

Supplementary Materials

Structural analysis of the novel variants of SARS-CoV-2 and forecasting in North America

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Table S1. Alteration of some amino acids of SARS-CoV-2 variants are presented relative to ancestral sequence of the Wuhan isolate

Variants	Amino acid positions relative to ancestral sequence of the Wuhan isolate																			
	69	70	80	144	215	242	243	244	417	452	484	501	570	614	681	701	716	982	1118	1176
Wild type	H	V	D	-	D	L	A	L	K	L	E	N	A	G	P	A	T	S	D	V
B.1.1.7	-	-	*	-	*	*	*	*	*	*	*	Y	D	*	H	*	I	A	H	*
B.1.351	*	*	A	Y	G	-	-	-	N	*	K	Y	*	*	*	V	*	*	*	*
P.1	*	*	*	Y	*	*	*	*	*	*	K	*	*	*	*	*	*	*	*	*
B.1.617	*	*	*	Y	*	*	*	*	*	R	Q	*	*	*	R	*	*	*	*	*

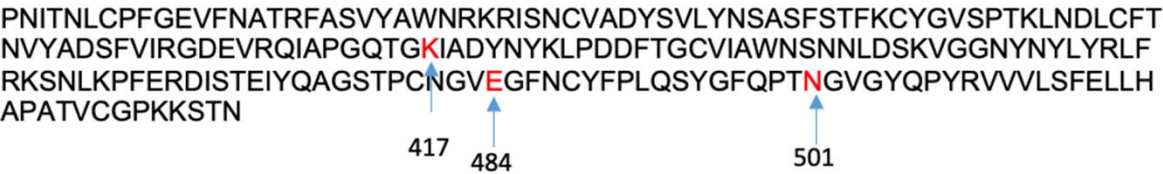
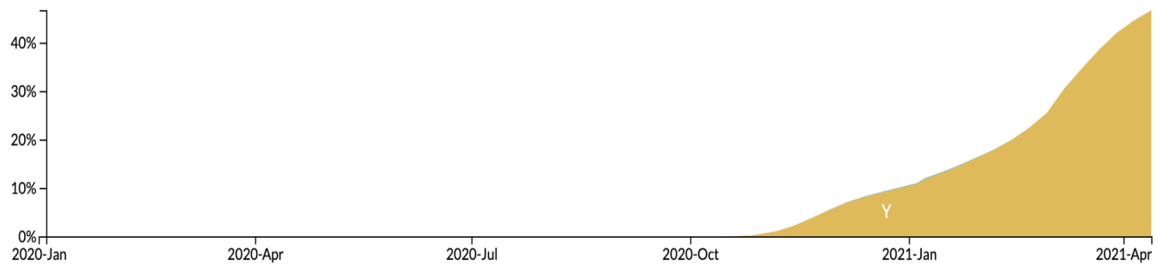
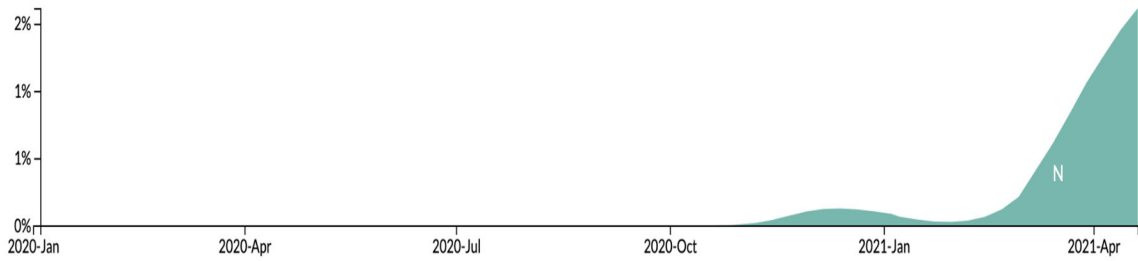


Figure S1. Sequence alignment of S-RBD of SARS-CoV-2 genes with mutations K417N, E484K, N501Y

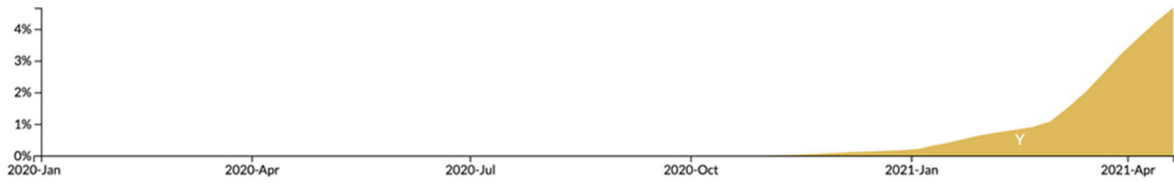
a



b



c



d

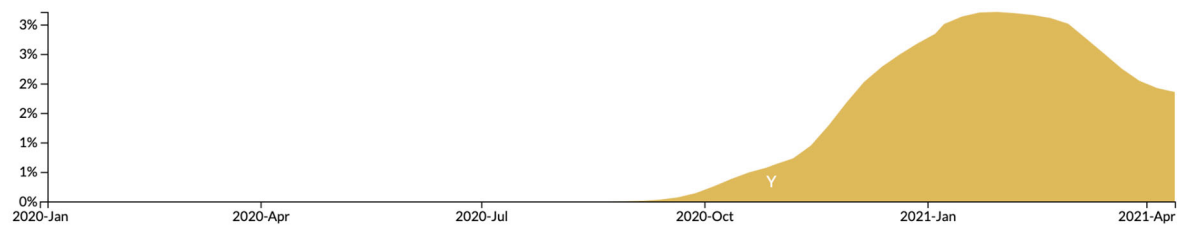


Figure S2: Frequency of novel variants of SARS-CoV 2 over time collected from North American subsample. a) B.1.1.7, b) B.1.617, c) P.1 and d) B.1.351

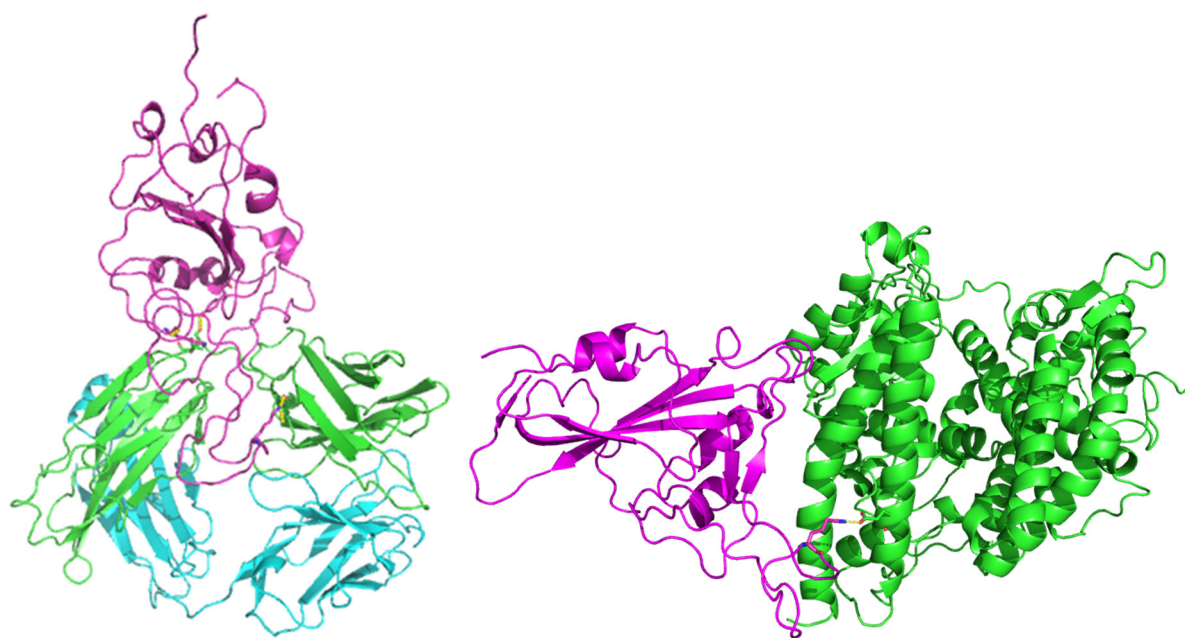


Figure S3: Docking structures of the interaction of E484K mutant of SARS-CoV-2 S-RBD protein in complex with a potent neutralizing CV30 antibody/hACE-2.

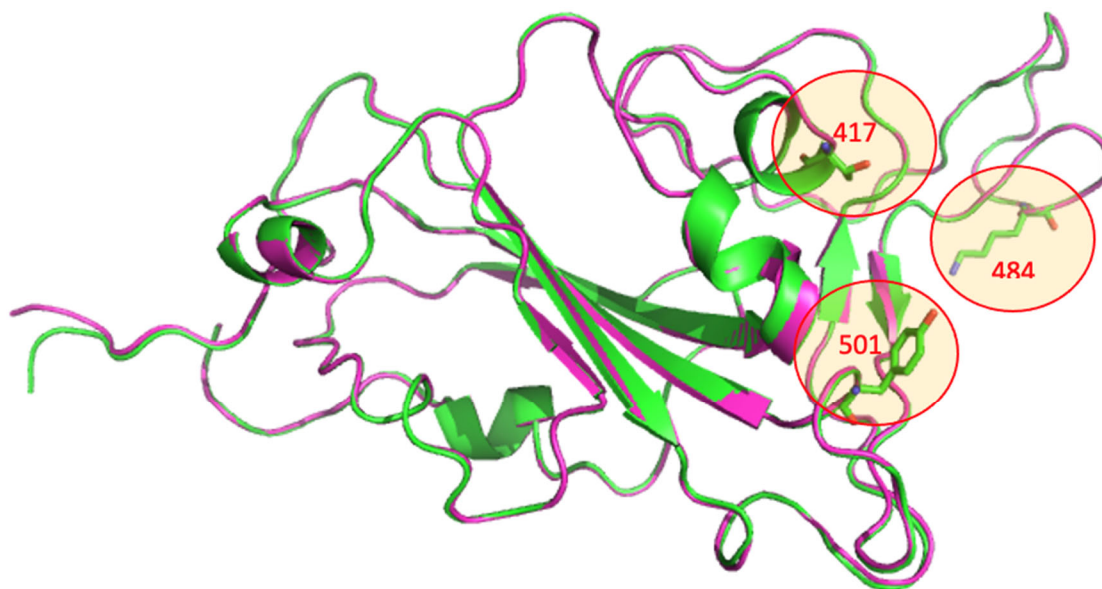
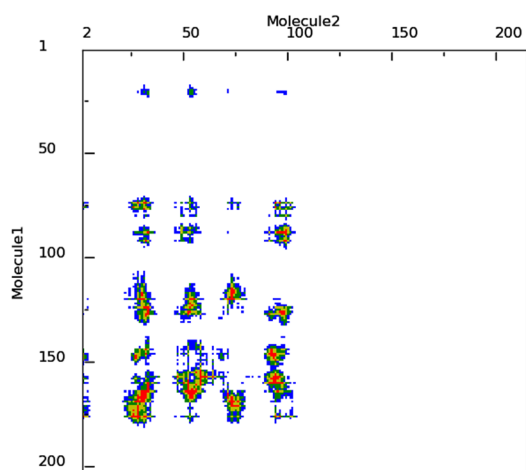
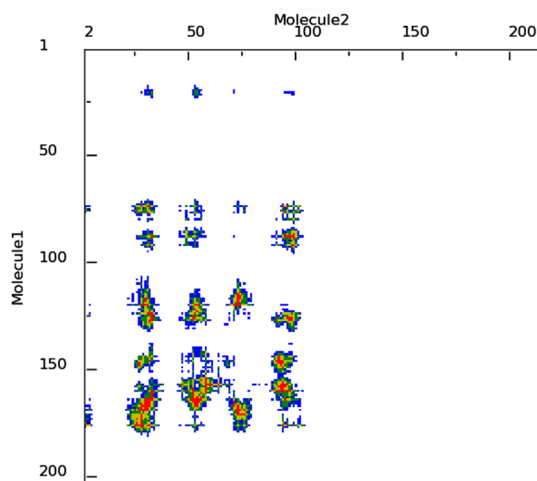


Figure S4. Superposition of wild/mutant SARS-CoV-2 S-RBD protein structures. The red rings in the photo indicate the three mutation points in the S-RBD that are in the flexible coil region. The structure displayed in purple indicates wild and the green color indicates mutated.

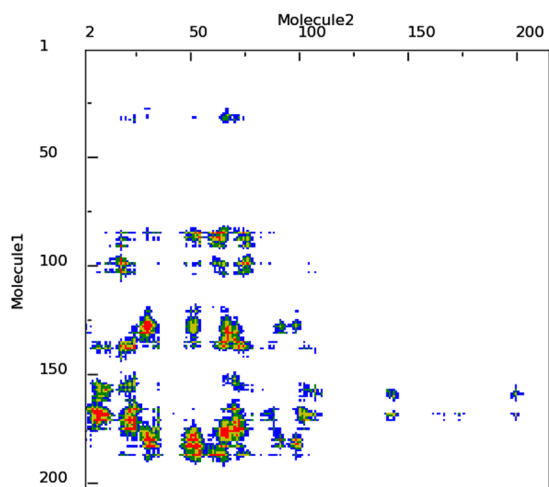
a) WT-CV30



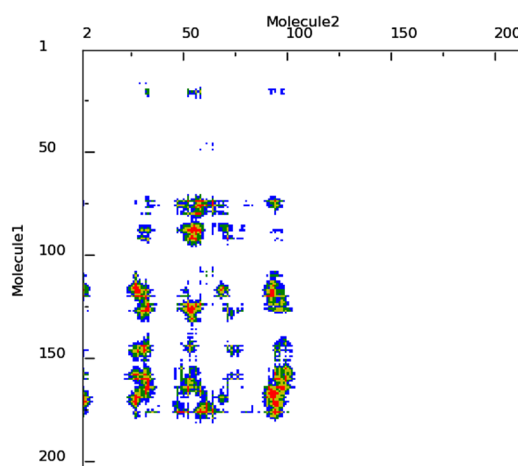
b) B.1.1.17-CV30



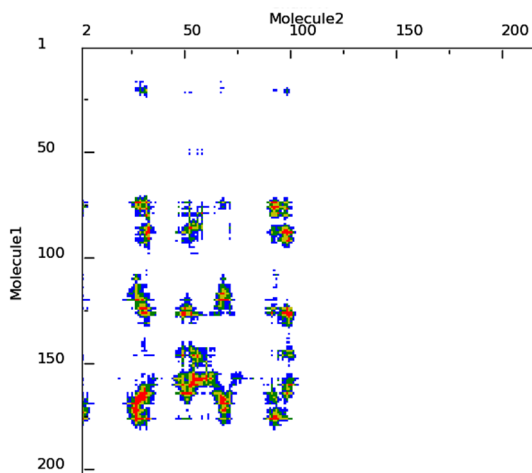
c) B.1.351-CV30



d) P.1-CV30



e) B.1.617-CV30



f) 484-CV30

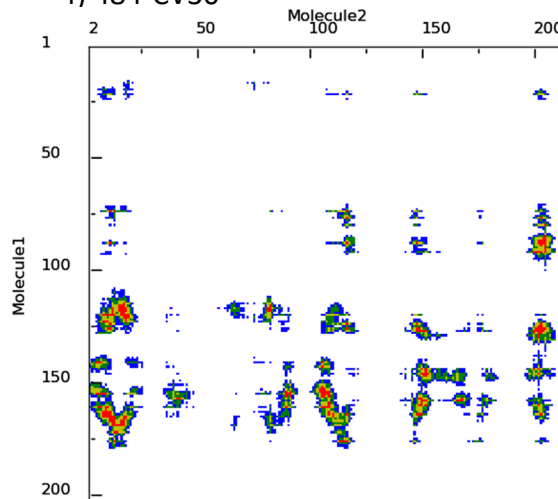
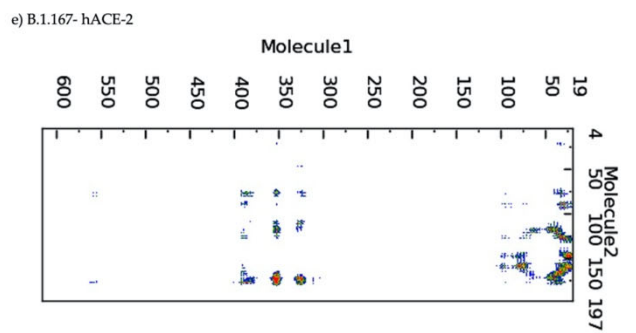
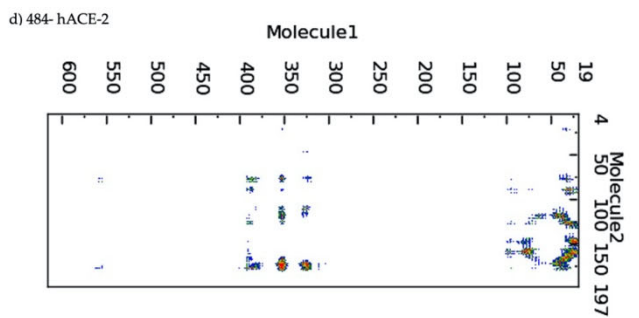
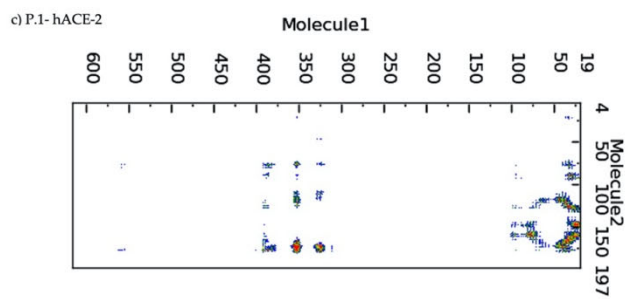
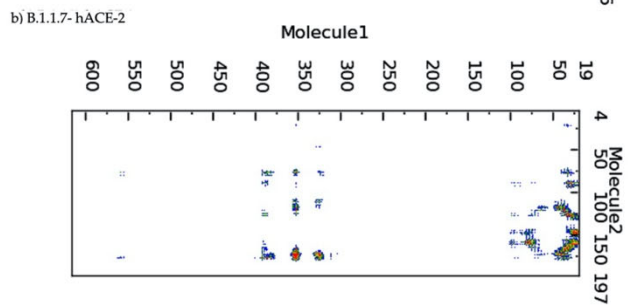
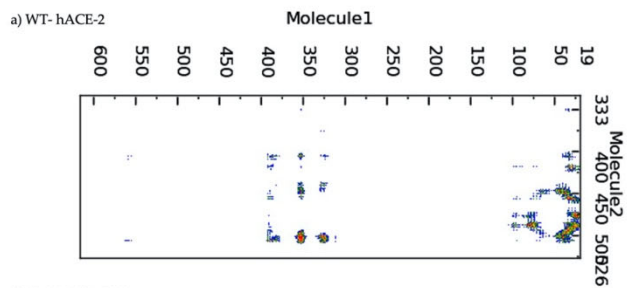


Figure S5: COCOMAPS distance contact maps for Interaction of different variants of SARS-CoV 2 spike with neutralizing antibody (CV30)/ACE-2. The color codes are reported in the legends under the maps.



7Å 10Å 13Å 16Å

Figure S5: COCOMAPS distance contact maps for Interaction of different variants of SARS-CoV-2 spike with neutralizing hACE-2. The color codes are reported in the legends under the maps.