Supporting Information

Assessing Potential Inhibitors for SARS-CoV-2 Main Protease from Available Drugs using Free Energy Perturbation Simulations

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Table S1. 2D docking conformation between the top 33 ZINC15 compounds and SARS-CoV-2 Mpro.

11a

Carmofur

His163

Cys145

Ser144

Thr25

His41

Ebselen

His163

Cys145

Asn142

Gly143

His41

Thr25

Leu141

11b

Disulfiram

His163

Cys145

Asn142

Gly143

His41

Thr25

Leu141

PX-12

Cys145

Asn142

Glu166

Ser144

Thr25

Thr24
Figure S1. Distribution of docking energy between 6363 ZINC15 compounds and SARS-CoV-2 Mpro.
Figure S2. All-atom RMSD of SARS-CoV-2 Mpro+inhibitors complexes during two independent 20ns-long MD simulations.
Figure S3. Desolvation free energy of experimentally characterized inhibitors of SARS-CoV-2 Mpro from solvated complex system (blue) and solvated ligand system (red). The difference between two metrics is the binding free energy between the ligand to SARS-CoV-2 Mpro, which obtained via FEP simulations.
Figure S4. Desolvation free energy of the top 33 ZINC15 compounds of SARS-CoV-2 Mpro from solvated complex system (blue) and solvated ligand system (red). The difference between two metrics is the binding free energy between the ligand to SARS-CoV-2 Mpro, which obtained via FEP simulation.