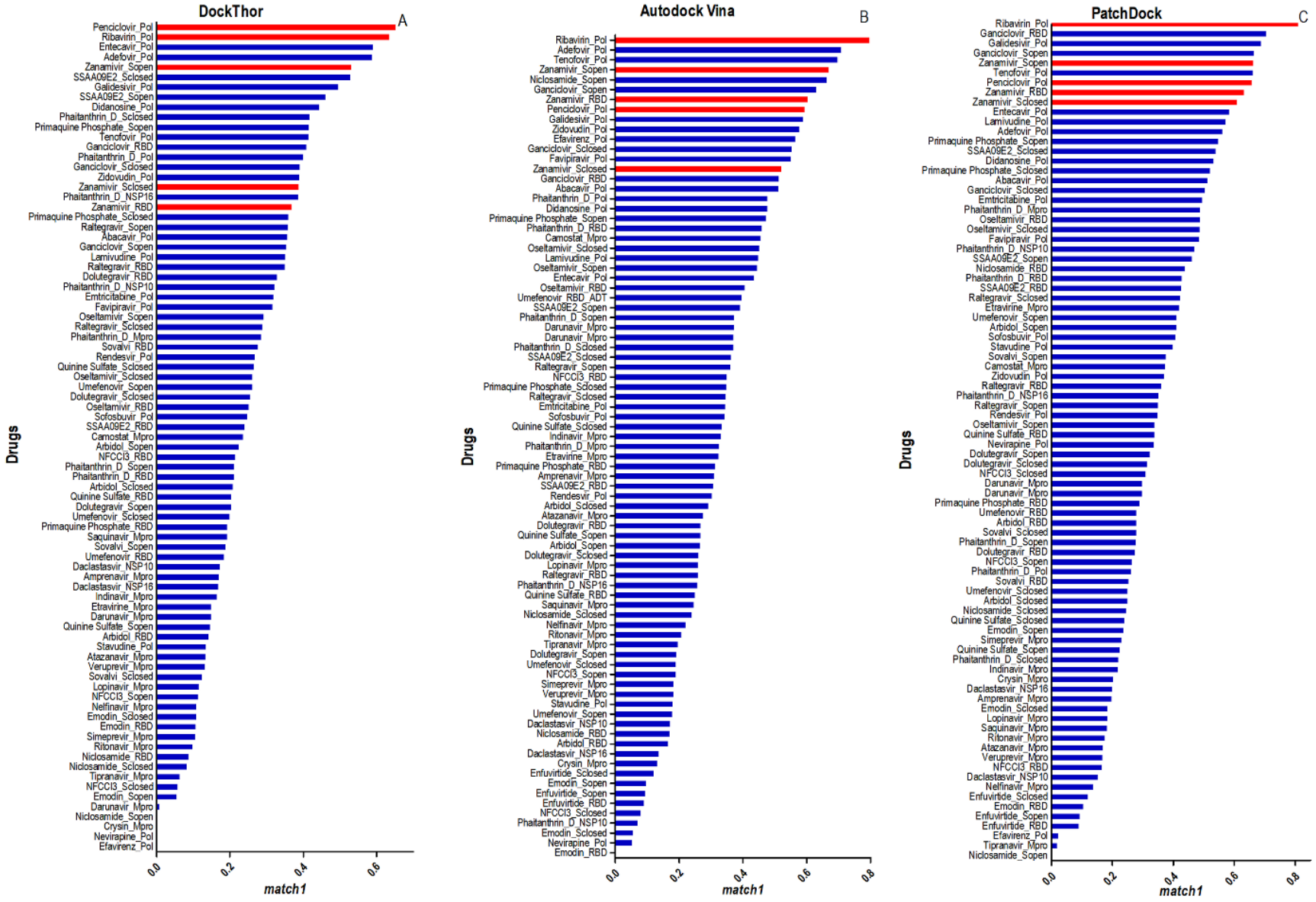
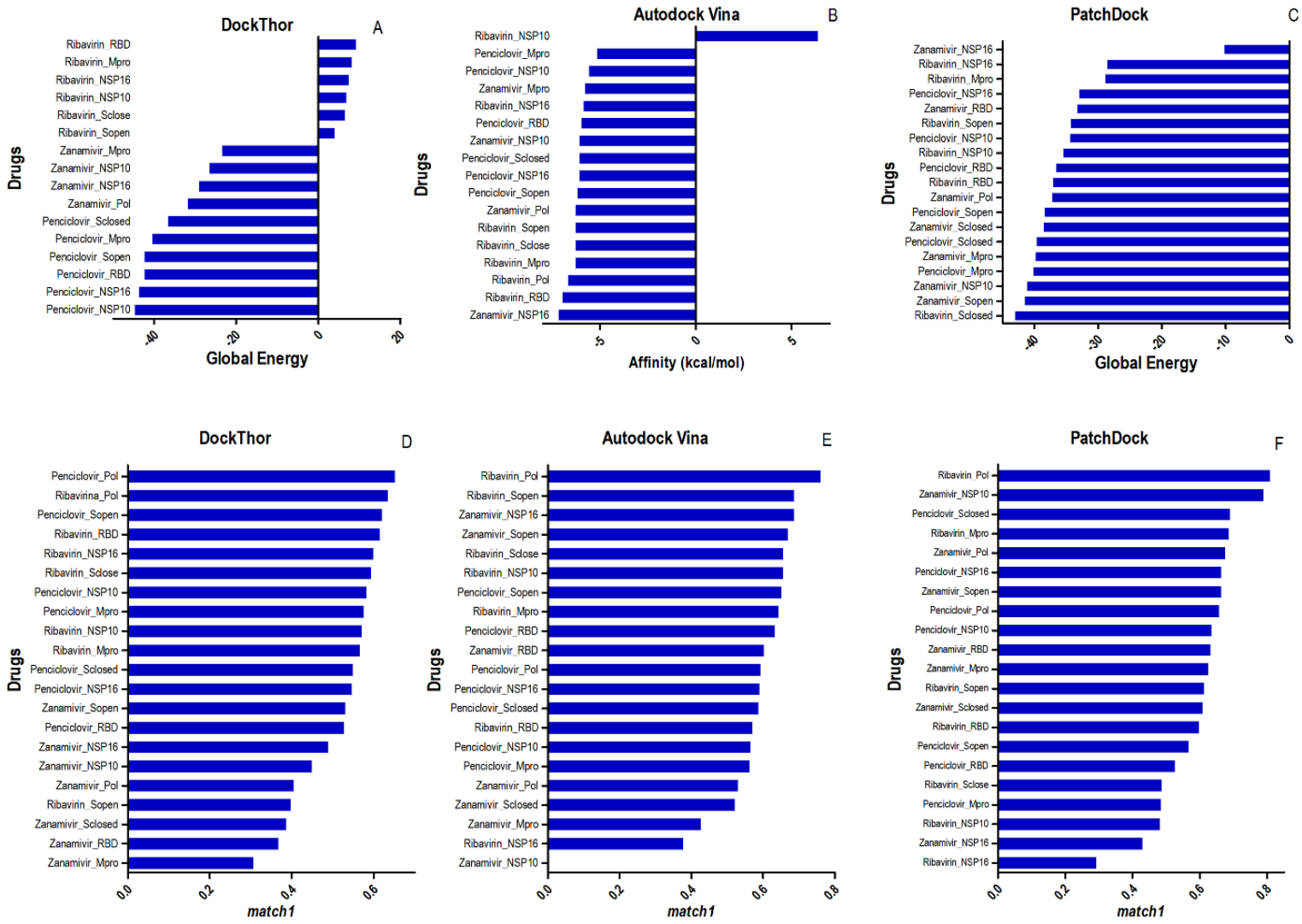
Supplementary Figures



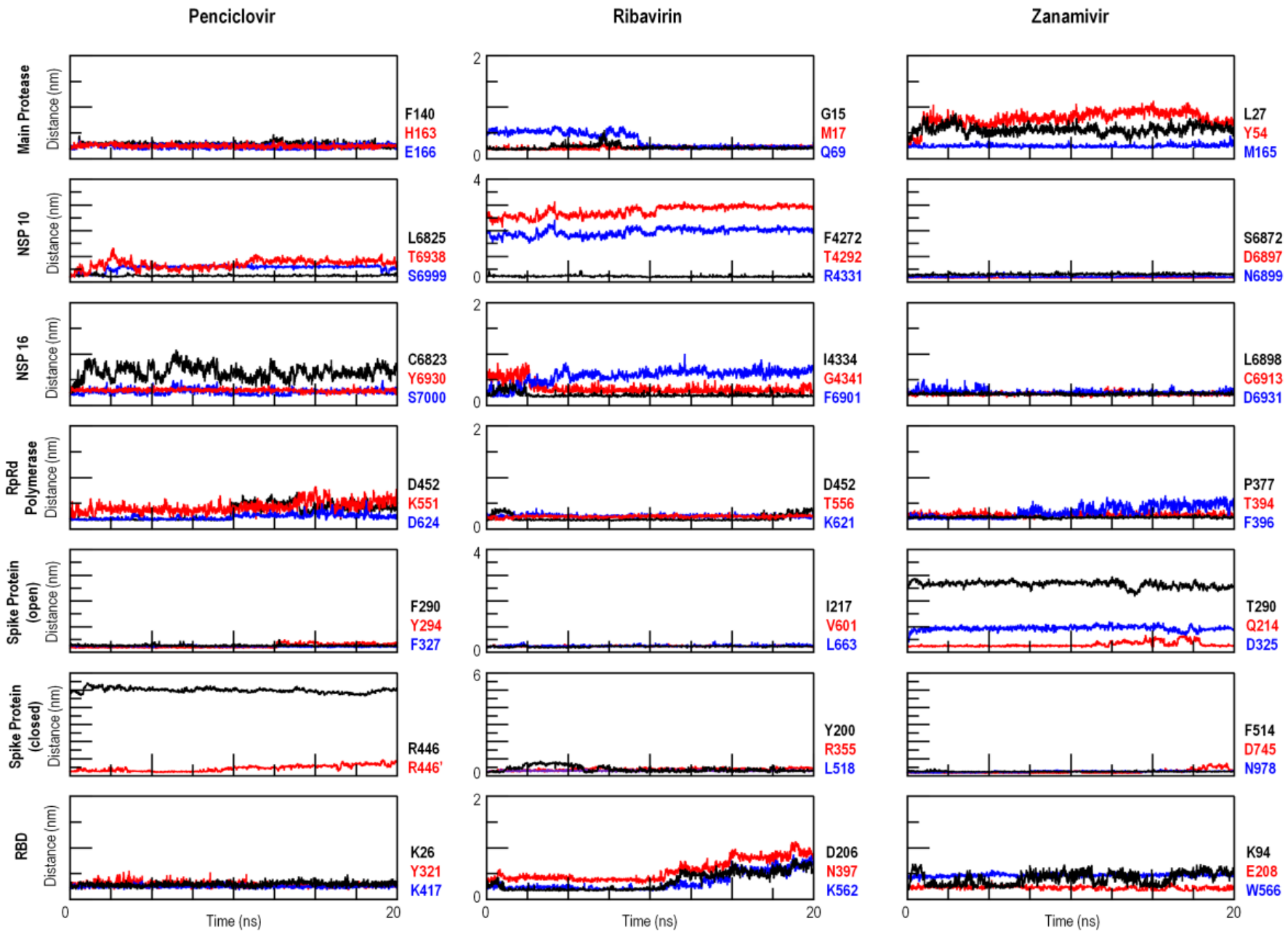
SFig 1. Global energy/Affinity data obtained from each docking software. Each bar represents a drug assigned to its putative target protein. In red are highlighted the docking results for complexes involving Penciclovir, Ribavirin, and Zanamivir. Results for Dockthor (A), Autodock Vina (B), and Patchdock (C).



SFig 2. Match1 ranking for each docking software obtained with Platinum for each software: Dockthor (A), Autodock Vina (B), and Patchdock (C). The threshold for selecting the best complexes was defined as *0.600.* In red are highlighted the docking results for complexes involving Penciclovir, Ribavirin, and Zanamivir.



SFig 3. Analysis of the interaction of the best compounds in each docking software. Individual global energy obtained for the best compounds against all viral proteins in each docking software (DockThor (A), Autodock Vina (B), PatchDock (C)) followed by analysis of Platinum unification of the results for each molecular docking software (DockThor (D), Autodock Vina (E), PatchDock (F)).



SFig 4. Analysis of the interaction between selected drugs and SARS-CoV-2 proteins via molecular dynamics. Distances between ligand (drug molecules) and receptor (contacting amino acids of the target protein) were measured to assess binding stability in physiological, time-dependent conditions.