

Table S25: Virtual screening of 70 validated anti-SARS-CoV-2 small molecule drugs. DrugID corresponds to the drug id in DrugBank. non-inhibitor_probs represents the probability of non-SARS-CoV-2 inhibitors. inhibitor_probs represents the probability of SARS-CoV-2 inhibitors.

DrugID	non-inhibitor_probs	inhibitor_probs
DB01078	1.88E-05	0.99998116
DB11544	6.96E-05	0.9999305
DB13467	7.81E-05	0.9999219
DB00441	0.000127156	0.9998728
DB06733	0.000423055	0.999577
DB01396	0.000441887	0.99955815
DB12167	0.001608472	0.99839145
DB01933	0.002126772	0.9978732
DB03172	0.002269188	0.9977308
DB08860	0.002693576	0.99730647
DB11925	0.003411441	0.9965886
DB12008	0.004869224	0.9951308
DB11836	0.00769462	0.99230534
DB11963	0.007864516	0.9921355
DB12731	0.010650054	0.9893499
DB12980	0.01098805	0.9890119
DB12191	0.016336948	0.9836631
DB05424	0.017515251	0.98248476
DB09274	0.018679384	0.98132056
DB12180	0.026367793	0.9736322
DB00773	0.030529208	0.9694708
DB16228	0.06574645	0.93425363
DB00220	0.0725568	0.9274432
DB12387	0.07817044	0.9218295
DB01667	0.085802235	0.91419774
DB11432	0.089807265	0.91019267
DB04865	0.090802744	0.90919733
DB14761	0.10425286	0.8957471
DB02587	0.11542233	0.88457763
DB13393	0.12973516	0.8702648
DB08437	0.13642898	0.86357105
DB13729	0.14483973	0.85516036
DB06469	0.17343509	0.8265649
DB12774	0.18150604	0.81849396
DB08916	0.19392926	0.80607074
DB11617	0.24374713	0.7562529
DB00276	0.2623714	0.73762864
DB15686	0.3348823	0.6651177
DB12598	0.37335983	0.62664014
DB00352	0.39709035	0.6029097
DB02010	0.4401818	0.5598182
DB06061	0.48684037	0.51315963
DB15408	0.5064007	0.49359924
DB06816	0.5371333	0.4628667

DB05239	0.68645936	0.31354067
DB00630	0.8108554	0.18914457
DB01033	0.8182946	0.1817054
DB14904	0.8200117	0.17998832
DB15254	0.8292575	0.17074253
DB08142	0.9157889	0.08421114
DB05983	0.96002465	0.039975315
DB13536	0.968111	0.03188905
DB12673	0.9783483	0.021651639
DB01204	0.9814736	0.018526396
DB12120	0.98246884	0.017531095
DB12933	0.98937875	0.010621207
DB12624	0.9905019	0.009498136
DB05013	0.99586725	0.004132716
DB03523	0.99608266	0.003917368
DB00694	0.997431	0.002569054
DB00439	0.9977557	0.002244335
DB06810	0.99794656	0.002053446
DB00993	0.9981153	0.001884712
DB12114	0.9981482	0.00185186
DB12241	0.9989208	0.001079185
DB06442	0.99926716	0.000732864
DB09053	0.9996747	0.000325358
DB15661	0.9996815	0.000318544
DB00482	0.9999987	1.28E-06
DB01609	0.99999976	1.98E-07