

**Fast Identification of Possible Drug Treatment of Coronavirus Disease -19 (COVID-19)
Through Computational Drug Repurposing Study**

(Supporting Information)

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Table S1. List of Glide docking scores and MM-PBSA-WSAS binding free energies for potential inhibitors binding to SARS-Cov-2 main protease (in kcal/mol). The net charge (NC) of charged molecules is shown in the parentheses.

Compound Name	Docking Score	ΔE_{EEL}	ΔE_{VDW}	ΔG_{PB}	ΔG_{SA}	ΔTS	ΔG_{bind}
DB01601 Docking Pose 2	-9.4	-51.6 ± 0.2	-18.2 ± 0.30	47.37 ± 0.2	-4.8 ± 0.0	-23.4 ± 0.06	-3.76 ± 0.2
10011418	-8.9	-46.9 ± 0.4	-69.7 ± 0.7	95.6 ± 0.7	-4.8 ± 0.0	-22.7 ± 0.1	-3.0 ± 0.3
6102717	-10.0	-47.2 ± 0.2	-22.4 ± 0.5	51.6 ± 0.6	-4.3 ± 0.0	-22.8 ± 0.1	0.4 ± 0.3
DB00183	-10.4	-43.3 ± 0.2	-27.4 ± 0.6	54.7 ± 1.2	-4.4 ± 0.0	-21.6 ± 0.1	1.3 ± 0.6
DB01072	-9.1	-46.8 ± 0.2	-16.8 ± 0.5	47.3 ± 0.5	-4.7 ± 0.0	-22.8 ± 0.2	1.8 ± 0.6
DB01204	-10.1	-51.1 ± 0.2	-31.2 ± 0.2	58.5 ± 0.6	-4.1 ± 0.0	-23.4 ± 0.0	-4.5 ± 0.4
DB01232	-9.0	-44.2 ± 0.4	-8.6 ± 0.4	34.7 ± 0.4	-4.4 ± 0.0	-21.0 ± 0.1	-1.4 ± 0.3
DB01264	-9.9	-37.2 ± 0.1	-31.2 ± 0.6	47.8 ± 0.6	-2.9 ± 0.0	-20.3 ± 0.1	-3.2 ± 0.2
DB01282	-8.7	-49.1 ± 0.5	-66.5 ± 0.4	91.8 ± 0.2	-4.4 ± 0.0	-23.8 ± 0.0	-4.5 ± 0.3
DB01328 (NC = 0)	-8.5	-37.2 ± 0.1	-23.9 ± 0.7	49.5 ± 0.6	-3.2 ± 0.0	-19.8 ± 0.1	5.0 ± 0.1
DB01328 (NC = -2)	-6.1	-44.8 ± 0.3	115.0 ± 0.8	-80.8 ± 0.7	-3.7 ± 0.0	-21.9 ± 0.1	7.5 ± 0.8
DB01698	-8.6	-48.4 ± 0.2	-46.0 ± 0.4	73.7 ± 0.4	-3.9 ± 0.0	-22.7 ± 0.1	-1.9 ± 0.8
DB03141 (NC = 0)	-9.8	-53.0 ± 0.3	-27.4 ± 0.4	62.8 ± 0.3	-4.6 ± 0.0	-22.4 ± 0.0	0.2 ± 0.2
DB03247 (NC = -2)	-7.4	-47.6 ± 0.5	74.0 ± 1.9	-39.5 ± 2.0	-3.6 ± 0.0	-21.8 ± 0.1	4.9 ± 0.3
DB03310 (NC = 0)	-8.7	-54.4 ± 0.4	-76.0 ± 0.9	107.8 ± 1.0	-4.2 ± 0.0	-26.1 ± 0.0	-0.8 ± 0.3
DB03310 (NC = -2)	-6.9	-39.5 ± 0.2	45.9 ± 2.6	-20.9 ± 2.8	-3.3 ± 0.0	-21.8 ± 0.0	4.0 ± 0.3
DB06441 (NC = -4)	-6.9	-52.5 ± 0.4	194.4 ± 2.8	-141.3 ± 2.1	-4.3 ± 0.0	-24.4 ± 0.0	20.7 ± 0.8
DB06717 (NC = -2)	-8.5	-34.8 ± 0.7	177.4 ± 4.9	-136.8 ± 2.2	-3.4 ± 0.0	-21.1 ± 0.1	23.4 ± 2.1
DB08818 (NC = 0)	-9.1	-44.1 ± 0.3	-80.2 ± 0.3	105.4 ± 0.5	-4.6 ± 0.0	-23.8 ± 0.1	0.4 ± 0.4
DB08818 (NC = -2)	-9.3	-44.9 ± 0.1	75.9 ± 1.5	-49.2 ± 1.3	-4.3 ± 0.0	-22.8 ± 0.0	0.4 ± 0.6
DB09059	-9.0	-61.3 ± 0.2	-33.8 ± 0.7	75.1 ± 0.8	-5.0 ± 0.0	-25.8 ± 0.1	0.8 ± 0.6
DB09065	-9.0	-58.2 ± 0.1	-14.3 ± 0.1	48.2 ± 0.4	-5.3 ± 0.0	-25.4 ± 0.1	-4.1 ± 0.3
DB11602	-8.9	-52.6 ± 0.4	-33.1 ± 0.4	73.0 ± 0.2	-5.1 ± 0.0	-24.7 ± 0.1	7.0 ± 0.2
DB13074	-9.2	-40.0 ± 0.3	-22.7 ± 0.8	45.2 ± 0.4	-3.3 ± 0.0	-20.0 ± 0.1	-0.7 ± 0.1