

## Comparative binding efficacy of Ivermectin and Remdesivir against the spike protein of Omicron variants: an *in-silico* perspective

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### Supplementary Data

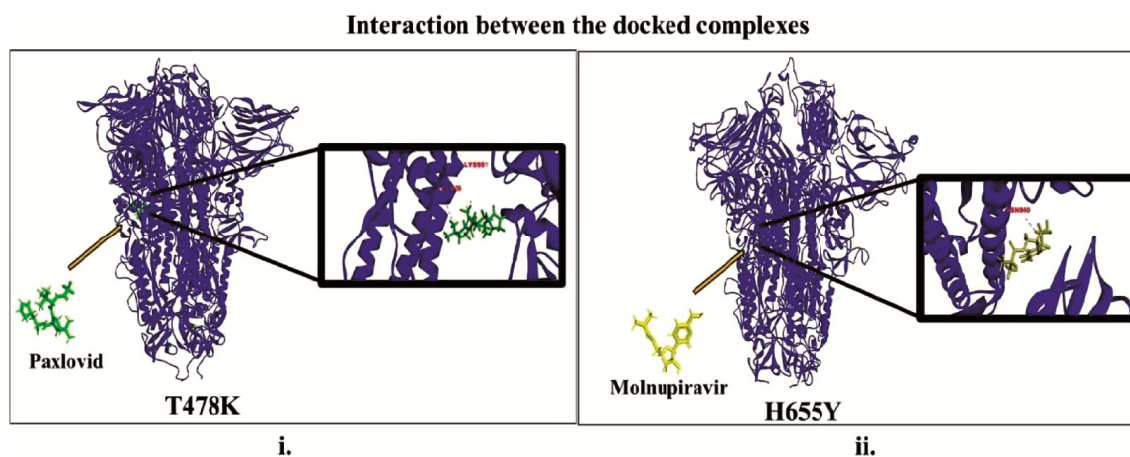


Fig. S1 — Interactions between the docked complex; i. Paxlovid-T478K complex ii. Molnupiravir-H655Y complex

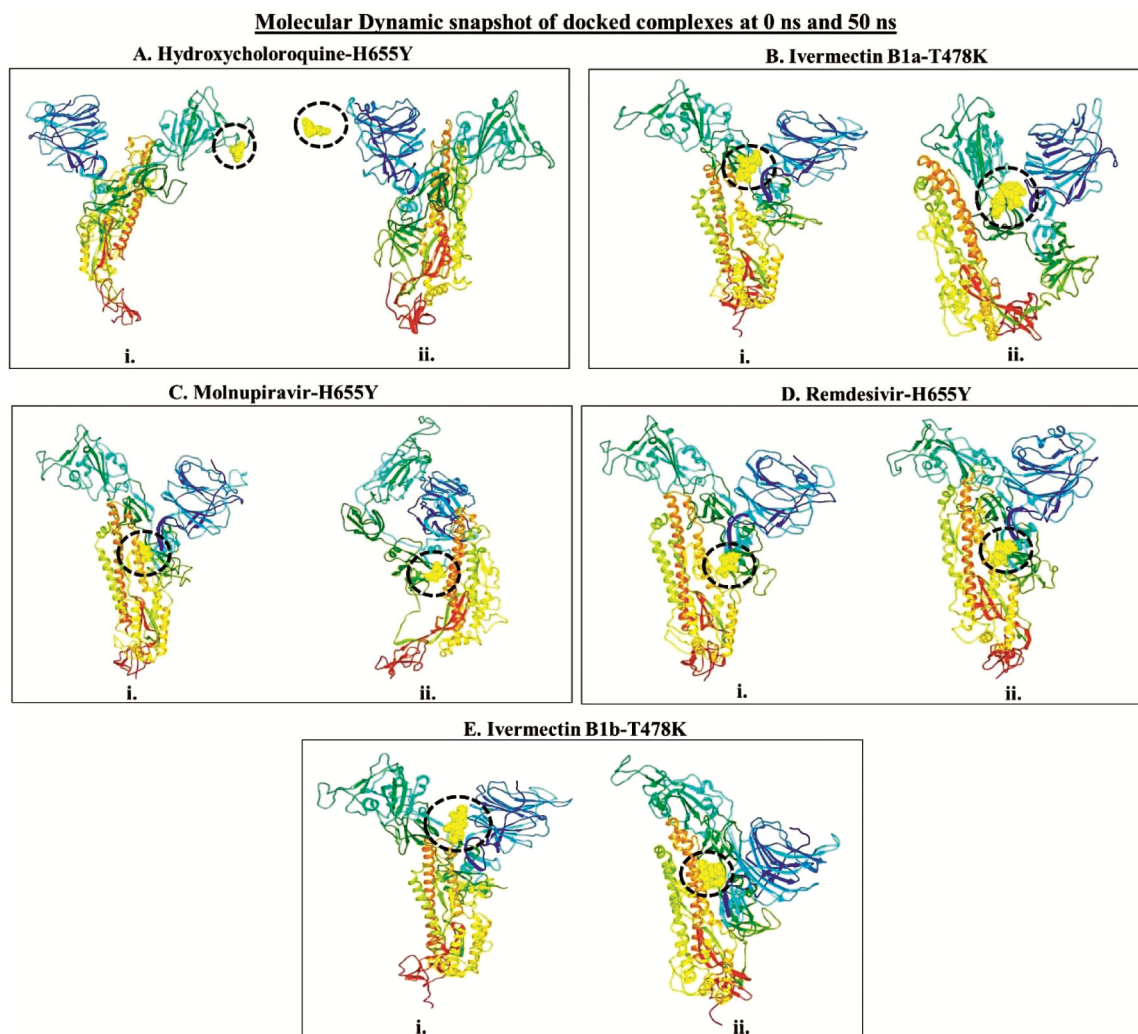


Fig. S2 — Molecular Dynamic snapshot of docked complexes at 0 ns and 50 ns; A. Hydroxychloroquine-H655Y i. at 0 ns, ii. at 50 ns, B. Ivermectin B1a-T478K i. at 0 ns, ii. at 50 ns, C. Molnupiravir-H655Y i. at 0 ns, ii. at 50 ns, D. Remdesivir-H655Y i. at 0 ns, ii. at 50 ns, E. Ivermectin B1b-T478K i. at 0 ns, ii. at 50 ns.

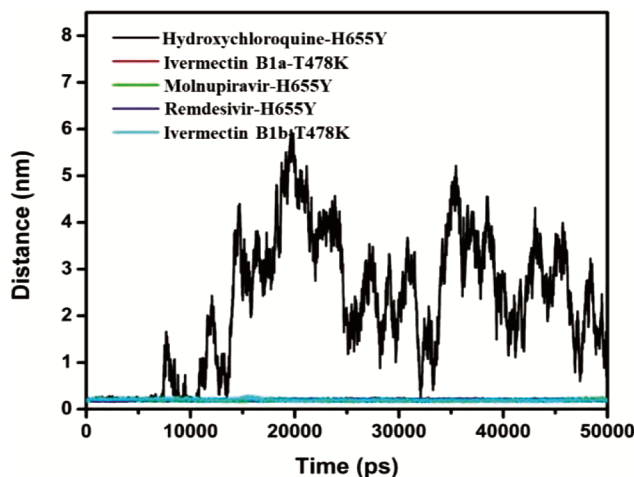


Fig. S3 — The distance vs time plot of ligand and protein over simulation periods; Hydroxychloroquine-H655Y shown in black, Ivermectin B1a-T478K shown in red, Molnupiravir-H655Y shown in green, Remdesivir-H655Y shown in blue, and Ivermectin B1b-T478K shown in cyan.

Table S1 — Docking score of all the mutant variant of omicron with the five drugs of interest.

Target Protein	E total						
	Ivermectin		Remdesivir	Hydroxychloroquine	Favipiravir	Paxlovid	Molnupiravir
	Ivermectin B1A	Ivermectin B1B					
Wild Type	-424.63	-332.81	-290.3	-1066.04	-83.9	-242.90	-193.63
E484A	-430.36	-340.93	-276.5	-1038.41	-84.0	-242.38	-207.89
G339D	-415.14	-331.40	-284.1	-1076.91	-71.7	-244.80	-202.10
G446S	-429.80	-339.72	-279.0	-1075.37	-80.9	-248.38	-193.66
G496S	-422.07	-332.41	-278.1	-1047.63	-77.0	-244.38	-205.10
K417N	-427.20	-331.66	-283.6	-1080.32	-75.9	-240.00	-204.93
N440K	-421.71	-334.32	-284.3	-1012.73	-75.9	-246.68	-201.04
N501Y	-425.56	-332.05	-285.8	-1038.67	-77.91	-245.44	-210.85
Q493R	-426.88	-334.87	-278.0	-1032.88	-85.7	-251.04	-193.38
Q498R	-424.64	-336.54	-287.5	-1031.88	-80.6	-244.31	-209.99
S373P	-420.72	-333.48	-288.4	-1038.89	-70.5	-244.68	-203.17
S375F	-422.84	-339.00	-278.8	-1075.55	-81.1	-246.36	-193.48
S477N	-422.01	-339.32	-278.7	-1075.36	-80.8	-244.07	-194.88
T478K	-430.56	-339.37	-278.7	-1047.60	-80.4	-251.67	-193.66
Y505H	-426.06	-333.89	-282.1	-1046.01	-74.7	-242.53	-201.42
A67V	-345.88	-286.90	-353.16	-1437.47	-133.91	-202.36	-231.46
HV69-70del	-344.64	-281.05	-339.52	-1482.48	-139.47	-210.25	-229.04
T95I	-340.01	-280.72	-321.71	-1474.79	-130.65	-207.40	-222.23
G142D	-426.19	-331.07	-285.82	-1051.61	-76.42	-245.60	-206.18
VYY143-145del	-348.55	-300.91	-328.39	-1472.49	-162.61	-205.04	-215.33
N211del	-350.19	-286.60	-348.09	-1481.36	-133.56	-199.73	-217.90
L212I	-336.14	-282.19	-320.17	-1471.70	-130.15	-214.25	-223.35
ins214EPE	-337.76	-286.04	-323.99	-1544.67	-121.71	-195.19	-222.00
S371L	-422.63	-329.60	-285.99	-1048.27	-77.15	-241.71	-205.02
T547K	-350.17	-287.49	-325.62	-1344.00	-133.10	-217.50	-226.50
D614G	-47.36	-54.65	-41.43	-963.81	-100.29	-162.94	-52.44
H655Y	-342.64	-283.91	-352.78	-1456.44	-133.93	-211.26	-226.60
N679K	-328.14	-289.18	-287.21	-1418.37	-130.29	-217.98	-225.42
P681H	-429.84	-333.91	-281.31	-1120.55	-82.04	-226.87	-192.87
N764K	-350.03	-281.15	-329.75	-1350.07	-140.71	-237.81	-228.98
D796Y	-344.71	-280.68	-339.12	-1452.14	-141.49	-235.10	-225.04
N856K	-329.38	-284.18	-270.44	-1374.27	-143.84	-227.74	-216.93
Q954H	-334.72	-288.74	-359.51	-1459.29	-135.91	-206.03	-238.07
N969K	-345.03	-284.18	-329.39	-1238.14	-134.74	-223.35	-229.94
L981F	-348.81	-289.78	-322.66	-1485.89	-130.63	-204.36	-223.52
All Mutations	-403.1	-325.7	-275.0	-331.5	-143.1	-426.0	-202.7