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Publisher Correction: Virtual screening and molecular dynamics simulations provide insight into repurposing drugs against SARS-CoV-2 variants Spike protein/ACE2 interface

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Correction to: *Scientific reports* <https://doi.org/10.1038/s41598-023-28716-8>, published online 27 January 2023

The original version of this Article contained errors in Table 2, where data in the heading row was displaced. As a result, the values in the columns ΔG_{bind} , $\Delta G_{\text{Coulomb}}$, $\Delta G_{\text{Covalent}}$, ΔG_{Hbond} , ΔG_{Lipo} , ΔG_{SolvGB} and ΔG_{vdW} appeared under an incorrect column heading. Additionally, the column heading “ $\Delta G_{\text{Coulomb}}$ ” was incorrectly stated as “ ΔG_{Coulom} ”. The original Table 2 and accompanying legend appear below.

The original Article has been corrected.

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ligand	ΔG_{bind}	ΔG_{Coulom}	$\Delta G_{\text{Covalent}}$	ΔG_{Hbondd}	ΔG_{Lipo}	ΔG_{SolvGB}	ΔG_{vdW}	
#1	ZINC000000004319	-59.54	0.12	1.23	-2.94	-13.79	-15.71	-26.22
#2	ZINC000003824921	-54.8	-37.26	4.57	-3.47	-18.48	35.68	-31.99
#3	ZINC000067665085	-54.76	-18.6	1.33	-2.31	-17.91	28.05	-42.13
#4	ZINC000035644633	-51.87	-57.74	3.44	-2.32	-17.69	61.48	-34.59
#5	ZINC000085540202	-51.64	6.63	5.41	-1.82	-15.39	3.93	-47.05
#6	ZINC000000607910	-51.46	-21.8	-0.94	-2.45	-13.77	19.15	-25.85
#7	ZINC000000538509	-50.78	4.91	2.05	-1.6	-17.78	-3.98	-30.29
#8	ZINC000053073961	-50.18	41.13	3.07	-1.16	-17.26	-33.41	-36.14
#9	ZINC000003810860	-50.05	-26.04	4.45	-1.71	-19.57	27.55	-29.34
#10	ZINC000022446634	-49.42	28.75	5.74	-1.13	-17.62	-29.46	-32.19
#11	ZINC000003816292	-48.55	42.49	9.34	-2.06	-9.41	-50.72	-35.51
#12	ZINC000001530886	-48.14	31.35	2.7	-2.59	-17.89	-23.82	-28.71
#13	ZINC000006716957	-47.99	-13.17	9.96	-1.89	-18.8	21.94	-38.49
#14	ZINC000077313075	-47.94	-63.1	8.9	-2.92	-19.73	72.88	-39.91
#15	ZINC000030731084	-47.58	-23.59	5.78	-4.24	-13.51	31.38	-41.64
#16	ZINC000000537928	-47.34	22.02	3.74	-0.54	-26.3	-11.93	-29.88
#17	ZINC000150339331	-47.3	11.6	7.07	-1.84	-14.58	-9.06	-33.73
#18	ZINC000000001003	-47.24	-15.85	2.57	-1.03	-15.88	13.98	-25.87
#19	ZINC000000608266	-47.12	61.92	5.59	-0.65	-22.26	-55.54	-32.12
#20	ZINC000001552042	-47.11	-77.88	2.11	-1.33	-16.25	86.71	-34.63

Table 2. Binding energy (kcal/mol) and individual energy terms of Delta RBD-ligand systems calculated by Prime MM-GBSA.



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