

7 TABLES AND FIGURES

Table S1 - Represents the mutations that are present in the Multiple Sequence Alignment between the BA.1.1 Omicron variant and the wildtype.

A67V	Q493R
69-70del	G496S
T95I	Q498R
GVYY142-145D	N501Y
NL211-212I	Y505H
ins214EPE	T547K
G339D	D614G
R346K	H655Y
S371L	N679K
S373P	P681H
S375F	N764K
K417N	D796Y
N440K	N856K
G446S	Q954H
S477N	N969K
T478K	L981F
E484A	

Table S2.1: Amino acid composition comparison between the whole spike protein sequence of the Omicron BA.1.1 with reference to wild type (wuhan-Hu-1)

	Wuhan-Hu-1-Whole Spike	Omicron-Whole Spike (BA.1.1)
Ala (A)%	6.2%	6.2%
Arg (R)%	3.3%	3.4%
Asn (N)%	6.9%	6.5%
Asp (D)%	4.9%	4.9%
Cys (C)%	3.1%	3.1%
Gln (Q)%	4.9%	4.6%
Glu (E)%	3.8%	3.9%
Gly (G)%	6.4%	6.2%
His (H)%	1.3%	1.4%
Ile (I)%	6.0%	6.1%
Leu (L)%	8.5%	8.4%
Lys (K)%	4.8%	5.4%
Met (M)%	1.1%	1.1%
Phe (F)%	6.0%	6.2%
Pro (P)%	4.6%	4.6%
Ser (S)%	7.8%	7.6%
Thr (T)%	7.6%	7.4%
Trp (W)%	0.9%	0.9%
Tyr (Y)%	4.2%	4.3%
Val (V)%	7.6%	7.6%
Pyl (O)%	0.0%	0.0%
Sec (U)%	0.0%	0.0%

Table S2.2: Amino acid composition comparison between the Receptor-binding Domain (RBD) sequence of the Omicron BA.1.1 with reference to wild type (wuhan-Hu-1)

	Wuhan-Hu-1 RBD	Omicron-RBD (BA.1.1)
Ala (A)%	5.2%	6.1%
Arg (R)%	4.8%	6.5%
Asn (N)%	9.2%	10.7%
Asp (D)%	3.9%	2.8%
Cys (C)%	3.9%	4.2%
Gln (Q)%	3.1%	1.9%
Glu (E)%	3.1%	3.3%
Gly (G)%	6.6%	4.2%
His (H)%	3.1%	0.9%
Ile (I)%	3.9%	4.2%
Leu (L)%	6.1%	6.1%
Lys (K)%	5.2%	7.0%
Met (M)%	0.0%	0.0%
Phe (F)%	7.0%	7.9%
Pro (P)%	5.7%	6.5%
Ser (S)%	7.4%	7.0%
Thr (T)%	5.7%	5.1%
Trp (W)%	0.9%	1.4%
Tyr (Y)%	6.6%	4.7%
Val (V)%	8.7%	9.3%
Pyl (O)%	0.0%	0.0%
Sec (U)%	0.0%	0.0%

Table S2.3: Amino acid composition comparison between the N-Terminal Domain (NTD) sequence of the Omicron BA.1.1 with reference to wild type (wuhan-Hu-1)

	Wuhan-Hu-1 NTD	Omicron-NTD (BA.1.1)
Ala (A)%	4.4%	4.1%
Arg (R)%	3.8%	3.8%
Asn (N)%	7.5%	7.2%
Asp (D)%	4.8%	5.2%
Cys (C)%	2.0%	2.1%
Gln (Q)%	3.4%	3.4%
Glu (E)%	3.4%	4.1%
Gly (G)%	5.8%	5.5%
His (H)%	2.0%	1.7%
Ile (I)%	4.4%	5.2%
Leu (L)%	9.6%	9.3%
Lys (K)%	5.1%	5.2%
Met (M)%	0.7%	0.7%
Phe (F)%	7.8%	7.9%
Pro (P)%	5.1%	5.5%
Ser (S)%	0.7%	8.3%
Thr (T)%	8.5%	8.3%
Trp (W)%	1.4%	1.4%
Tyr (Y)%	5.1%	4.5%
Val (V)%	6.8%	6.6%
Pyl (O)%	0.0%	0.0%
Sec (U)%	0.0%	0.0%

Table S3: Secondary structure prediction and comparison of Omicron Spike Protein, RBD and NTD (B.A.1.1) variant with reference to wild type (Wuhan-Hu-1)

	Wuhan-Hu-1-whole Spike	Omicron Spike (BA.1.1)
Alpha helix (Hh)	21.52%	22.91%
Extended strand (Ee)	22.07%	20.87%
Random coil (Cc)	56.40%	56.22%
	Wuhan-Hu-1 RBD	Omicron RBD (BA.1.1)
Alpha helix (Hh)	6.55%	5.61%
Extended strand (Ee)	22.71%	23.36%
Random coil (Cc)	70.74%	71.03%
	Wuhan-Hu-1 NTD	Omicron NTD (BA.1.1)
Alpha helix (Hh)	12.97%	14.83%
Extended strand (Ee)	25.26%	23.79%
Random coil (Cc)	61.77%	61.38%

Table S4.1: Expasy protparam (Whole Spike protein)

	WT	BA.1.1
No of amino acids	1273	1270
Molecular weight	141178.47	141300.09
Theoretical pI	6.24	7.14
Total number of negatively charged residues (Asp + Glu)	110	111
Total number of positively charged residues (Arg + Lys)	103	111
Instability index	33.01	34.69
Aliphatic index	84.67	84.95
Grand average of hydropathicity (GRAVY)	-0.079	-0.080

Table S4.2: Expasy protparam (RBD)

	WT	BA.1.1
No of amino acids	229	214
Molecular weight	25745.11	24441.05
Theoretical pI	8.91	9.64
Total number of negatively charged residues (Asp + Glu)	16	13
Total number of positively charged residues (Arg + Lys)	23	29
Instability index	21.04	32.60
Aliphatic index	71.44	73.27
Grand average of hydropathicity (GRAVY)	-0.259	-0.289

Table S4.1: Expasy protparam (NTD)

	WT	BA.1.1
No of amino acids	293	290
Molecular weight	33224.64	32902.27
Theoretical pI	8.13	6.51
Total number of negatively charged residues (Asp + Glu)	24	27
Total number of positively charged residues (Arg + Lys)	26	26
Instability index	34.12	35.84
Aliphatic index	78.81	79.62
Grand average of hydropathicity (GRAVY)	-0.199	-0.210

Table S5: Intrinsically disordered prediction using PONDR®VLXT tool.

	No.of residues disordered	Overall percent disordered	Predicted disorder segments	Number Disordered Regions
Wuhan-HU-1	98	7.70	[17]-[20] [468]-[475] [601]-[608] [672]-[709] [869]-[871] [945]-[950] [982]-[986] [992]-[994] [1023]-[1023] [1174]-[1194] [1264]-[1264]	11
Wuhan-RBD	18	7.86	[317]-[322] [468]-[473]	2
Wuhan-NTD	0	0.00	-	0
Omicron (BA.1.1)	85	6.69	[17]-[20] [208]-[221] [598]-[607] [675]-[706] [867]-[868] [1020]-[1020] [1171]-[1191] [1261]-[1261]	8
Omicron RBD (BA1.1)	6	2.62	[1]-[6]	1
Omicron NTD (BA.1.1)	14	4.83	[196]-[209]	1