

Supplementary Tables

Table S1: Binding affinity details: Gibbs free energy and dissociation constant for 21A Delta, 21K Omicron and 21L Omicron in Uttar Pradesh, India during the second and third waves.

Spike_A CE 2 complex	ΔG (kcal mol ⁻¹)	Kd (M) at 25.0 °C	ICs charge d- charge d	ICs charge d-polar	ICs charge d- apolar	ICs polar- polar	ICs polar- apolar	ICs apolar- apolar	NIS charged:	NIS apolar:
Delta (21A)	- 10.18±0. 932	7.75E- 08±7.1 9E-08	9.4±4.7 44	10.1±3. 130	17.3±3. 880	3.7±2.8 30	13.7±5. 381	12.3±5. 451	21.20%±0. 022	41.928±0.084 %
21K Omicron	- 8.95±0.8 12	6.42E- 07±8.6 7E-07	2.9±1.3 33	2.4±1.2 31	14±4.40 0	0.2±0.6 15	9.5±3.5 31	16.7±3. 672	21.58%±6. 640	41.79±0.0674 %
21L Omicron	- 10.68±1. 303	1.04E- 07±1.7 E-07	4.7±3.6 14	8.5±3.3 79	19.4±3. 816	5.7±3.7 0	18.3±4. 426	17.8±9. 185	21.413%±0 .028	41.3611±12. 731%

Table S2: Details of the binding energy and amino acids involved in *in silico* docking of 21A Delta, 21K Omicron and 21K Omicron Spike with host ACE2.

Spike_ACE2 complex	Binding energy	Free	Amino acids falling in Favourable and allowed region	Amino falling in disallowed region	acid in	Contacts and interface area
Delta (21A)	-20.2367±1.118		98.3	1.7%		17 amino acids of Delta spike with 18 amino acids of ACE2 chain, covering 1072Å ² ×1068 Å ² , involving 3 salt bridges, 6 hydrogen bonds and 125 non bonded contacts
21K Omicron	-13.03±2.196		97.4	2.6%		5 amino acids of 21K Spike with 17 amino acids of ACE2 chain, covering 524Å ² ×667 Å ² , involving 0 salt bridges, 3 hydrogen bonds and 145 non bonded contacts
21L Omicron	-61.8833±2.254		98.3	1.7%		13 amino acids of 21L Spike with 17 amino acids of ACE2 chain, covering 890Å ² ×951 Å ² , involving 5 salt bridges, 3 hydrogen bonds and 103 non bonded contacts

The data presented in this study are deposited in the GISAID repository under classification 'Asia/India/Uttar Pradesh/CDRI' with the following accession numbers;

For 1st wave: (released on 2nd August 2022)

EPI_ISL_14192906, EPI_ISL_14192907, EPI_ISL_14192904, EPI_ISL_14192905, EPI_ISL_14192869, EPI_ISL_14192902, EPI_ISL_14192903, EPI_ISL_14192867, EPI_ISL_14192900, EPI_ISL_14192868, EPI_ISL_14192901, EPI_ISL_14192908, EPI_ISL_14192909, EPI_ISL_14192865, EPI_ISL_14192866, EPI_ISL_14192863, EPI_ISL_14192864, EPI_ISL_14192861, EPI_ISL_14192862, EPI_ISL_14192860, EPI_ISL_14192858, EPI_ISL_14192935, EPI_ISL_14192859, EPI_ISL_14192936,

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For 2nd wave: (released on 3rd august)

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For 3rd wave, released date 4th august

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