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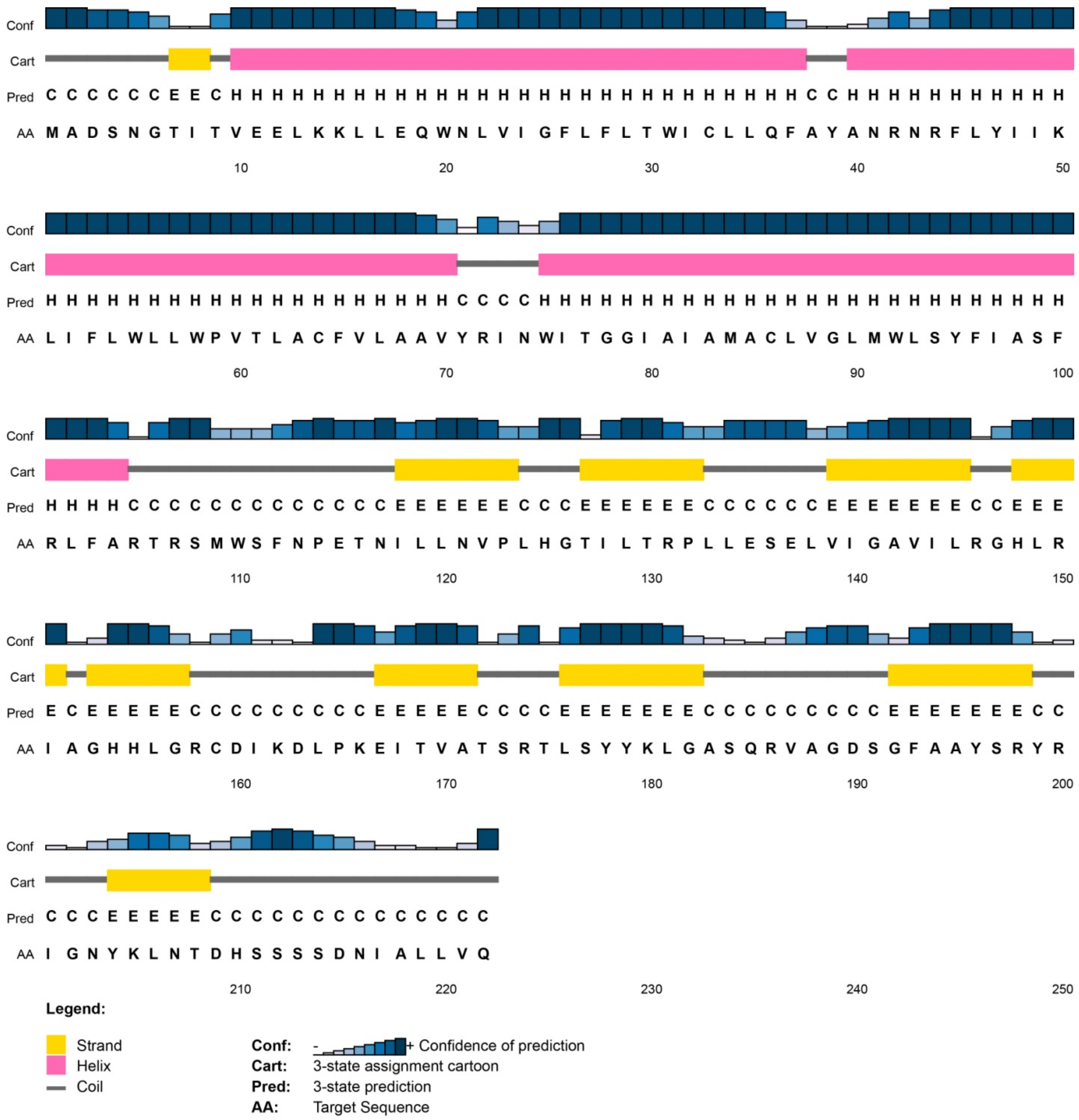
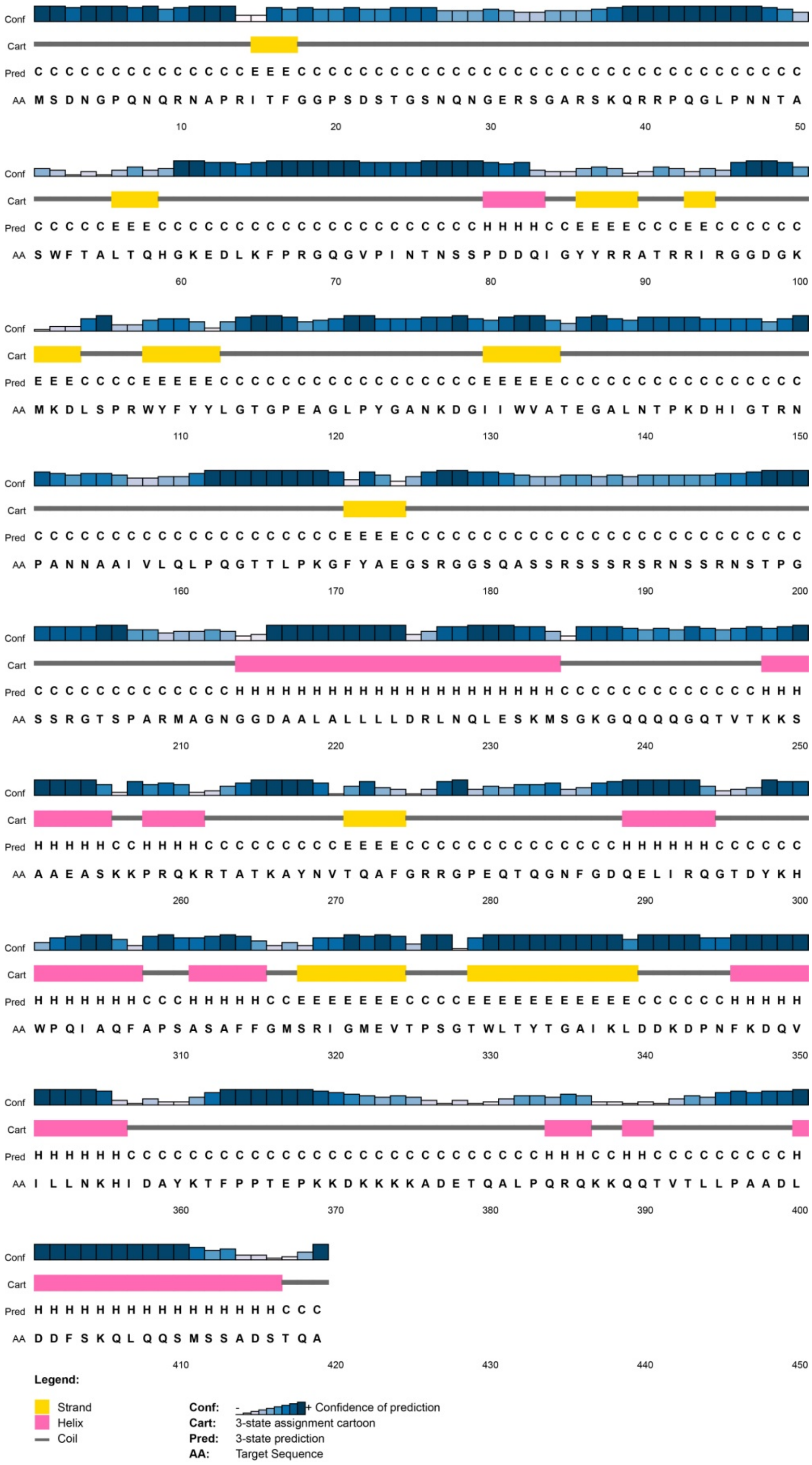
Supplementary Table 10. Mutations observed in the 34 non-allergenic and non-toxic linear B-cell epitopes.

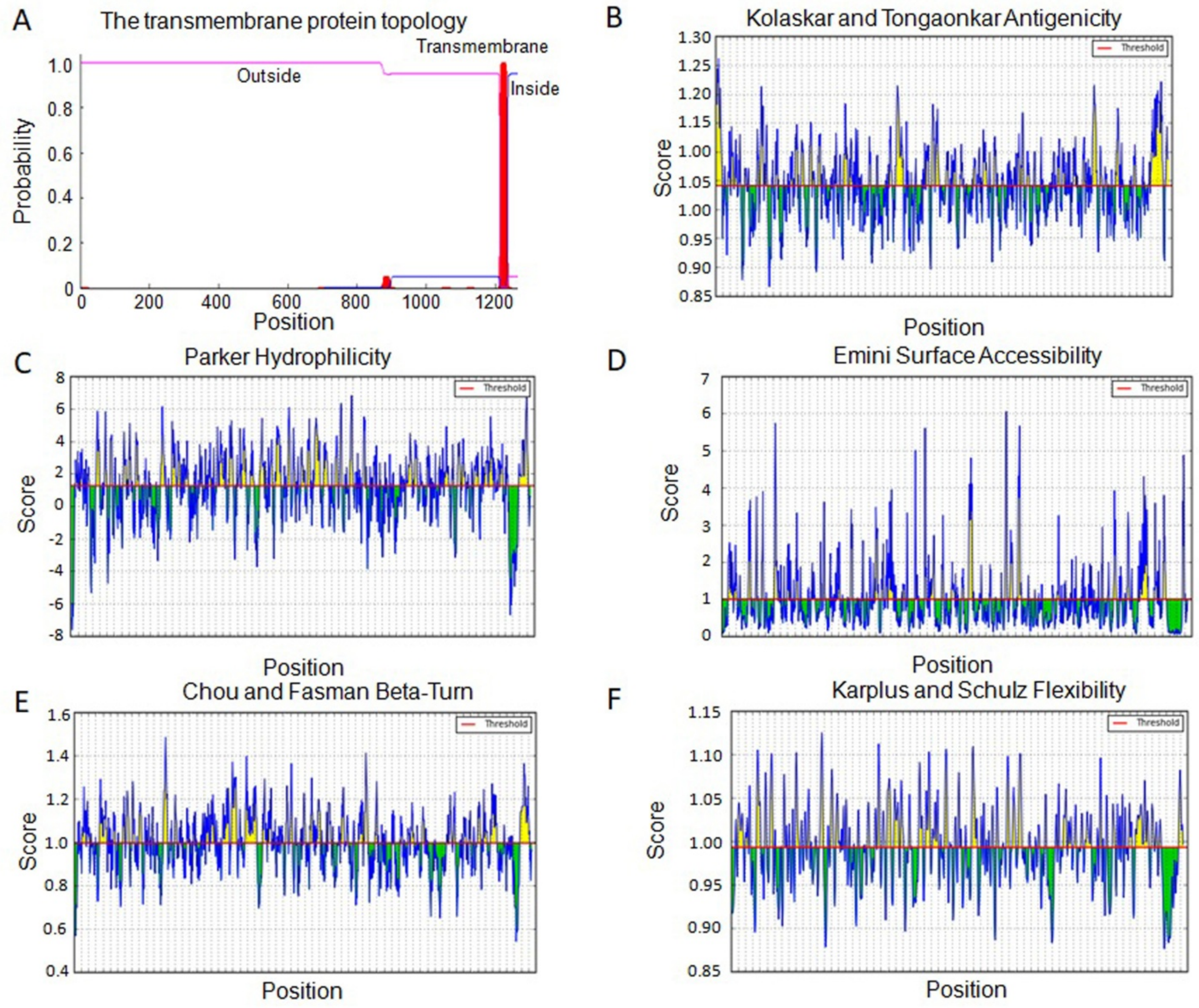
Supplementary Figure 1. Secondary structure predicted for the S protein of SARS-CoV-2.



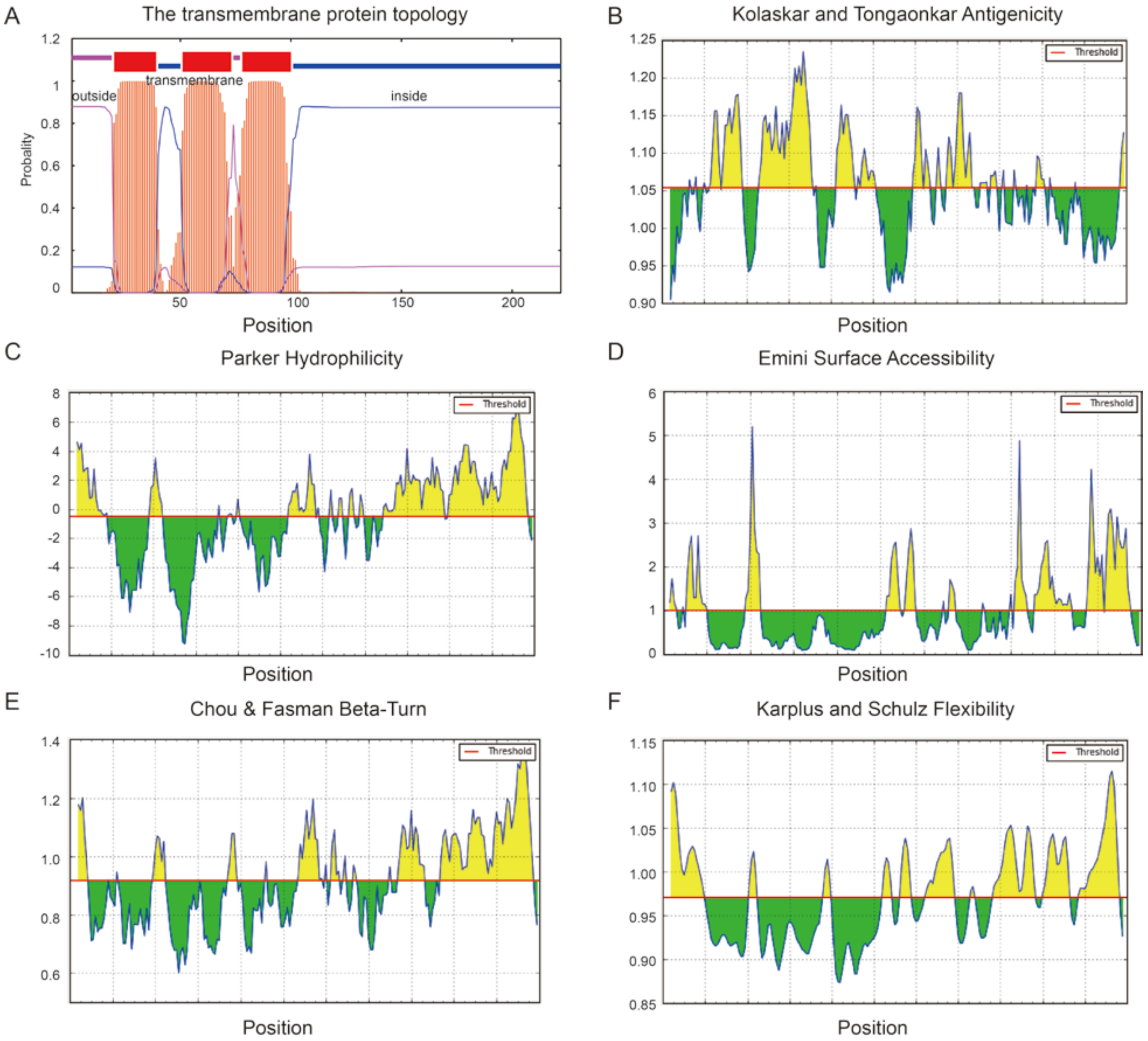
Supplementary Figure 2. Secondary structure predicted for the M protein of SARS-CoV-2.



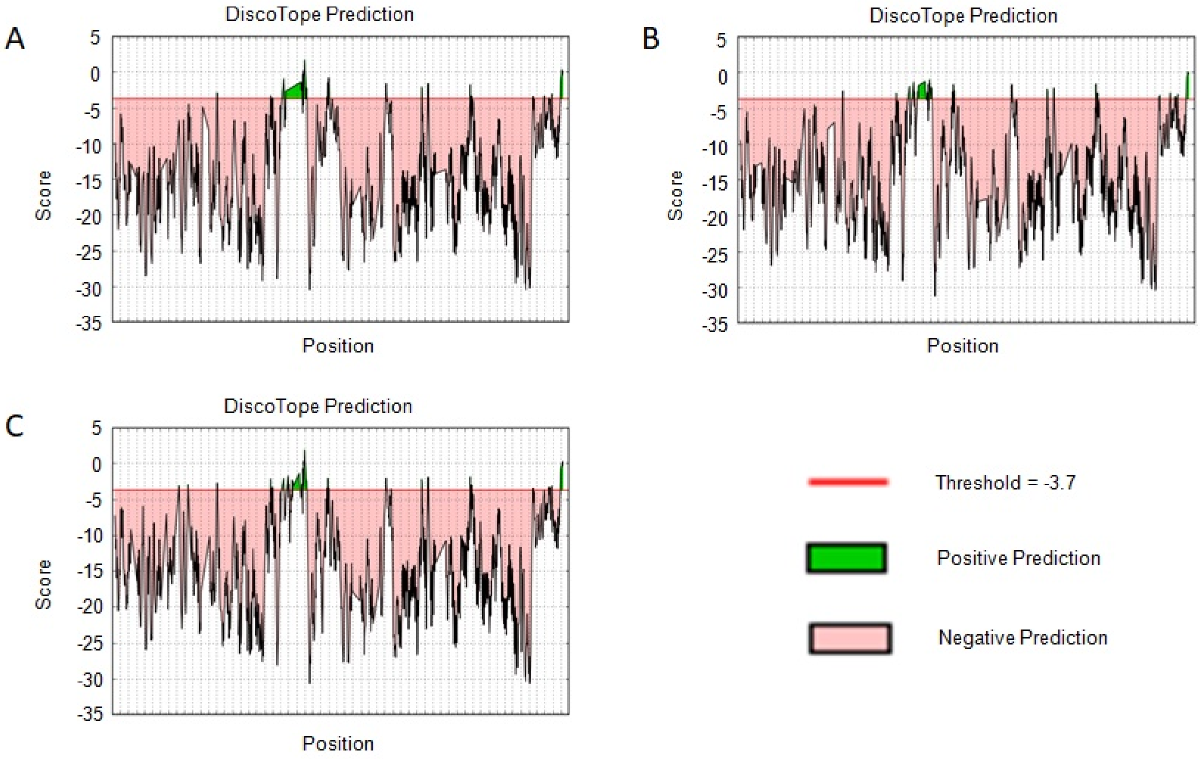
Supplementary Figure 3. Secondary structure predicted for the N protein of SARS-CoV-2.



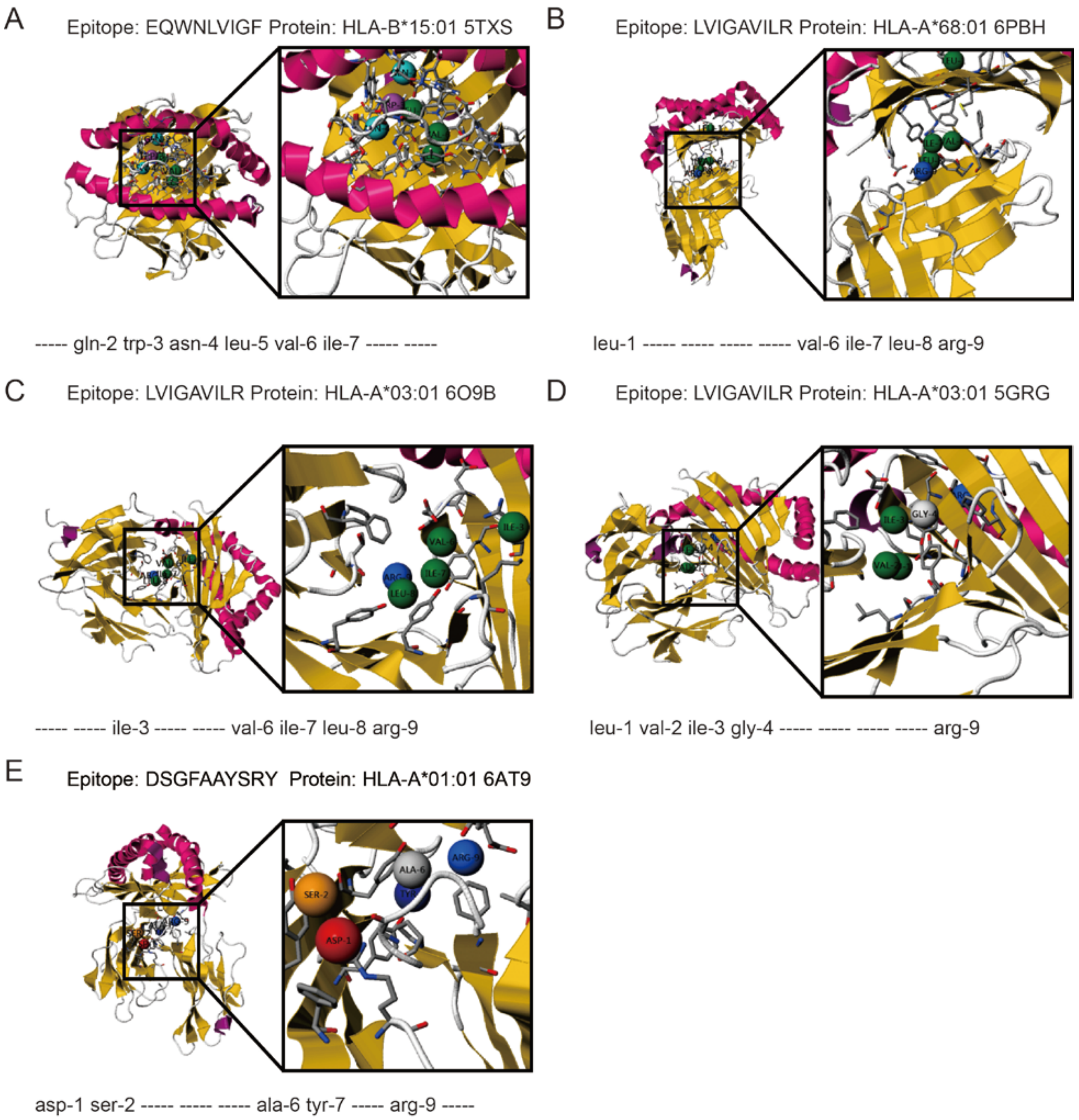
Supplementary Figure 4. Antigenicity estimation of the full-length S protein. (A) The transmembrane protein topology predicted by TMHMM; (B) Antigenicity prediction using Kolaskar and Tongaonkar antigenicity scale; (C) Hydrophilicity prediction using Parker hydrophilicity; (D) Surface accessibility by Emini surface accessibility; (E) Beta turns prediction by Chou and Fasman beta-turn; (F) Flexibility by Karplus and Schulz flexibility.



Supplementary Figure 5. Antigenicity estimation of the full-length M protein. (A) The transmembrane protein topology predicted by TMHMM; (B) Antigenicity prediction using Kolaskar and Tongaonkar antigenicity scale; (C) Hydrophilicity prediction using Parker hydrophilicity; (D) Surface accessibility by Emini surface accessibility; (E) Beta turns prediction by Chou and Fasman beta-turn; (F) Flexibility by Karplus and Schulz flexibility.



Supplementary Figure 6. The score value of discontinuous epitopes predicted by discotope using Chain_A (A), Chain_B (B), and Chain_C (C) of the SARS-CoV-2 S protein.



A Epitope: EQWNLVIGF Protein: HLA-B*15:01 5TXS

----- gln-2 trp-3 asn-4 leu-5 val-6 ile-7 ----- -----

B Epitope: LVIGAVILR Protein: HLA-A*68:01 6PBH

leu-1 ----- ----- ----- ----- val-6 ile-7 leu-8 arg-9

C Epitope: LVIGAVILR Protein: HLA-A*03:01 6O9B

----- ----- ile-3 ----- ----- val-6 ile-7 leu-8 arg-9

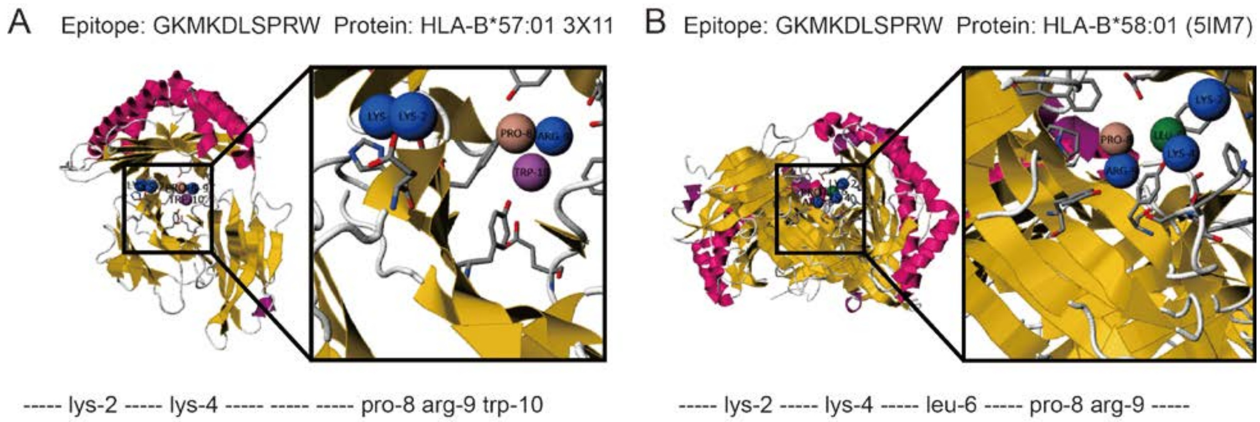
D Epitope: LVIGAVILR Protein: HLA-A*03:01 5GRG

leu-1 val-2 ile-3 gly-4 ----- ----- ----- ----- arg-9

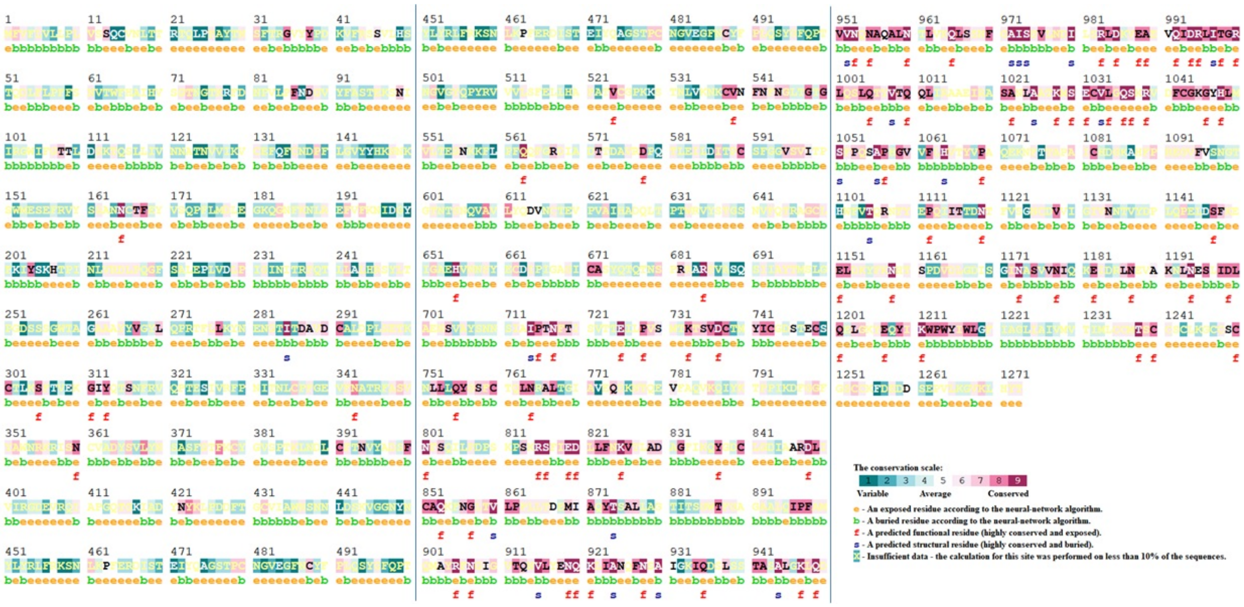
E Epitope: DSGFAAYSRY Protein: HLA-A*01:01 6AT9

asp-1 ser-2 ----- ----- ----- ala-6 tyr-7 ----- arg-9 -----

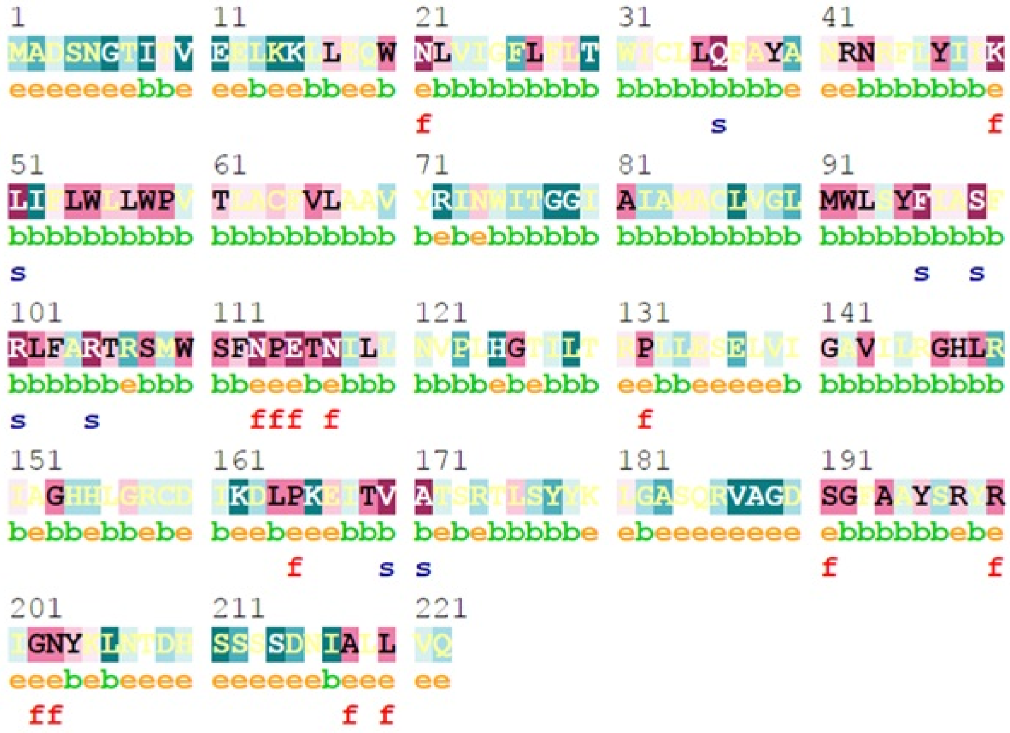
Supplementary Figure 7. The graphical presentation of predicted interactions between MHC class I binding T-cell epitopes from M protein and HLA alleles. ‘EQWNLVIGF’ with HLA-B:*15:01(PDB ID 5TXS) (A), ‘LVIGAVILR’ with HLA-A*68:01 (PDB ID 6PBH) (B), HLA-A*03:01 (PDB ID 6O9B) (C) and HLA-A*03:01 (PDB ID 5GRG) (D), and ‘DSGFAAYSRY’ with HLA-A*01:01(PDB ID 6AT9) (E), respectively.



Supplementary Figure 8. The graphical presentation of predicted interactions between MHC class I binding T-cell epitopes from N protein and HLA alleles. ‘GKMKDLSPRW’ with HLA-B:*57:01(PDB ID 3X11) (A) and HLA-A*58:01 (PDB ID 5IM7) (B), respectively.



Supplementary Figure 9. The conservation status of S protein in the coronaviruses. Seven known coronaviruses includes SARS-CoV-2 (YP_009724390.1), SARS-CoV (NP_828851.1), MERS-CoV (YP_009047204.1), alpha coronavirus 229E (NP_073551.1), alpha coronavirus NL63 (AFV53148.1), beta coronavirus OC43 (YP_009555241.1) and beta coronavirus HKU1 (AAT98580.1).



Legend:

The conservation scale:

e - An exposed residue according to the neural-network algorithm.

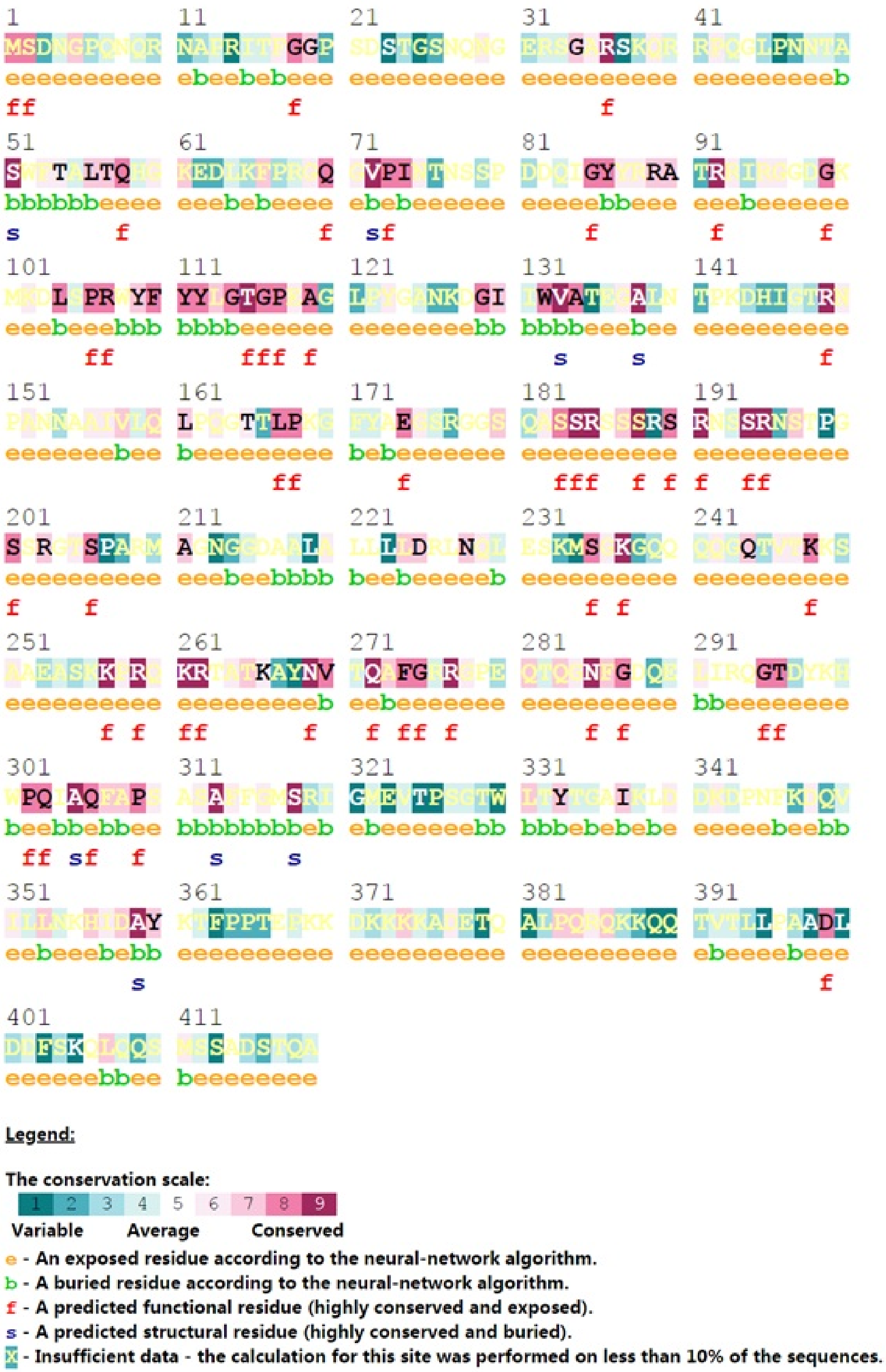
b - A buried residue according to the neural-network algorithm.

f - A predicted functional residue (highly conserved and exposed).

s - A predicted structural residue (highly conserved and buried).

X - Insufficient data - the calculation for this site was performed on less than 10% of the sequences.

Supplementary Figure 10. The conservation status of M protein in the coronaviruses. Seven known coronaviruses includes SARS-CoV-2 (YP_009724390.1), SARS-CoV (NP_828851.1), MERS-CoV (YP_009047204.1), alpha coronavirus 229E (NP_073551.1), alpha coronavirus NL63 (AFV53148.1), beta coronavirus OC43 (YP_009555241.1) and beta coronavirus HKU1 (AAT98580.1).



Supplementary Figure 11. The conservation status of N protein in the coronaviruses. Seven known coronaviruses includes SARS-CoV-2 (YP_009724390.1), SARS-CoV (NP_828851.1), MERS-CoV (YP_009047204.1), alpha coronavirus 229E (NP_073551.1), alpha coronavirus NL63 (AFV53148.1), beta coronavirus OC43 (YP_009555241.1) and beta coronavirus HKU1 (AAT98580.1).

Supplementary Table 1: PhysicoChemical parameters of S, M and N protein computed through ExPASy ProtParam.

S: spike

Parameters	**SARS-CoV-2 S protein**
Mol. Weight	141178.47 Dalton
No. of amino acids	1273
Theoretical *pI*	6.24
Instability index (II)	33.01 (stable)
No. of Negatively Charged Residues (Asp + Glu)	110
No. of Positively Charged Residues (Arg + Lys)	103
Aliphatic Index	84.67
Grand average of Hydropathicity (GRAVY)	-0.079
Atomic Composition	Carbon 6336
	Hydrogen 9770
	Nitrogen 1656
	Oxygen 1894
	Sulfur 54
Amino Acid Composition	Ala (A) 79 6.2%
	Arg (R) 42 3.3%
	Asn (N) 88 6.9%
	Asp (D) 62 4.9%
	Cys (C) 40 3.1%
	Gln (Q) 62 4.9%
	Glu (E) 48 3.8%
	Gly (G) 82 6.4%
	His (H) 17 1.3%
	Ile (I) 76 6.0%
	Leu (L) 108 8.5%
	Lys (K) 61 4.8%
	Met (M) 14 1.1%
	Phe (F) 77 6.0%
	Pro (P) 58 4.6%
	Ser (S) 99 7.8%
	Thr (T) 97 7.6%
	Trp (W) 12 0.9%
	Tyr (Y) 54 4.2%
	Val (V) 97 7.6%
	Pyl (O) 0 0%
	Sec (U) 0 0%

M: membrane_glycoprotein

Parameters		SARS-CoV-2 M protein
Mol. Weight		25146.62
No. of amino acids		222
Theoretical pI		9.51
Instability index (II)		39.14
No. of Negatively Charged Residues (Asp + Glu)		13
No. of Positively Charged Residues (Arg + Lys)		21
Aliphatic Index		120.86
Grand average of Hydropathicity (GRAVY)		0.446
Atomic Composition	Carbon C	1165
	Hydrogen H	1823
	Nitrogen N	303
	Oxygen O	301
	Sulfur S	8
Amino Acid Composition	Ala (A) 19	8.60%
	Arg (R) 14	6.30%
	Asn (N) 11	5.00%
	Asp (D) 6	2.70%
	Cys (C) 4	1.80%
	Gln (Q) 4	1.80%
	Glu (E) 7	3.20%
	Gly (G) 14	6.30%
	His (H) 5	2.30%
	Ile (I) 20	9.00%
	Leu (L) 35	15.80%
	Lys (K) 7	3.20%
	Met (M) 4	1.80%
	Phe (F) 11	5.00%
	Pro (P) 5	2.30%
	Ser (S) 15	6.80%
	Thr (T) 13	5.90%
	Trp (W) 7	3.20%
	Tyr (Y) 9	4.10%
	Val (V) 12	5.40%
	Pyl (O) 0	0.00%
	Sec (U) 0	0.00%

N: nucleocapsid_phosphoprotein

Parameters		**SARS-CoV-2 N protein**
Mol. Weight		45625.7
No. of amino acids		419
Theoretical pI		10.07
Instability index (II)		55.09
No. of Negatively Charged Residues (Asp + Glu)		36
No. of Positively Charged Residues (Arg + Lys)		60
Aliphatic Index		52.53
Grand average of Hydropathicity (GRAVY)		-0.971
Atomic Composition	Carbon C	1971
	Hydrogen H	3137
	Nitrogen N	607
	Oxygen O	629
	Sulfur S	7
Amino Acid Composition	Ala (A) 37	8.80%
	Arg (R) 29	6.90%
	Asn (N) 22	5.30%
	Asp (D) 24	5.70%
	Cys (C) 0	0.00%
	Gln (Q) 35	8.40%
	Glu (E) 12	2.90%
	Gly (G) 43	10.30%
	His (H) 4	1.00%
	Ile (I) 14	3.30%
	Leu (L) 27	6.40%
	Lys (K) 31	7.40%
	Met (M) 7	1.70%
	Phe (F) 13	3.10%
	Pro (P) 28	6.70%
	Ser (S) 37	8.80%
	Thr (T) 32	7.60%
	Trp (W) 5	1.20%
	Tyr (Y) 11	2.60%
	Val (V) 8	1.90%
	Pyl (O) 0	0.00%
	Sec (U) 0	0.00%

Supplementary Table 2: Predicted disulphide bonds within residues of S, M and N protein by DiANNA 1.1.

S protein:

Serial no	positions	peptide bonds	scores
1	15 - 1240	LVSSQCVNLTT - CCMTSCCSCLK	0.9725
2	131 - 391	VVIKVCEFQFC - KLNDLCFTNVY	0.986
3	136 - 662	CEFQFCNDPFL - NNSYECDIPIG	0.9966
4	166 - 1236	SSANNCTFEYV - TIMLCCMTSCC	0.9983
5	291 - 671	TDAVDCALDPL - IGAGICASYQT	0.9094
6	301 - 336	LSETKCTLKSF - NITNLCPFGEV	0.9941
7	361 - 488	KRISNCVADYS - VEGFNCYFPLQ	0.997
8	379 - 743	FSTFKCYGVSP - CTMYICGDSTE	0.9972
9	432 - 1235	DDFTGCVIAWN - VTIMLCCMTSC	0.9988
10	480 - 1248	AGSTPCNGVEG - CLKGCCSCGSC	0.9987
11	525 - 1247	APATVCGPKKS - SCLKGCCSCGS	0.5136
12	538 - 1043	LVKNKCVNFNF - KRVDFCGKGYH	0.9995
13	590 - 617	LDITPCSFGGV - YQDVNCTEVPV	1
14	649 - 1241	QTRAGCLIGAE - CMTSCCSCLKG	0.9997
15	738 - 1243	KTSVDCTMYIC - TSCCSCLKGCC	0.0104
16	749 - 1126	GDSTECSNLLL - FVSGNCDVVIG	0.9914
17	760 - 1250	QYGSFCTQLNR - KGCCSCGSCCK	0.8063
18	840 - 1032	KQYGDCLGDIA - TKMSECVLGQS	0.9756
19	851 - 1254	ARDLICAQKFN - SCGSCCKFDED	0.9996
20	1082 - 1253	TAPAICHDGKA - CSCGSCCKFDE	0.0575

M protein:

Serial No.	Positions	Peptide bonds	Score
1	33 - 64	FLTWICLLQFA-PVTLACFVLAA	0.01039
2	33 - 86	FLTWICLLQFA-AIAMACLVGLM	0.01063
3	33 - 159	FLTWICLLQFA-HHLGRCDIKDL	0.012
4	64 - 86	PVTLACFVLAA-AIAMACLVGLM	0.01037
5	64 - 159	PVTLACFVLAA-HHLGRCDIKDL	0.0107
6	86 - 159	AIAMACLVGLM-HHLGRCDIKDL	0.01043

N protein:

No disulfide bonds are possible for this sequence, the prediction will not be attempted

Supplementary Table 3A. B-cell epitopes predicted by IEDB with antigenicity evaluated by VaxiJen.

start	end	peptide	vaxijen	method	Protein	Peptide Length
21	31	RTQLPPAYTNS	0.871	Bepipred	S	11
71	81	SGTNGTKRFDN	0.5906	Bepipred	S	11
181	186	GKQGNF	2.1342	Bepipred	S	6
249	261	LTPGDSSSGWTAG	0.495	Bepipred	S	13
282	287	NGTITD	1.1184	Bepipred	S	6
318	324	FRVQPTE	1.6729	Bepipred	S	7
407	420	VRQIAPGQTGKIAD	1.2606	Bepipred	S	14
423	428	YKLPDD	-0.9691	Bepipred	S	6
439	447	NNLDSKVGG	0.8904	Bepipred	S	9
473	483	YQAGSTPCNGV	0.0881	Bepipred	S	11
495	506	YGFQPTNGVGYQ	0.7136	Bepipred	S	12
523	532	TVCGPKKSTN	-0.0257	Bepipred	S	10
567	580	RDIADTTDAVRDPQ	0.44	Bepipred	S	14
597	606	VITPGTNTSN	0.4217	Bepipred	S	10
675	687	QTQTNSPRRARSV	0.1763	Bepipred	S	13
772	780	VEQDKNTQE	0.0684	Bepipred	S	9
788	797	IYKTPPIKDF	-0.1626	Bepipred	S	10
805	816	ILPDPSKPSKRS	0.5322	Bepipred	S	12
936	941	DSLSST	0.7417	Bepipred	S	6
1069	1077	PAQEKNFTT	0.382	Bepipred	S	9
1137	1148	VYDPLQPELDSF	0.0903	Bepipred	S	12
1157	1167	KNHTSPDVDLG	1.4039	Bepipred	S	11
1256	1265	FDEDDSEPVL	0.3154	Bepipred	S	10
13	37	SQCVNLTTRTQLPPAYTNSFTRGVY	0.686	Bepipred2.0	S	25
59	81	FSNVTWFHAIHVSGTNGTKRFDN	0.6767	Bepipred2.0	S	23
138	154	DPFLGVYYHKNNKSWME	0.5821	Bepipred2.0	S	17
177	189	MDLEGKQGNFKNL	1.2592	Bepipred2.0	S	13
206	221	KHTPINLVRDLPQGFS	0.6403	Bepipred2.0	S	16
250	260	TPGDSSSGWTA	0.2473	Bepipred2.0	S	11
304	322	KSFTVEKGIYQTSNFRVQP	0.5729	Bepipred2.0	S	19
329	363	FPNITNLCPFGEVFNATRFASVYAWNRKRISNCVA	0.4466	Bepipred2.0	S	35
369	393	YNSASFSTFKCYGVSPTKLNDLCFT	1.4031	Bepipred2.0	S	25
404	426	GDEVRQIAPGQTGKIADYNYKLP	1.1017	Bepipred2.0	S	23
440	501	NLDSKVGGNYNYLYRLFRKSNLKPFERDISTEIYQAGSTPCNGVEGFNCYFPLQSYGFQPTN	0.3951	Bepipred2.0	S	62
516	536	ELLHAPATVCGPKKSTNLVKN	0.0029	Bepipred2.0	S	21
555	562	SNKKFLPF	1.3952	Bepipred2.0	S	8
616	632	NCTEVPVAIHADQLTPT	0.3987	Bepipred2.0	S	17
634	644	RVYSTGSNVFQ	-0.1	Bepipred2.0	S	11
656	666	VNNSYECDIPI	0.6124	Bepipred2.0	S	11
672	690	ASYQTQTNSPRRARSVASQ	0.2556	Bepipred2.0	S	19
695	710	YTMSLGAENSVAYSNN	0.6434	Bepipred2.0	S	16
773	779	EQDKNTQ	0.1017	Bepipred2.0	S	7
786	800	KQIYKTPPIKDFGGF	-0.3896	Bepipred2.0	S	15
807	814	PDPSKPSK	0.0621	Bepipred2.0	S	8
828	842	LADAGFIKQYGDCLG	0.2071	Bepipred2.0	S	15
1035	1043	GQSKRVDFC	1.779	Bepipred2.0	S	9
1107	1118	RNFYEPQIITTD	0.3529	Bepipred2.0	S	12
1133	1172	VNNTVYDPLQPELDSFKEELDKYFKNHTSPDVDLGDISGI	0.1613	Bepipred2.0	S	40
1252	1267	SCCKFDEDDSEPVLKG	0.4347	Bepipred2.0	S	16
4	18	FLVLLPLVSSQCVNL	0.8302	Kolaskar and Tongaonkar antigenicity	S	15
34	41	RGVYYPDK	1.0191	Kolaskar and Tongaonkar antigenicity	S	8
44	51	RSSVLHST	0.5459	Kolaskar and Tongaonkar antigenicity	S	8
53	60	DLFLPFFS	-0.3099	Kolaskar and Tongaonkar antigenicity	S	8
65	70	FHAIHV	1.6766	Kolaskar and Tongaonkar antigenicity	S	6
81	87	NPVLPFN	0.5863	Kolaskar and Tongaonkar antigenicity	S	7
115	121	QSLLIVN	0.8168	Kolaskar and Tongaonkar antigenicity	S	7
125	134	NVVIKVCEFQ	-0.1498	Kolaskar and Tongaonkar antigenicity	S	10
136	146	CNDPFLGVYYH	0.4109	Kolaskar and Tongaonkar antigenicity	S	11
168	174	FEYVSQP	0.9073	Kolaskar and Tongaonkar antigenicity	S	7
210	216	INLVRDL	-0.3198	Kolaskar and Tongaonkar antigenicity	S	7
223	230	LEPLVDLP	-0.3271	Kolaskar and Tongaonkar antigenicity	S	8
239	248	QTLLALHRSY	0.5596	Kolaskar and Tongaonkar antigenicity	S	10
263	270	AAYYVGYL	0.5218	Kolaskar and Tongaonkar antigenicity	S	8
272	278	PRTFLLK	-1.3917	Kolaskar and Tongaonkar antigenicity	S	7
288	295	AVDCALDP	0.773	Kolaskar and Tongaonkar antigenicity	S	8
333	339	TNLCPFG	1.1812	Kolaskar and Tongaonkar antigenicity	S	7
359	371	SNCVADYSVLYNS	-0.1828	Kolaskar and Tongaonkar antigenicity	S	13
376	385	TFKCYGVSPT	1.5059	Kolaskar and Tongaonkar antigenicity	S	10
430	435	TGCVIA	0.4716	Kolaskar and Tongaonkar antigenicity	S	6
488	495	CYFPLQSY	0.9394	Kolaskar and Tongaonkar antigenicity	S	8
505	527	YQPYRVVVLSFELLHAPATVCGP	0.4697	Kolaskar and Tongaonkar antigenicity	S	23
592	599	FGGVSVIT	0.7715	Kolaskar and Tongaonkar antigenicity	S	8
607	615	QVAVLYQDV	0.265	Kolaskar and Tongaonkar antigenicity	S	9
617	627	CTEVPVAIHAD	0.0499	Kolaskar and Tongaonkar antigenicity	S	11
647	653	AGCLIGA	0.1743	Kolaskar and Tongaonkar antigenicity	S	7
667	674	GAGICASY	0.521	Kolaskar and Tongaonkar antigenicity	S	8
687	693	VASQSII	-0.0188	Kolaskar and Tongaonkar antigenicity	S	7
723	730	TTEILPVS	1.2071	Kolaskar and Tongaonkar antigenicity	S	8
735	741	SVDCTMY	1.0932	Kolaskar and Tongaonkar antigenicity	S	7
750	763	SNLLLQYGSFCTQL	0.7599	Kolaskar and Tongaonkar antigenicity	S	14
781	788	VFAQVKQI	0.5854	Kolaskar and Tongaonkar antigenicity	S	8
803	808	SQILPD	-0.1542	Kolaskar and Tongaonkar antigenicity	S	6
837	843	YGDCLGD	-0.5555	Kolaskar and Tongaonkar antigenicity	S	7
847	853	RDLICAQ	1.1443	Kolaskar and Tongaonkar antigenicity	S	7
858	864	LTVLPPL	0.6786	Kolaskar and Tongaonkar antigenicity	S	7
873	880	YTSALLAG	0.3798	Kolaskar and Tongaonkar antigenicity	S	8
959	966	LNTLVKQL	-0.7591	Kolaskar and Tongaonkar antigenicity	S	8
973	979	ISSVLND	0.0414	Kolaskar and Tongaonkar antigenicity	S	7
1002	1011	QSLQTYVTQQ	-0.1009	Kolaskar and Tongaonkar antigenicity	S	10
1030	1037	SECVLGQS	-0.011	Kolaskar and Tongaonkar antigenicity	S	8
1057	1070	PHGVVFLHVTYVPA	0.8058	Kolaskar and Tongaonkar antigenicity	S	14

1079	1085	PAICHDG	-1.01	Kolaskar and Tongaonkar antigenicity	S	7
1123	1132	SGNCDVVIGI	0.7421	Kolaskar and Tongaonkar antigenicity	S	10
1174	1179	ASVVNI	0.8671	Kolaskar and Tongaonkar antigenicity	S	6
1221	1256	IAGLIAIVMVTIMLCCMTSCCSCLKGCCSCGSCCKF	0.143	Kolaskar and Tongaonkar antigenicity	S	36
1262	1270	EPVLKGVKL	1.2301	Kolaskar and Tongaonkar antigenicity	S	9
14	20	QCVNLTT	1.5916	Parker hydrophilicity	S	7
28	33	YTNSFT	-0.7122	Parker hydrophilicity	S	6
47	52	VLHSTQ	0.8948	Parker hydrophilicity	S	6
70	80	VSGTNGTKRFD	0.8493	Parker hydrophilicity	S	11
94	100	STEKSNI	0.6662	Parker hydrophilicity	S	7
109	115	TLDSKTQ	1.2584	Parker hydrophilicity	S	7
145	153	YHKNNKSWM	0.3388	Parker hydrophilicity	S	9
161	167	SSANNCT	-0.4197	Parker hydrophilicity	S	7
180	188	EGKQGNFKN	1.1232	Parker hydrophilicity	S	9
248	263	YLTPGDSSSGWTAGAA	0.465	Parker hydrophilicity	S	16
280	292	NENGTITDAVDCA	0.5014	Parker hydrophilicity	S	13
295	302	PLSETKCT	1.2573	Parker hydrophilicity	S	8
316	325	SNFRVQPTES	1.2078	Parker hydrophilicity	S	10
356	364	KRISNCVAD	0.0005	Parker hydrophilicity	S	9
381	388	GVSPTKLN	1.9197	Parker hydrophilicity	S	8
404	409	GDEVRQ	0.6701	Parker hydrophilicity	S	6
411	425	APGQTGKIADYNYKL	1.4441	Parker hydrophilicity	S	15
437	449	NSNNLDSKVGGNY	0.6657	Parker hydrophilicity	S	13
464	470	FERDIST	-1.2261	Parker hydrophilicity	S	7
472	485	IYQAGSTPCNGVEG	-0.0612	Parker hydrophilicity	S	14
496	507	GFQPTNGVGYQP	0.6299	Parker hydrophilicity	S	12
522	535	ATVCGPKKSTNLVK	0.0422	Parker hydrophilicity	S	14
550	557	GVLTESNK	0.7779	Parker hydrophilicity	S	8
565	581	FGRDIADTTDAVRDPQT	0.0859	Parker hydrophilicity	S	17
599	607	TPGTNTSNQ	0.5029	Parker hydrophilicity	S	9
614	620	DVNCTEV	2.2015	Parker hydrophilicity	S	7
637	647	STGSNVFQTRA	0.502	Parker hydrophilicity	S	11
654	662	EHVNNSYEC	1.068	Parker hydrophilicity	S	9
672	689	ASYQTQTNSPRRARSVAS	0.2963	Parker hydrophilicity	S	18
699	712	LGAENSVAYSNNSI	0.608	Parker hydrophilicity	S	14
731	738	MTKTSVDC	1.5932	Parker hydrophilicity	S	8
743	750	CGDSTECS	0.0977	Parker hydrophilicity	S	8
771	781	AVEQDKNTQEV	0.3969	Parker hydrophilicity	S	11
806	814	LPDPSKPSK	-0.1058	Parker hydrophilicity	S	9
837	842	YGDCLG	-0.4941	Parker hydrophilicity	S	6
926	944	QFNSAIGKIQDSLSSTASA	0.3983	Parker hydrophilicity	S	19
949	958	QDVVNQNAQA	0.2037	Parker hydrophilicity	S	10
966	972	LSSNFGA	0.6114	Parker hydrophilicity	S	7
1033	1046	VLGQSKRVDFCGKG	1.3582	Parker hydrophilicity	S	14
1053	1058	PQSAPH	0.141	Parker hydrophilicity	S	6
1069	1077	PAQEKNFTT	0.382	Parker hydrophilicity	S	9
1081	1091	ICHDGKAHFPR	-0.8542	Parker hydrophilicity	S	11
1114	1128	IITTDNTFVSGNCDV	0.1092	Parker hydrophilicity	S	15
1141	1154	LQPELDSFKEELDK	-0.7047	Parker hydrophilicity	S	14
1156	1168	FKNHTSPDVDLGD	1.0616	Parker hydrophilicity	S	13
1187	1194	NEVAKNLN	-0.0646	Parker hydrophilicity	S	8
1238	1264	TSCCSCLKGCCSCGSCCKFDEDDSEPV	0.1337	Parker hydrophilicity	S	27
18	32	LTTRTQLPPAYTNSF	0.79	Emini surface accessibility	S	15
35	43	GVYYPDKVF	0.0652	Emini surface accessibility	S	9
73	80	TNGTKRFD	0.2041	Emini surface accessibility	S	8
110	115	LDSKTQ	1.3071	Emini surface accessibility	S	6
144	153	YYHKNNKSWM	0.3777	Emini surface accessibility	S	10
179	185	LEGKQGN	1.8367	Emini surface accessibility	S	7
202	208	KIYSKHT	0.7773	Emini surface accessibility	S	7
250	255	TPGDSS	0.3268	Emini surface accessibility	S	6
278	284	KYNENGT	0.9414	Emini surface accessibility	S	7
314	323	QTSNFRVQPT	1.405	Emini surface accessibility	S	10
352	357	AWNRKR	1.632	Emini surface accessibility	S	6
419	428	ADYNYKLPDD	0.6956	Emini surface accessibility	S	10
437	442	NSNNLD	1.1859	Emini surface accessibility	S	6
455	468	LFRKSNLKPFERDI	0.361	Emini surface accessibility	S	14
495	500	YGFQPT	1.6231	Emini surface accessibility	S	6
569	581	IADTTDAVRDPQT	0.3018	Emini surface accessibility	S	13
601	606	GTNTSN	1.2831	Emini surface accessibility	S	6
627	636	DQLTPTWRVY	0.6489	Emini surface accessibility	S	10
655	660	HVNNSY	1.0629	Emini surface accessibility	S	6
674	685	YQTQTNSPRRAR	0.076	Emini surface accessibility	S	12
773	779	EQDKNTQ	0.1017	Emini surface accessibility	S	7
786	794	KQIYKTPPI	0.2705	Emini surface accessibility	S	9
808	817	DPSKPSKRSF	0.8148	Emini surface accessibility	S	10
914	920	NVLYENQ	0.4689	Emini surface accessibility	S	7
1068	1076	VPAQEKNFT	1.0107	Emini surface accessibility	S	9
1105	1111	TQRNFYE	0.219	Emini surface accessibility	S	7
1139	1162	DPLQPELDSFKEELDKYFKNHTSP	-0.3378	Emini surface accessibility	S	24
1179	1186	IQKEIDRL	-1.0253	Emini surface accessibility	S	8
1202	1210	ELGKYEQYI	0.5415	Emini surface accessibility	S	9
1256	1261	FDEDDS	-0.0685	Emini surface accessibility	S	6
23	34	QLPPAYTNSFTR	-0.0689	Chou and Fasman beta turn	S	12
36	43	VYYPDKVF	0.0301	Chou and Fasman beta turn	S	8
71	91	SGTNGTKRFDNPVLPFNDGVY	0.3544	Chou and Fasman beta turn	S	21
109	115	TLDSKTQ	1.2584	Chou and Fasman beta turn	S	7
135	142	FCNDPFLG	0.1982	Chou and Fasman beta turn	S	8
145	152	YHKNNKSW	0.4099	Chou and Fasman beta turn	S	8
161	167	SSANNCT	-0.4197	Chou and Fasman beta turn	S	7
181	188	GKQGNFKN	1.0999	Chou and Fasman beta turn	S	8
248	260	YLTPGDSSSGWTA	0.627	Chou and Fasman beta turn	S	13
279	285	YNENGTI	0.508	Chou and Fasman beta turn	S	7
292	298	ALDPLSE	0.5276	Chou and Fasman beta turn	S	7

313	320	YQTSNFRV	0.371	Chou and Fasman beta turn	S	8
367	374	VLYNSASF	0.1765	Chou and Fasman beta turn	S	8
380	389	YGVSPTKLND	1.4531	Chou and Fasman beta turn	S	10
411	430	APGQTGKIADYNYKLPDDFT	1.0425	Chou and Fasman beta turn	S	20
436	452	WNSNNLDSKVGGNYNYL	0.8074	Chou and Fasman beta turn	S	17
474	507	QAGSTPCNGVEGFNCYFPLQSYGFQPTNGVGYQP	0.5024	Chou and Fasman beta turn	S	34
523	535	TVCGPKKSTNLVK	0.0426	Chou and Fasman beta turn	S	13
537	548	KCVNFNFNGLTG	1.6969	Chou and Fasman beta turn	S	12
588	594	TPCSFGG	1.6632	Chou and Fasman beta turn	S	7
599	606	TPGTNTSN	0.5249	Chou and Fasman beta turn	S	8
636	643	YSTGSNVF	-0.1992	Chou and Fasman beta turn	S	8
655	666	HVNNSYECDIPI	0.6752	Chou and Fasman beta turn	S	12
674	683	YQTQTNSPRR	-0.2647	Chou and Fasman beta turn	S	10
705	714	VAYSNNSIAI	1.0545	Chou and Fasman beta turn	S	10
740	750	MYICGDSTECS	-0.3346	Chou and Fasman beta turn	S	11
789	802	YKTPPIKDFGGFNF	0.2117	Chou and Fasman beta turn	S	14
804	815	QILPDPSKPSKR	0.2594	Chou and Fasman beta turn	S	12
835	842	KQYGDCLG	0.4129	Chou and Fasman beta turn	S	8
926	931	QFNSAI	-0.1194	Chou and Fasman beta turn	S	6
934	943	IQDSLSSTAS	0.4491	Chou and Fasman beta turn	S	10
966	972	LSSNFGA	0.6114	Chou and Fasman beta turn	S	7
1033	1038	VLGQSK	1.2255	Chou and Fasman beta turn	S	6
1040	1048	VDFCGKGYH	0.375	Chou and Fasman beta turn	S	9
1052	1058	FPQSAPH	-0.3069	Chou and Fasman beta turn	S	7
1082	1088	CHDGKAH	-0.2298	Chou and Fasman beta turn	S	7
1096	1101	VSNGTH	0.7888	Chou and Fasman beta turn	S	6
1119	1128	NTFVSGNCDV	-0.5646	Chou and Fasman beta turn	S	10
1136	1146	TVYDPLQPELD	0.3454	Chou and Fasman beta turn	S	11
1155	1173	YFKNHTSPDVDLGDISGIN	0.88	Chou and Fasman beta turn	S	19
1237	1264	MTSCCSCLKGCCSCGSCCKFDEDDSEPV	0.1043	Chou and Fasman beta turn	S	28
19	34	TTRTQLPPAYTNSFTR	0.3477	Karplus and Schulz flexibility	S	16
39	47	PDKVFRSSV	-0.7314	Karplus and Schulz flexibility	S	9
49	54	HSTQDL	0.4956	Karplus and Schulz flexibility	S	6
71	83	SGTNGTKRFDNPV	0.3648	Karplus and Schulz flexibility	S	13
94	99	STEKSN	1.0006	Karplus and Schulz flexibility	S	6
108	116	TTLDSKTQS	1.0106	Karplus and Schulz flexibility	S	9
147	152	KNNKSW	0.4346	Karplus and Schulz flexibility	S	6
180	190	EGKQGNFKNLR	1.0042	Karplus and Schulz flexibility	S	11
205	210	SKHTPI	0.7317	Karplus and Schulz flexibility	S	6
214	220	RDLPQGF	1.1398	Karplus and Schulz flexibility	S	7
248	258	YLTPGDSSSGW	0.624	Karplus and Schulz flexibility	S	11
279	287	YNENGTITD	0.765	Karplus and Schulz flexibility	S	9
294	305	DPLSETKCTLKS	0.9204	Karplus and Schulz flexibility	S	12
383	389	SPTKLND	0.839	Karplus and Schulz flexibility	S	7
403	408	RGDEVR	-2.2527	Karplus and Schulz flexibility	S	6
411	417	APGQTGK	1.7614	Karplus and Schulz flexibility	S	7
424	430	KLPDDFT	-0.051	Karplus and Schulz flexibility	S	7
437	448	NSNNLDSKVGGN	0.6962	Karplus and Schulz flexibility	S	12
457	471	RKSNLKPFERDISTE	0.4847	Karplus and Schulz flexibility	S	15
475	484	AGSTPCNGVE	0.0244	Karplus and Schulz flexibility	S	10
498	503	QPTNGV	0.0716	Karplus and Schulz flexibility	S	6
526	537	GPKKSTNLVKNK	0.4692	Karplus and Schulz flexibility	S	12
545	558	GLTGTGVLTESNKK	1.0227	Karplus and Schulz flexibility	S	14
564	582	QFGRDIADTTDAVRDPQTL	0.1344	Karplus and Schulz flexibility	S	19
599	607	TPGTNTSNQ	0.5029	Karplus and Schulz flexibility	S	9
614	619	DVNCTE	2.375	Karplus and Schulz flexibility	S	6
627	632	DQLTPT	0.7329	Karplus and Schulz flexibility	S	6
637	642	STGSNV	0.3608	Karplus and Schulz flexibility	S	6
675	691	QTQTNSPRRARSVASQS	0.1698	Karplus and Schulz flexibility	S	17
744	750	GDSTECS	0.111	Karplus and Schulz flexibility	S	7
773	780	EQDKNTQE	0.0364	Karplus and Schulz flexibility	S	8
789	798	YKTPPIKDFG	0.02	Karplus and Schulz flexibility	S	10
806	816	LPDPSKPSKRS	0.5972	Karplus and Schulz flexibility	S	11
836	841	QYGDCL	0.1281	Karplus and Schulz flexibility	S	6
880	885	GTITSG	-0.0576	Karplus and Schulz flexibility	S	6
932	943	GKIQDSLSSTAS	0.5659	Karplus and Schulz flexibility	S	12
946	956	GKLQDVVNQNA	0.3966	Karplus and Schulz flexibility	S	11
961	969	TLVKQLSSN	-0.5178	Karplus and Schulz flexibility	S	9
982	988	SRLDKVE	0.0966	Karplus and Schulz flexibility	S	7
994	1011	DRLITGRLQSLQTYVTQQ	-0.2656	Karplus and Schulz flexibility	S	18
1034	1039	LGQSKR	2.0011	Karplus and Schulz flexibility	S	6
1070	1078	AQEKNFTTA	0.7576	Karplus and Schulz flexibility	S	9
1116	1125	TTDNTFVSGN	0.3035	Karplus and Schulz flexibility	S	10
1134	1172	NNTVYDPLQPELDSFKEELDKYFKNHTSPDVDLGDISGI	0.1406	Karplus and Schulz flexibility	S	39
1179	1187	IQKEIDRLN	-0.4173	Karplus and Schulz flexibility	S	9
1191	1196	KNLNES	0.863	Karplus and Schulz flexibility	S	6
1202	1207	ELGKYE	0.4595	Karplus and Schulz flexibility	S	6
1256	1269	FDEDDSEPVLKGVK	0.6734	Karplus and Schulz flexibility	S	14
1	8	MADSNGTI	0.0793	Bepipred	M	8
185	194	QRVAGDSGFA	0.198	Bepipred	M	10
206	215	LNTDHSSSSD	0.2535	Bepipred	M	10
4	19	NGTITVEELKKLLEQW	-0.1969	Bepipred2	M	16
131	136	PLLESE	0.8069	Bepipred2	M	6
179	190	KLGASQRVAGDS	0.0439	Bepipred2	M	12
198	217	YRIGNYKLNTDHSSSSDNIA	0.2216	Bepipred2	M	20
39	44	YANRNR	0.342	Chou	M	6
107	118	RSMWSFNPETNI	0.5882	Chou	M	12
154	166	HHLGRCDIKDLPK	0.3852	Chou	M	13
174	217	RTLSYYKLGASQRVAGDSGFAAYSRYRIGNYKLNTDHSSSSDNI	0.3707	Chou	M	44
11	20	EELKKLLEQW	-1.3465	Emini	M	10
38	44	AYANRNR	0.674	Emini	M	7
103	109	FARTRSM	0.5616	Emini	M	7
162	167	KDLPKE	-1.1446	Emini	M	6

171	188	ATSRTLSYYKLGASQRVA	0.6107	Emini	M	18
195	202	AYSRYRIG	0.5894	Emini	M	8
204	215	YKLNTDHSSSSD	0.0168	Emini	M	12
4	19	SNGTITVEELKKLLEQ	0.0264	Karplus	M	16
124	138	LHGTILTRPLLESEL	0.1462	Karplus	M	15
157	176	GRCDIKDLPKEITVATSRTL	0.6445	Karplus	M	20
180	193	KLGASQRVAGDSGF	0.3608	Karplus	M	14
197	216	SRYRIGNYKLNTDHSSSSDN	0.1004	Karplus	M	20
29	38	LTWICLLQFA	1.0412	Kolaskar	M	10
46	71	LYIIKLIFLWLLWPVTLACFVLAAVY	0.7033	Kolaskar	M	26
83	91	AMACLVGLM	0.6251	Kolaskar	M	9
93	101	LSYFIASFR	0.3283	Kolaskar	M	9
135	148	ESELVIGAVILRGH	0.6733	Kolaskar	M	14
4	18	SNGTITVEELKKLLE	0.1513	Parker	M	15
38	44	AYANRNR	0.674	Parker	M	7
104	116	ARTRSMWSFNPET	1.0549	Parker	M	13
149	177	LRIAGHHLGRCDIKDLPKEITVATSRTLS	0.3861	Parker	M	29
180	217	KLGASQRVAGDSGFAAYSRYRIGNYKLNTDHSSSSDNI	0.3675	Parker	M	38

Supplementary Table 3B. B-cell epitopes predicted by BCEPRED with antigenicity evaluated by VaxiJen.

start	end	peptide	vaxijen	method	Protein	Peptide Length
17	47	NLTTRTQLPPAYTNSFTRGVYYPDKVFRSS	0.3475	Accessibility	S	31
71	84	SGTNGTKRFDNPV	0.3648	Accessibility	S	14
91	103	YFASTEKSNIIR	-0.0942	Accessibility	S	13
108	118	TTLDSKTQSL	0.99	Accessibility	S	11
142	161	GVYYHKNNKSWMESEFRVY	0.4302	Accessibility	S	20
177	193	MDLEGKQGNFKNLREF	0.8263	Accessibility	S	17
200	212	YFKIYSKHTPIN	0.7893	Accessibility	S	13
268	285	GYLQPRTFLLKYNENGT	0.4239	Accessibility	S	18
294	326	DPLSETKCTLKSFTVEKGIYQTSNFRVQPTES	0.6225	Accessibility	S	33
350	362	VYAWNRKRISNC	0.3253	Accessibility	S	13
383	391	SPTKLNDL	1.0358	Accessibility	S	9
417	431	KIADYNYKLPDDFT	0.9567	Accessibility	S	15
437	446	NSNNLDSKV	0.6019	Accessibility	S	10
447	472	GNYNYLYRLFRKSNLKPFERDISTE	0.1595	Accessibility	S	26
503	512	VGYQPYRVV	1.4383	Accessibility	S	10
525	538	CGPKKSTNLVKNK	0.1411	Accessibility	S	14
552	562	LTESNKKFLP	0.6681	Accessibility	S	11
573	584	TDAVRDPQTLE	0.2349	Accessibility	S	12
599	609	TPGTNTSNQV	0.4224	Accessibility	S	11
654	664	EHVNNSYECD	0.827	Accessibility	S	11
672	689	ASYQTQTNSPRRARSVA	0.3628	Accessibility	S	18
771	783	AVEQDKNTQEVF	0.2192	Accessibility	S	13
806	821	LPDPSKPSKRSFIED	0.0476	Accessibility	S	16
913	924	QNVLYENQKLI	0.2774	Accessibility	S	12
982	990	SRLDKVEA	0.1615	Accessibility	S	9
1000	1012	RLQSLQTYVTQQ	0.1103	Accessibility	S	13
1035	1043	GQSKRVDF	1.9298	Accessibility	S	9
1067	1080	YVPAQEKNFTTAP	0.6578	Accessibility	S	14
1104	1114	VTQRNFYEPQ	0.6509	Accessibility	S	11
1134	1164	NNTVYDPLQPELDSFKEELDKYFKNHTSPD	-0.2097	Accessibility	S	31
1178	1198	NIQKEIDRLNEVAKNLNESL	-0.0099	Accessibility	S	21
1201	1214	QELGKYEQYIKWP	0.3709	Accessibility	S	14
1254	1265	CKFDEDDSEPV	0.2159	Accessibility	S	12
1	21	MFVFLVLLPLVSSQCVNLTT	0.8317	Antigenic_Propensity	S	21
36	63	VYYPDKVFRSSVLHSTQDLFLPFFSNV	0.0327	Antigenic_Propensity	S	28
114	122	TQSLLIVN	0.6517	Antigenic_Propensity	S	9
124	148	TNVVIKVCEFQFCNDPFLGVYYHK	0.072	Antigenic_Propensity	S	25
166	178	CTFEYVSQPFLM	0.2955	Antigenic_Propensity	S	13
207	219	HTPINLVRDLPQ	-0.1335	Antigenic_Propensity	S	13
223	234	LEPLVDLPIGI	0.8222	Antigenic_Propensity	S	12
265	274	YYVGYLQPR	1.4692	Antigenic_Propensity	S	10
332	343	ITNLCPFGEVF	0.3094	Antigenic_Propensity	S	12
364	372	DYSVLYNS	0.1757	Antigenic_Propensity	S	9
374	386	FSTFKCYGVSPT	0.8097	Antigenic_Propensity	S	13
389	397	DLCFTNVY	1.8569	Antigenic_Propensity	S	9
449	458	YNYLYRLFR	-0.8692	Antigenic_Propensity	S	10
486	496	FNCYFPLQSY	0.8219	Antigenic_Propensity	S	11
505	520	YQPYRVVVLSFELLH	0.9711	Antigenic_Propensity	S	16
584	602	ILDITPCSFGGVSVITPG	1.1031	Antigenic_Propensity	S	19
610	623	VLYQDVNCTEVPV	0.619	Antigenic_Propensity	S	14
736	745	VDCTMYICG	-0.7197	Antigenic_Propensity	S	10
748	761	ECSNLLLQYGSFC	0.8661	Antigenic_Propensity	S	14
857	868	GLTVLPPLLTD	0.5484	Antigenic_Propensity	S	12
946	955	GKLQDVVNQ	0.3499	Antigenic_Propensity	S	10
961	969	TLVKQLSS	-0.4822	Antigenic_Propensity	S	9
975	983	SVLNDILS	-0.6172	Antigenic_Propensity	S	9
1001	1014	LQSLQTYVTQQLI	-0.1517	Antigenic_Propensity	S	14
1028	1039	KMSECVLGQSK	0.1391	Antigenic_Propensity	S	12
1057	1070	PHGVVFLHVTYVP	0.9305	Antigenic_Propensity	S	14
1122	1135	VSGNCDVVIGIVN	0.7251	Antigenic_Propensity	S	14
1136	1144	TVYDPLQP	0.3135	Antigenic_Propensity	S	9
1227	1257	IVMVTIMLCCMTSCCSCLKGCCSCGSCCKF	0.0464	Antigenic_Propensity	S	31
1262	1274	EPVLKGVKLHYT	1.4118	Antigenic_Propensity	S	13
144	154	YYHKNNKSWM	0.3777	Exposed_Surface	S	11
351	361	YAWNRKRISN	0.5855	Exposed_Surface	S	11
456	464	FRKSNLKP	1.1111	Exposed_Surface	S	9
526	534	GPKKSTNL	0.7072	Exposed_Surface	S	9
552	560	LTESNKKF	0.7708	Exposed_Surface	S	9
677	686	QTNSPRRAR	-0.118	Exposed_Surface	S	10
772	782	VEQDKNTQEV	0.2465	Exposed_Surface	S	11
784	797	QVKQIYKTPPIKD	0.3607	Exposed_Surface	S	14
808	818	DPSKPSKRSF	0.8148	Exposed_Surface	S	11
1148	1161	FKEELDKYFKNHT	-0.967	Exposed_Surface	S	14

1179	1187	IQKEIDRL	-1.0253	Exposed_Surface	S	9
68	77	IHVSGTNGT	0.8621	Flexibility	S	10
90	98	VYFASTEK	0.9206	Flexibility	S	9
108	116	TTLDSKTQ	1.0912	Flexibility	S	9
247	256	SYLTPGDSS	0.7324	Flexibility	S	10
351	359	YAWNRKRI	0.7206	Flexibility	S	9
439	447	NNLDSKVG	1.2952	Flexibility	S	9
454	462	RLFRKSNL	0.2128	Flexibility	S	9
522	532	ATVCGPKKST	-0.1151	Flexibility	S	11
550	558	GVLTESNK	0.7779	Flexibility	S	9
597	606	VITPGTNTS	0.2753	Flexibility	S	10
672	685	ASYQTQTNSPRRA	0.107	Flexibility	S	14
742	750	ICGDSTEC	-0.2546	Flexibility	S	9
770	779	IAVEQDKNT	0.4823	Flexibility	S	10
804	816	QILPDPSKPSKR	0.2594	Flexibility	S	13
932	940	GKIQDSLS	0.2746	Flexibility	S	9
1031	1040	ECVLGQSKR	0.9377	Flexibility	S	10
1254	1262	CKFDEDDS	-0.1581	Flexibility	S	9
70	79	VSGTNGTKR	0.9855	Hydrophilicity	S	10
250	258	TPGDSSSG	0.0924	Hydrophilicity	S	9
278	288	KYNENGTITD	0.9589	Hydrophilicity	S	11
437	449	NSNNLDSKVGGN	0.6962	Hydrophilicity	S	13
525	533	CGPKKSTN	-0.2855	Hydrophilicity	S	9
568	579	DIADTTDAVRD	0.8257	Hydrophilicity	S	12
673	685	SYQTQTNSPRRA	0.0145	Hydrophilicity	S	13
743	752	CGDSTECSN	0.1786	Hydrophilicity	S	10
771	782	AVEQDKNTQEV	0.3969	Hydrophilicity	S	12
807	817	PDPSKPSKRS	0.8374	Hydrophilicity	S	11
1157	1166	KNHTSPDVD	0.7809	Hydrophilicity	S	10
144	161	YYHKNNKSWMESEFRVY	0.3439	Polarity	S	18
185	197	NFKNLREFVFKN	0.1722	Polarity	S	13
201	209	FKIYSKHT	1.1661	Polarity	S	9
298	311	ETKCTLKSFTVEK	0.5711	Polarity	S	14
351	362	YAWNRKRISNC	0.4749	Polarity	S	12
402	410	IRGDEVRQ	-0.6918	Polarity	S	9
452	472	LYRLFRKSNLKPFERDISTE	-0.0464	Polarity	S	21
552	561	LTESNKKFL	0.3167	Polarity	S	10
679	689	NSPRRARSVA	0.2502	Polarity	S	11
809	821	PSKPSKRSFIED	0.3363	Polarity	S	13
982	993	SRLDKVEAEVQ	0.3878	Polarity	S	12
1013	1021	IRAAEIRA	0.2791	Polarity	S	9
1082	1095	CHDGKAHFPREGV	-0.4141	Polarity	S	14
1144	1161	ELDSFKEELDKYFKNHT	-0.8623	Polarity	S	18
1179	1192	IQKEIDRLNEVAK	-0.1773	Polarity	S	14
1201	1212	QELGKYEQYIK	0.2086	Polarity	S	12
1253	1265	CCKFDEDDSEPV	0.4603	Polarity	S	13
134	142	QFCNDPFL	-0.243	Turns	S	9
145	153	YHKNNKSW	0.4099	Turns	S	9
160	169	YSSANNCTF	-0.1036	Turns	S	10
435	445	AWNSNNLDSK	1.0198	Turns	S	11
538	547	CVNFNFNGL	1.7985	Turns	S	10
601	609	GTNTSNQV	0.7179	Turns	S	9
653	662	AEHVNNSYE	0.8405	Turns	S	10
706	714	AYSNNSIA	0.5473	Turns	S	9
1156	1164	FKNHTSPD	0.5003	Turns	S	9
9	20	TVEELKKLLEQW	-0.7598	Accessibility	M	12
38	47	AYANRNRFLY	0.1565	Accessibility	M	10
101	117	RLFARTRSMWSFNPETN	0.5366	Accessibility	M	17
131	137	RPLLESE	0.1952	Accessibility	M	7
160	169	DIKDLPKEIT	0.7112	Accessibility	M	10
172	186	TSRTLSYYKLGASQR	0.7675	Accessibility	M	15
194	216	AAYSRYRIGNYKLNTDHSSSSDN	0.2438	Accessibility	M	23
21	37	NLVIGFLFLTWICLLQF	1.0402	Antigenic	M	17
44	62	RFLYIIKLIFLWLLWPVTL	0.5893	Antigenic	M	19
86	93	CLVGLMWL	0.8376	Antigenic	M	8
117	140	NILLNVPLHGTILTRPLLESELVI	-0.0316	Antigenic	M	24
143	149	VILRGHL	-0.2078	Antigenic	M	7
175	182	TLSYYKLG	0.9387	Antigenic	M	8
9	15	TVEELKK	0.2727	Exposed	M	7
160	168	DIKDLPKEI	0.5528	Exposed	M	9
169	175	TVATSRT	0.7772	Flexibility	M	7
204	215	YKLNTDHSSSSD	0.0168	Flexibility	M	12
1	9	MADSNGTIT	0.4187	Hydrophilicity	M	9
207	217	NTDHSSSSDNI	0.3291	Hydrophilicity	M	11
9	20	TVEELKKLLEQW	-0.7598	Polarity	M	12

101	107	RLFARTR	0.2275	Polarity	M	7
131	137	RPLLESE	0.1952	Polarity	M	7
144	168	ILRGHLRIAGHHLGRCDIKDLPKEI	0.1626	Polarity	M	25
205	218	KLNTDHSSSSDNIA	0.06	Turns	M	14

Supplementary Table 3C. B-cell epitopes predicted by both IEDB and BCEPRED with antigenicity evaluated by VaxiJen > 0.9.

start	end	peptide	vaxijen	method	server	Protein	Peptide Length	RBD	Topology	Allergenicity	Toxicity
108	117	TTLDSKTQSL	0.99	Accessibility	BcePred	S	10	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
383	390	SPTKLNDL	1.0358	Accessibility	BcePred	S	8	RBD	Outside	Non-Toxin	ALLERGEN
417	430	KIADYNYKLPDDFT	0.9567	Accessibility	BcePred	S	14	RBD	Outside	Non-Toxin	NON-ALLERGEN
503	511	VGYQPYRVV	1.4383	Accessibility	BcePred	S	9	RBD	Outside	Non-Toxin	ALLERGEN
1035	1042	GQSKRVDF	1.9298	Accessibility	BcePred	S	8	nonRBD	Outside	Non-Toxin	ALLERGEN
21	37	NLVIGFLFLTWICLLQF	1.0402	Antigenic	BcePred	M	17	NA	Transmembrane	Toxin	NON-ALLERGEN
175	182	TLSYYKLG	0.9387	Antigenic	BcePred	M	8	NA	Inside	Non-Toxin	ALLERGEN
265	273	YYVGYLQPR	1.4692	Antigenic_Propensity	BcePred	S	9	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
389	396	DLCFTNVY	1.8569	Antigenic_Propensity	BcePred	S	8	RBD	Outside	Non-Toxin	ALLERGEN
505	519	YQPYRVVVLSFELLH	0.9711	Antigenic_Propensity	BcePred	S	15	RBD	Outside	Non-Toxin	NON-ALLERGEN
584	601	ILDITPCSFGGVSVITPG	1.1031	Antigenic_Propensity	BcePred	S	18	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
1057	1069	PHGVVFLHVTYVP	0.9305	Antigenic_Propensity	BcePred	S	13	nonRBD	Outside	Non-Toxin	ALLERGEN
1262	1273	EPVLKGVKLHYT	1.4118	Antigenic_Propensity	BcePred	S	12	nonRBD	Inside	Non-Toxin	NON-ALLERGEN
181	186	GKQGNF	2.1342	Bepipred	IEDB	S	6	nonRBD	Outside	Non-Toxin	ALLERGEN
282	287	NGTITD	1.1184	Bepipred	IEDB	S	6	nonRBD	Outside	Non-Toxin	ALLERGEN
318	324	FRVQPTE	1.6729	Bepipred	IEDB	S	7	RBD	Outside	Non-Toxin	ALLERGEN
407	420	VRQIAPGQTGKIAD	1.2606	Bepipred	IEDB	S	14	RBD	Outside	Non-Toxin	NON-ALLERGEN
1157	1167	KNHTSPDVDLG	1.4039	Bepipred	IEDB	S	11	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
177	189	MDLEGKQGNFKNL	1.2592	Bepipred2.0	IEDB	S	13	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
369	393	YNSASFSTFKCYGVSPTKLNDLCFT	1.4031	Bepipred2.0	IEDB	S	25	RBD	Outside	Non-Toxin	NON-ALLERGEN
404	426	GDEVRQIAPGQTGKIADYNYKLP	1.1017	Bepipred2.0	IEDB	S	23	RBD	Outside	Non-Toxin	NON-ALLERGEN
555	562	SNKKFLPF	1.3952	Bepipred2.0	IEDB	S	8	nonRBD	Outside	Non-Toxin	ALLERGEN
1035	1043	GQSKRVDFC	1.779	Bepipred2.0	IEDB	S	9	nonRBD	Outside	Non-Toxin	ALLERGEN
109	115	TLDSKTQ	1.2584	Chou and Fasman beta turn	IEDB	S	7	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
181	188	GKQGNFKN	1.0999	Chou and Fasman beta turn	IEDB	S	8	nonRBD	Outside	Non-Toxin	ALLERGEN
380	389	YGVSPTKLND	1.4531	Chou and Fasman beta turn	IEDB	S	10	RBD	Outside	Non-Toxin	NON-ALLERGEN
411	430	APGQTGKIADYNYKLPDDFT	1.0425	Chou and Fasman beta turn	IEDB	S	20	RBD	Outside	Non-Toxin	NON-ALLERGEN
537	548	KCVNFNFNGLTG	1.6969	Chou and Fasman beta turn	IEDB	S	12	RBD	Outside	Non-Toxin	NON-ALLERGEN
588	594	TPCSFGG	1.6632	Chou and Fasman beta turn	IEDB	S	7	nonRBD	Outside	Non-Toxin	ALLERGEN
705	714	VAYSNNSIAI	1.0545	Chou and Fasman beta turn	IEDB	S	10	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
1033	1038	VLGQSK	1.2255	Chou and Fasman beta turn	IEDB	S	6	nonRBD	Outside	Non-Toxin	ALLERGEN
110	115	LDSKTQ	1.3071	Emini surface accessibility	IEDB	S	6	nonRBD	Outside	Non-Toxin	ALLERGEN
179	185	LEGKQGN	1.8367	Emini surface accessibility	IEDB	S	7	nonRBD	Outside	Non-Toxin	ALLERGEN
278	284	KYNENGT	0.9414	Emini surface accessibility	IEDB	S	7	nonRBD	Outside	Non-Toxin	ALLERGEN
314	323	QTSNFRVQPT	1.405	Emini surface accessibility	IEDB	S	10	RBD	Outside	Non-Toxin	ALLERGEN
352	357	AWNRKR	1.632	Emini surface accessibility	IEDB	S	6	RBD	Outside	Non-Toxin	ALLERGEN
437	442	NSNNLD	1.1859	Emini surface accessibility	IEDB	S	6	RBD	Outside	Non-Toxin	ALLERGEN
495	500	YGFQPT	1.6231	Emini surface accessibility	IEDB	S	6	RBD	Outside	Non-Toxin	ALLERGEN
601	606	GTNTSN	1.2831	Emini surface accessibility	IEDB	S	6	nonRBD	Outside	Non-Toxin	ALLERGEN
655	660	HVNNSY	1.0629	Emini surface accessibility	IEDB	S	6	nonRBD	Outside	Non-Toxin	ALLERGEN
1068	1076	VPAQEKNFT	1.0107	Emini surface accessibility	IEDB	S	9	nonRBD	Outside	Non-Toxin	ALLERGEN
456	463	FRKSNLKP	1.1111	Exposed_Surface	BcePred	S	8	RBD	Outside	Non-Toxin	ALLERGEN
90	97	VYFASTEK	0.9206	Flexibility	BcePred	S	8	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
108	115	TTLDSKTQ	1.0912	Flexibility	BcePred	S	8	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
439	446	NNLDSKVG	1.2952	Flexibility	BcePred	S	8	RBD	Outside	Non-Toxin	ALLERGEN
1031	1039	ECVLGQSKR	0.9377	Flexibility	BcePred	S	9	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
70	78	VSGTNGTKR	0.9855	Hydrophilicity	BcePred	S	9	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
278	287	KYNENGTITD	0.9589	Hydrophilicity	BcePred	S	10	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
94	99	STEKSN	1.0006	Karplus and Schulz flexibility	IEDB	S	6	nonRBD	Outside	Non-Toxin	ALLERGEN
108	116	TTLDSKTQS	1.0106	Karplus and Schulz flexibility	IEDB	S	9	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
180	190	EGKQGNFKNLR	1.0042	Karplus and Schulz flexibility	IEDB	S	11	nonRBD	Outside	Non-Toxin	ALLERGEN
214	220	RDLPQGF	1.1398	Karplus and Schulz flexibility	IEDB	S	7	nonRBD	Outside	Non-Toxin	ALLERGEN
294	305	DPLSETKCTLKS	0.9204	Karplus and Schulz flexibility	IEDB	S	12	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
411	417	APGQTGK	1.7614	Karplus and Schulz flexibility	IEDB	S	7	RBD	Outside	Non-Toxin	ALLERGEN
545	558	GLTGTGVLTESNKK	1.0227	Karplus and Schulz flexibility	IEDB	S	14	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
614	619	DVNCTE	2.375	Karplus and Schulz flexibility	IEDB	S	6	nonRBD	Outside	Non-Toxin	ALLERGEN
1034	1039	LGQSKR	2.0011	Karplus and Schulz flexibility	IEDB	S	6	nonRBD	Outside	Non-Toxin	ALLERGEN
29	38	LTWICLLQFA	1.0412	Kolaskar	IEDB	M	10	NA	Transmembrane	Non-Toxin	ALLERGEN
34	41	RGVYYPDK	1.0191	Kolaskar and Tongaonkar antigenicity	IEDB	S	8	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
65	70	FHAIHV	1.6766	Kolaskar and Tongaonkar antigenicity	IEDB	S	6	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
168	174	FEYVSQP	0.9073	Kolaskar and Tongaonkar antigenicity	IEDB	S	7	nonRBD	Outside	Non-Toxin	ALLERGEN
333	339	TNLCPFG	1.1812	Kolaskar and Tongaonkar antigenicity	IEDB	S	7	RBD	Outside	Non-Toxin	NON-ALLERGEN
376	385	TFKCYGVSPT	1.5059	Kolaskar and Tongaonkar antigenicity	IEDB	S	10	RBD	Outside	Non-Toxin	ALLERGEN
488	495	CYFPLQSY	0.9394	Kolaskar and Tongaonkar antigenicity	IEDB	S	8	RBD	Outside	Non-Toxin	ALLERGEN
723	730	TTEILPVS	1.2071	Kolaskar and Tongaonkar antigenicity	IEDB	S	8	nonRBD	Outside	Non-Toxin	ALLERGEN
735	741	SVDCTMY	1.0932	Kolaskar and Tongaonkar antigenicity	IEDB	S	7	nonRBD	Outside	Non-Toxin	ALLERGEN
847	853	RDLICAQ	1.1443	Kolaskar and Tongaonkar antigenicity	IEDB	S	7	nonRBD	Outside	Non-Toxin	ALLERGEN
1262	1270	EPVLKGVKL	1.2301	Kolaskar and Tongaonkar antigenicity	IEDB	S	9	nonRBD	Inside	Non-Toxin	NON-ALLERGEN
104	116	ARTRSMWSFNPET	1.0549	Parker	IEDB	M	13	NA	Inside	Non-Toxin	NON-ALLERGEN
14	20	QCVNLTT	1.5916	Parker hydrophilicity	IEDB	S	7	nonRBD	Outside	Non-Toxin	ALLERGEN
109	115	TLDSKTQ	1.2584	Parker hydrophilicity	IEDB	S	7	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
180	188	EGKQGNFKN	1.1232	Parker hydrophilicity	IEDB	S	9	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
295	302	PLSETKCT	1.2573	Parker hydrophilicity	IEDB	S	8	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
316	325	SNFRVQPTES	1.2078	Parker hydrophilicity	IEDB	S	10	RBD	Outside	Non-Toxin	ALLERGEN
381	388	GVSPTKLN	1.9197	Parker hydrophilicity	IEDB	S	8	RBD	Outside	Non-Toxin	ALLERGEN
411	425	APGQTGKIADYNYKL	1.4441	Parker hydrophilicity	IEDB	S	15	RBD	Outside	Non-Toxin	NON-ALLERGEN
614	620	DVNCTEV	2.2015	Parker hydrophilicity	IEDB	S	7	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
654	662	EHVNNSYEC	1.068	Parker hydrophilicity	IEDB	S	9	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
731	738	MTKTSVDC	1.5932	Parker hydrophilicity	IEDB	S	8	nonRBD	Outside	Non-Toxin	ALLERGEN
1033	1046	VLGQSKRVDFCGKG	1.3582	Parker hydrophilicity	IEDB	S	14	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
1156	1168	FKNHTSPDVDLGD	1.0616	Parker hydrophilicity	IEDB	S	13	nonRBD	Outside	Non-Toxin	NON-ALLERGEN
201	208	FKIYSKHT	1.1661	Polarity	BcePred	S	8	nonRBD	Outside	Non-Toxin	ALLERGEN
435	444	AWNSNNLDSK	1.0198	Turns	BcePred	S	10	RBD	Outside	Non-Toxin	ALLERGEN
538	546	CVNFNFNGL	1.7985	Turns	BcePred	S	9	RBD	Outside	Non-Toxin	ALLERGEN

Supplementry Table 3D. Antigenicity score of predicted B-cell epitopes curated from literature.

start	end	protein	peptide	reference	vaxijen
524	598	S	VCGPKKSTNLVKNKCVNFNFNGLTGTGVLTESNKKFLPFQQFGRDIADTTDAVRDPQTLEILDITPCSFGGVSVI	Grifoni A. et al. Cell Host & Microbe, 2020	0.7634
888	909	S	FGAGAALQIPFAMQMAYRFNGI	Grifoni A. et al. Cell Host & Microbe, 2020	0.76
132	151	M	PLLESELVIGAVILRGHLRI	Grifoni A. et al. Cell Host & Microbe, 2020	0.6678
601	640	S	GTNTSNQVAVLYQDVNCTEVPVAIHADQLTPTWRVYSTGS	Grifoni A. et al. Cell Host & Microbe, 2020	0.6197
355	401	N	NKHIDAYKTFPPTEPKKDKKKKTDEAQPLPQRQKKQPTVTLLPAADM	Grifoni A. et al. Cell Host & Microbe, 2020	0.525
287	317	S	DAVDCALDPLSETKCTLKSFTVEKGIYQTSN	Grifoni A. et al. Cell Host & Microbe, 2020	0.5013
42	62	N	RPQGLPNNTASWFTALTQHGK	Grifoni A. et al. Cell Host & Microbe, 2020	0.3821
1	24	M	MADSNGTITVEELKKLLEQWNLVI	Grifoni A. et al. Cell Host & Microbe, 2020	0.1533
153	172	N	NNNAATVLQLPQGTTLPKGF	Grifoni A. et al. Cell Host & Microbe, 2020	0.1411
802	819	S	FSQILPDPSKPSKRSFIE	Grifoni A. et al. Cell Host & Microbe, 2020	0.0988
17	28	ORF3a	QGEIKDATPSDF	Srivastava S, et al, Biorxiv,2020	1.1542
71	96	ORF7a	VKHVYQLRARSVSPKLFIRQEEVQEL	Srivastava S, et al, Biorxiv,2020	0.6123
226	267	N protein	RLNQLESKMSGKGQQQQGQTVTKKSAAEASKKPRQKRTATKA	Srivastava S, et al, Biorxiv,2020	0.5627
329	363	S	FPNITNLCPFGEVFNATRFASVYAWNRKRISNCVA	Srivastava S, et al, Biorxiv,2020	0.4466
23	45	ORF8	QSCTQHQPYVVDDPCPIHFYSKW	Srivastava S, et al, Biorxiv,2020	0.4371
440	501	S	NLDSKVGGNYNYLYRLFRKSNLKPFERDISTEIYQAGSTPCNGVEGFNCYFPLQSYGFQPTN	Srivastava S, et al, Biorxiv,2020	0.3951
48	56	ORF8	RVGARKSAP	Srivastava S, et al, Biorxiv,2020	0.3698
4157	4176	ORF1ab	GTTQTACTDDNALAYYNTTK	Srivastava S, et al, Biorxiv,2020	0.3601
159	164	ORF3a	PYNSVT	Srivastava S, et al, Biorxiv,2020	0.3244
250	260	S	TPGDSSSGWTA	Srivastava S, et al, Biorxiv,2020	0.2473
180	191	Membrane Protein	KLGASQRVAGDS	Srivastava S, et al, Biorxiv,2020	0.0439
17	25	ORF7a	LYHYQECVR	Srivastava S, et al, Biorxiv,2020	0.024

Supplementary Table 3E. Discontinuous B-cell epitopes predicted by DiscoTope 2 with the discotope score threshold of -3.7 (default setting).

chain_id	residue_id	residue_name	contact_number	propensity_score	discotope_score	locations on the 3D structure of SARS-CoV-2 (PDB ID: 6VSB)
A	281	GLU	0	-3.366	-2.979	stem
A	282	ASN	7	-2.664	-3.162	stem
A	415	THR	0	-3.819	-3.38	head
A	420	ASP	4	-3.618	-3.662	head
A	449	TYR	4	-0.567	-0.962	head
A	450	ASN	11	-1.78	-2.841	head
A	454	ARG	14	-1.224	-2.694	head
A	491	PRO	7	-0.72	-1.442	head
A	492	LEU	15	-0.95	-2.565	head
A	493	GLN	9	-0.572	-1.541	head
A	494	SER	7	-0.846	-1.553	head
A	496	GLY	3	0.041	-0.309	head
A	498	GLN	4	0.68	0.142	head
A	499	PRO	5	0.178	-0.417	head
A	500	THR	0	1.907	1.688	head
A	503	VAL	5	-1.856	-2.218	head
A	505	TYR	8	-1.528	-2.272	head
A	556	ASN	2	-3.79	-3.584	stem
A	558	LYS	2	-1.479	-1.539	head
A	560	LEU	2	-1.137	-1.236	stem
A	561	PRO	0	-0.961	-0.851	head
A	562	PHE	0	-2.061	-1.824	head
A	703	ASN	4	-2.02	-2.248	stem
A	704	SER	3	-1.469	-1.645	stem
A	705	VAL	10	-2.821	-3.646	stem
A	793	PRO	1	-2.278	-2.131	stem
A	794	ILE	1	-2.5	-2.327	stem
A	809	PRO	4	-2.691	-2.841	stem
A	810	SER	9	-0.669	-1.627	stem
A	914	ASN	7	-1.117	-1.794	stem
A	917	TYR	9	-2.702	-3.426	stem
A	918	GLU	13	-2.285	-3.517	stem
A	1071	GLN	9	-2.775	-3.491	stem
A	1099	GLY	1	-3.789	-3.468	stem
A	1100	THR	0	-3.877	-3.431	stem
A	1101	HIS	8	-2.903	-3.489	stem
A	1111	GLU	19	-1.693	-3.684	stem
A	1118	ASP	4	-3.016	-3.129	stem
A	1140	PRO	7	-0.961	-1.656	root
A	1141	LEU	5	-0.257	-0.802	root
A	1142	GLN	7	0.318	-0.523	root
A	1143	PRO	6	1.067	0.255	root
A	1144	GLU	6	0.716	-0.056	root
A	1145	LEU	5	0.162	-0.431	root
A	1146	ASP	5	0.731	0.072	root
B	187	LYS	9	-2.398	-3.158	stem
B	209	PRO	1	-3.243	-2.985	head
B	281	GLU	0	-4.065	-3.597	stem
B	282	ASN	6	-2.337	-2.758	stem
B	415	THR	0	-2.448	-2.167	head
B	417	LYS	15	-2.055	-3.544	head
B	420	ASP	5	-3.2	-3.407	head
B	449	TYR	3	-1.991	-2.107	head
B	460	ASN	15	-0.073	-1.79	head
B	462	LYS	2	-3.079	-2.955	head
B	469	SER	1	-2.505	-2.332	head
B	471	GLU	1	-2.616	-2.43	head
B	472	ILE	3	-3.202	-3.179	head
B	473	TYR	11	-2.078	-3.104	head
B	487	ASN	0	-1.605	-1.42	head
B	488	CYS	3	-2.718	-2.75	head
B	489	TYR	6	-3.009	-3.353	head
B	493	GLN	12	-2.368	-3.476	head
B	494	SER	8	-2.189	-2.858	head
B	496	GLY	1	-0.693	-0.728	head
B	497	PHE	18	-1.153	-3.091	head
B	498	GLN	7	1.188	0.246	head

B	499	PRO	5	0.294	-0.315	head
B	500	THR	1	2.231	1.86	head
B	503	VAL	6	-1.621	-2.124	head
B	504	GLY	0	-2.702	-2.392	head
B	505	TYR	9	-1.67	-2.513	head
B	556	ASN	2	-3.692	-3.497	stem
B	558	LYS	2	-2.13	-2.115	stem
B	560	LEU	1	-3.858	-3.529	stem
B	561	PRO	0	-3.986	-3.528	stem
B	703	ASN	4	-2.12	-2.336	stem
B	704	SER	3	-1.967	-2.086	stem
B	705	VAL	10	-2.857	-3.678	stem
B	716	THR	10	-2.78	-3.61	stem
B	793	PRO	0	-2.542	-2.25	stem
B	794	ILE	3	-2.633	-2.675	stem
B	809	PRO	4	-3.089	-3.193	stem
B	810	SER	9	-1.014	-1.932	stem
B	914	ASN	6	-1.369	-1.901	stem
B	917	TYR	9	-2.268	-3.042	stem
B	918	GLU	11	-2.251	-3.257	stem
B	1071	GLN	7	-3.08	-3.53	stem
B	1111	GLU	19	-1.343	-3.373	stem
B	1114	ILE	8	-2.852	-3.444	stem
B	1118	ASP	5	-2.997	-3.228	stem
B	1140	PRO	8	-0.677	-1.519	root
B	1141	LEU	5	-0.017	-0.59	root
B	1142	GLN	7	0.372	-0.476	root
B	1143	PRO	6	0.629	-0.134	root
B	1144	GLU	4	0.704	0.163	root
B	1145	LEU	5	0.171	-0.424	root
B	1146	ASP	4	0.724	0.181	root
C	281	GLU	0	-3.898	-3.45	stem
C	282	ASN	3	-2.566	-2.616	stem
C	415	THR	0	-3.378	-2.989	head
C	449	TYR	3	-1.844	-1.977	head
C	460	ASN	11	-0.126	-1.376	head
C	462	LYS	1	-2.996	-2.767	head
C	469	SER	5	-2.411	-2.708	head
C	470	THR	12	-2.535	-3.624	head
C	471	GLU	2	-1.882	-1.896	head
C	487	ASN	0	-1.487	-1.316	head
C	488	CYS	0	-2.512	-2.223	head
C	489	TYR	7	-2.629	-3.132	head
C	493	GLN	9	-2.288	-3.06	head
C	494	SER	7	-2.316	-2.854	head
C	496	GLY	1	-1.754	-1.668	head
C	498	GLN	3	-0.804	-1.057	head
C	503	VAL	10	-2.855	-3.677	head
C	504	GLY	0	-2.423	-2.145	head
C	505	TYR	9	-2.339	-3.105	head
C	556	ASN	0	-3.139	-2.778	stem
C	558	LYS	1	-1.819	-1.725	stem
C	560	LEU	1	-2.713	-2.516	stem
C	561	PRO	0	-3.804	-3.367	stem
C	703	ASN	3	-2.135	-2.235	stem
C	704	SER	3	-1.544	-1.711	stem
C	793	PRO	0	-2.671	-2.364	stem
C	794	ILE	4	-2.452	-2.63	stem
C	809	PRO	4	-3.118	-3.22	stem
C	810	SER	9	-1.295	-2.181	stem
C	914	ASN	9	-0.693	-1.648	stem
C	917	TYR	9	-2.612	-3.347	stem
C	918	GLU	12	-1.782	-2.957	stem
C	1071	GLN	7	-2.99	-3.451	stem
C	1074	ASN	7	-2.785	-3.27	stem
C	1100	THR	0	-3.348	-2.963	stem
C	1111	GLU	18	-1.566	-3.456	stem
C	1114	ILE	8	-2.926	-3.51	stem
C	1118	ASP	4	-3.023	-3.136	stem
C	1140	PRO	8	-1.41	-2.168	root

C	1141	LEU	3	-0.304	-0.614	root
C	1142	GLN	6	0.278	-0.444	root
C	1143	PRO	6	0.79	0.009	root
C	1144	GLU	4	0.433	-0.077	root
C	1145	LEU	4	0.405	-0.101	root
C	1146	ASP	4	0.234	-0.253	root

Supplementary Table 4. Discontinuous epitopes in the spike head of S protein.

Chain	Residue	Residue	Contact number	Propensity	Discotope
A	415	THR	0	-3.819	-3.38
A	420	ASP	4	-3.618	-3.662
A	449	TYR	4	-0.567	-0.962
A	450	ASN	11	-1.78	-2.841
A	454	ARG	14	-1.224	-2.694
A	491	PRO	7	-0.72	-1.442
A	492	LEU	15	-0.95	-2.565
A	493	GLN	9	-0.572	-1.541
A	494	SER	7	-0.846	-1.553
A	496	GLY	3	0.041	-0.309
A	498	GLN	4	0.68	0.142
A	499	PRO	5	0.178	-0.417
A	500	THR	0	1.907	1.688
A	503	VAL	5	-1.856	-2.218
A	505	TYR	8	-1.528	-2.272
A	558	LYS	2	-1.479	-1.539
A	561	PRO	0	-0.961	-0.851
A	562	PHE	0	-2.061	-1.824
B	209	PRO	1	-3.243	-2.985
B	415	THR	0	-2.448	-2.167
B	417	LYS	15	-2.055	-3.544
B	420	ASP	5	-3.2	-3.407
B	449	TYR	3	-1.991	-2.107
B	460	ASN	15	-0.073	-1.79
B	462	LYS	2	-3.079	-2.955
B	469	SER	1	-2.505	-2.332
B	471	GLU	1	-2.616	-2.43
B	472	ILE	3	-3.202	-3.179
B	487	ASN	0	-1.605	-1.42
B	488	CYS	3	-2.718	-2.75
B	489	TYR	6	-3.009	-3.353
B	493	GLN	12	-2.368	-3.476
B	494	SER	8	-2.189	-2.858
B	496	GLY	1	-0.693	-0.728
B	497	PHE	18	-1.153	-3.091
B	498	GLN	7	1.188	0.246
B	499	PRO	5	0.294	-0.315
B	500	THR	1	2.231	1.86
B	503	VAL	6	-1.621	-2.124
B	504	GLY	0	-2.702	-2.392
B	505	TYR	9	-1.67	-2.513
C	415	THR	0	-3.378	-2.989
C	449	TYR	3	-1.844	-1.977
C	460	ASN	11	-0.126	-1.376
C	462	LYS	1	-2.996	-2.767
C	469	SER	5	-2.411	-2.708
C	470	THR	12	-2.535	-3.624
C	471	GLU	2	-1.882	-1.896
C	487	ASN	0	-1.487	-1.316
C	488	CYS	0	-2.512	-2.223
C	489	TYR	7	-2.629	-3.132
C	493	GLN	9	-2.288	-3.06
C	494	SER	7	-2.316	-2.854
C	496	GLY	1	-1.754	-1.668
C	498	GLN	3	-0.804	-1.057
C	503	VAL	10	-2.855	-3.677
C	504	GLY	0	-2.423	-2.145

Supplementary Table 5A. Allergenicity, toxicity, hydro and physiochemical properties of the ten linear B-cell epitopes without allergenicity and toxicity in RBD of S protein.

Peptide Sequence	Allergenicity	Toxicity	Hydrophobicity	Hydropathicity	Hydrophilicity	Charge	pI	Mol wt
APGQTGKIADYNYKL	NA	NT	-0.16	-0.81	-0.01	1	8.76	1639.06
APGQTGKIADYNYKLPDDFT	NA	NT	-0.17	-0.93	0.15	-1	4.43	2214.7
GDEVRQIAPGQTGKIADYNYKLP	NA	NT	-0.21	-0.89	0.25	0	6.46	2534.17
KCVNFNFNGLTG	NA	NT	-0.05	0.02	-0.51	1	8.57	1313.67
KIADYNYKLPDDFT	NA	NT	-0.22	-0.99	0.26	-1	4.43	1703.07
TNLCPFG	NA	NT	0.06	0.41	-0.79	0	5.85	750.96
VRQIAPGQTGKIAD	NA	NT	-0.17	-0.37	0.21	1	9.1	1453.87
YGVSPTKLND	NA	NT	-0.17	-0.77	0.05	0	6.18	1093.34
YNSASFSTFKCYGVSPTKLNDLCFT	NA	NT	-0.08	-0.05	-0.41	1	8.33	2794.49
YQPYRVVVLSFELLH	NA	NT	0	0.47	-0.73	0.5	7.1	1863.42

NA non-allergic, NT non-toxic.

Supplementary Table 5B. Non-digesting enzymes of the ten linear B-cell epitopes without allergenicity and toxicity in RBD of S protein.

Peptide	Non-digesting enzymes
APGQTGKIADYNYKL	Cyanogen_Bromide,Clostripain,Staph_Protease,Trypsin_R,IodosoBenzoate
APGQTGKIADYNYKLPDDFT	Cyanogen_Bromide,Clostripain,Staph_Protease,Trypsin_R,IodosoBenzoate
GDEVRQIAPGQTGKIADYNYKLP	Cyanogen_Bromide,IodosoBenzoate
KCVNFNFNGLTG	Proline_Endopept,Cyanogen_Bromide,AspN,Clostripain,Staph_Protease,Trypsin_R,IodosoBenzoate
KIADYNYKLPDDFT	Cyanogen_Bromide,Clostripain,Staph_Protease,Trypsin_R,IodosoBenzoate
TNLCPFG	Trypsin,Cyanogen_Bromide,Trypsin_K,AspN,Clostripain,Staph_Protease,Trypsin_R,IodosoBenzoate
VRQIAPGQTGKIAD	Chymotrypsin,Cyanogen_Bromide,Staph_Protease,Chymotrypsin(modified),IodosoBenzoate
YGVSPTKLND	Cyanogen_Bromide,Clostripain,Staph_Protease,Trypsin_R,IodosoBenzoate
YNSASFSTFKCYGVSPTKLNDLCFT	Cyanogen_Bromide,Clostripain,Staph_Protease,Trypsin_R,IodosoBenzoate
YQPYRVVVLSFELLH	Cyanogen_Bromide,Trypsin_K,AspN,IodosoBenzoate

Supplementary Table 6A. MHC class-I allele binding epitopes from S protein.

Peptide	Antigenicity	Nr_alleles	Alleles
IPFAMQMAYR	1.5145	3	A*68:01, B*35:01, A*33:01
VVFLHVTYV	1.5122	3	A*02:03, A*02:06, A*68:02
FPNITNLCPF	1.3964	4	B*53:01, B*35:01, B*51:01, B*07:02
KWPWYIWLGF	1.3904	3	A*24:02, A*23:01, A*32:01
LPIGINITRF	1.3027	3	B*53:01, B*35:01, B*51:01
IAIVMVTIM	1.1339	4	B*58:01, B*51:01, B*53:01, B*35:01
ESNKKFLPF	1.0278	4	B*15:01, B*08:01, A*26:01, A*32:01
LPFFSNVTW	1.0808	3	B*53:01, B*51:01, B*57:01
FAMQMAYRF	1.0278	6	B*35:01, B*53:01, A*23:01, B*58:01, A*24:02, B*08:01

Supplementary Table 6B. MHC class-I allele binding epitopes from M protein.

Peptide	Antigenicity	Nr_alleles	Alleles
EQWNLVIGF	1.3869	6	B*44:03,A*32:01,B*15:01,B*44:02,B*40:01,A*26:01
LVIGAVILR	1.1027	5	A*68:01,A*33:01,A*31:01,A*11:01,A*03:01
RTRSMWSF	1.4716	4	B*57:01,A*30:01,A*32:01,B*58:01
LAAVYRINW	1.4322	4	B*58:01,B*57:01,B*53:01,A*32:01
VIGFLFLTW	1.1465	3	A*32:01,B*58:01,B*57:01
GTITVEELK	1.0976	3	A*11:01,A*68:01,A*03:01
LEQWNLVIGF	1.0564	3	B*44:03,B*44:02,B*40:01
VLAAVYRINW	1.1808	3	B*58:01,B*57:01,A*32:01
DSGFAAYSRY	1.0869	3	A*26:01,A*01:01,A*30:02

Supplementary Table 6C. MHC class-I allele binding epitopes from N protein.

Peptide	Antigenicity	Nr_alleles	Alleles
KMKDLSPRW	1.7462	8	A*32:01,B*57:01,B*58:01,B*15:01,A*30:02,A*23:01,B*53:01,A*24:02
KLDDKDPNF	2.6591	6	A*32:01,A*02:06,A*02:01,A*01:01,A*30:02,B*15:01
KMKDLSPRWY	1.5032	6	A*30:02,B*15:01,A*03:01,A*01:01,A*32:01,B*57:01
DLSPRWYFY	1.7645	5	A*26:01,A*01:01,A*30:02,A*33:01,B*35:01
SSRGTSPAR	1.2455	4	A*31:01,A*30:01,A*33:01,A*68:01
GKMKDLSPRW	1.3748	3	B*57:01,B*58:01,A*32:01
SSRSRNSSR	1.1218	3	A*31:01,A*30:01,A*33:01
NFKDQVILL	1.1677	3	A*23:01,A*24:02,B*08:01
DPNFKDQVI	1.7367	3	B*51:01,B*53:01,B*08:01

Supplementary Table 7A. MHC class-II allele binding epitopes from S protein.

Peptide	Antigenicity	Nr_alleles	Alleles
VGYQPYRVVVLSFEL	1.3858	6	DPA1*01:03/DPB1*04:01, DRB1*04:05, DPA1*02:01/DPB1*14:01, DPA1*01:03/DPB1*02:01, DRB1*07:01, DPA1*02:01/DPB1*05:01
FAMQMAYRFNGIGVT	1.3688	5	DRB3*02:02, DRB3*01:01, DRB1*08:02, DRB1*11:01, DRB5*01:01
IPFAMQMAYRFNGIG	1.2828	8	DRB4*01:01, DRB1*01:01, DRB5*01:01, DRB3*01:01, DRB3*02:02, DRB1*12:01, DRB1*15:01, DPA1*01:03/DPB1*04:01
NFTISVTTEILPVSM	1.2136	8	DRB1*07:01, DPA1*03:01/DPB1*04:02, DQA1*03:01/DQB1*03:02, DPA1*02:01/DPB1*01:01, DPA1*02:01/DPB1*14:01, DQA1*05:01/DQB1*02:01, DRB1*04:01, DRB3*02:02
LVLLPLVSSQCVNLT	1.2086	5	DRB4*01:01, DRB1*08:02, DRB1*04:01, DRB1*15:01, DRB1*04:05
VVFLHVTYVPAQEKN	1.172	10	DRB1*04:05, DPA1*01:03/DPB1*02:01, DRB1*08:02, DQA1*04:01/DQB1*04:02, DRB1*04:01, DRB5*01:01, DPA1*01:03/DPB1*04:01, DQA1*03:01/DQB1*03:02 , DPA1*02:01/DPB1*14:01, DQA1*05:01/DQB1*02:01
TNFTISVTTEILPVS	1.1691	9	DRB1*07:01, DRB1*09:01, DRB3*02:02, DQA1*03:01/DQB1*03:02, DQA1*05:01/DQB1*02:01, DRB1*04:01, DPA1*02:01/DPB1*01:01, DPA1*02:01/DPB1*14:01, DPA1*03:01/DPB1*04:02
QYIKWPWYIWLGFIA	1.1541	6	DPA1*01:03/DPB1*04:01, DPA1*02:01/DPB1*01:01, DPA1*01:03/DPB1*02:01, DQA1*01:01/DQB1*05:01, DPA1*02:01/DPB1*05:01, DPA1*03:01/DPB1*04:02
PTNFTISVTTEILPV	1.1349	8	DRB1*07:01, HLA-DRB1*09:01, DRB3*02:02, DQA1*03:01/DQB1*03:02, DQA1*05:01/DQB1*02:01, DPA1*02:01/DPB1*01:01, DRB1*04:01, DPA1*03:01/DPB1*04:02
GVVFLHVTYVPAQEK	1.1043	11	DRB1*04:05, DPA1*01:03/DPB1*02:01, DRB1*08:02, DRB1*04:01, DPA1*01:03/DPB1*04:01, DRB1*01:01, DQA1*05:01/DQB1*02:01 , DQA1*04:01/DQB1*04:02, DQA1*03:01/DQB1*03:02, DRB1*07:01, DPA1*02:01/DPB1*14:01
GYQPYRVVVLSFELL	1.074	11	DPA1*02:01/DPB1*01:01, DPA1*01:03/DPB1*02:01, DPA1*01:03/DPB1*04:01, DPA1*02:01/DPB1*05:01, DPA1*02:01/DPB1*14:01, DRB1*04:05, DRB4*01:01, DPA1*03:01/DPB1*04:02, DRB1*07:01, DRB1*15:01, DQA1*05:01/DQB1*02:01
VFLHVTYVPAQEKNF	1.0339	5	DRB5*01:01, DQA1*04:01/DQB1*04:02, DPA1*01:03/DPB1*02:01, DPA1*02:01/DPB1*14:01, DRB1*07:01
ALQIPFAMQMAYRFN	1.0112	10	DRB4*01:01, DRB5*01:01, DPA1*02:01/DPB1*14:01, DRB1*01:01, DRB1*12:01, DRB3*01:01, DRB3*02:02, DPA1*01:03/DPB1*04:01, DRB1*03:01, DRB1*15:01

Supplementary Table 7B. MHC class-II allele binding epitopes from M protein.

Peptide	Antigenicity	Nr_alleles	Alleles
LACFVLAAVYRINWI	1.2905	12	DRB1*07:01,DRB3*01:01,DRB5*01:01,DRB1*01:01,DPA1*01:03/DPB1*02:01,DPA1*02:01/DPB1*05:01,DPA1*01:03/DPB1*04:01,DRB1*12:01,DRB1*11:01,DRB1*04:01,DRB1*09:01,DQA1*01:01/DQB1*05:01
TLACFVLAAVYRINW	1.3132	11	DRB1*07:01,DRB3*01:01,DRB5*01:01,DRB1*01:01,DPA1*01:03/DPB1*02:01,DPA1*02:01/DPB1*05:01,DPA1*01:03/DPB1*04:01,DRB1*12:01,DRB1*04:01,DRB1*11:01,DRB1*09:01
VTLACFVLAAVYRIN	1.045	11	DRB1*07:01,DRB3*01:01,DRB5*01:01,DRB1*01:01,DPA1*01:03/DPB1*02:01,DPA1*02:01/DPB1*05:01,DPA1*01:03/DPB1*04:01,DRB1*09:01,DQA1*01:01/DQB1*05:01,DRB1*04:01,DRB1*04:05
ACFVLAAVYRINWIT	1.1115	10	DRB1*07:01,DRB3*01:01,DRB5*01:01,DRB1*01:01,DPA1*01:03/DPB1*02:01,DPA1*01:03/DPB1*04:01,DRB1*11:01,DRB1*04:01,DRB1*12:01,DRB1*09:01
CFVLAAVYRINWITG	1.0062	8	DRB1*07:01,DRB1*01:01,DRB5*01:01,DPA1*01:03/DPB1*02:01,DRB3*01:01,DRB1*04:01,DRB1*11:01,DPA1*01:03/DPB1*04:01
IGFLFLTWICLLQFA	1.1111	8	DPA1*03:01/DPB1*04:02,DPA1*01:03/DPB1*02:01,DPA1*02:01/DPB1*01:01,DQA1*01:01/DQB1*05:01,DQA1*05:01/DQB1*02:01,DPA1*01:03/DPB1*04:01,DPA1*02:01/DPB1*05:01,DRB1*07:01
YRINWITGGIAIAMA	1.1274	7	DQA1*01:02/DQB1*06:02,DQA1*05:01/DQB1*03:01,DRB3*02:02,DRB1*01:01,DRB1*13:02,DRB1*09:01,DPA1*02:01/DPB1*14:01
FVLAAVYRINWITGG	1.023	7	DRB1*07:01,DRB3*02:02,DRB3*01:01,DRB5*01:01,DRB1*11:01,DQA1*01:01/DQB1*05:01,DRB1*01:01
NLVIGFLFLTWICLL	1.2609	6	DPA1*01:03/DPB1*02:01,DPA1*03:01/DPB1*04:02,DPA1*02:01/DPB1*01:01,DPA1*02:01/DPB1*05:01,DQA1*01:01/DQB1*05:01,DRB1*15:01
LVIGFLFLTWICLLQ	1.0776	6	DPA1*03:01/DPB1*04:02,DPA1*01:03/DPB1*02:01,DPA1*02:01/DPB1*01:01,DQA1*01:01/DQB1*05:01,DPA1*02:01/DPB1*05:01,DRB1*15:01
WNLVIGFLFLTWICL	1.4689	6	DPA1*01:03/DPB1*02:01,DPA1*03:01/DPB1*04:02,DPA1*02:01/DPB1*05:01,DQA1*01:01/DQB1*05:01,DRB1*15:01,DRB1*07:01
LTWICLLQFAYANRN	1.2337	6	DRB1*12:01,DRB4*01:01,DPA1*01:03/DPB1*02:01,DPA1*01:03/DPB1*04:01,DRB5*01:01,DPA1*02:01/DPB1*01:01
LEQWNLVIGFLFLTW	1.0231	5	DPA1*01:03/DPB1*02:01,DPA1*02:01/DPB1*05:01,DRB1*15:01,DPA1*01:03/DPB1*04:01,DQA1*01:01/DQB1*05:01

Supplementary Table 8A. Allergenicity, toxicity, hydro and physiochemical properties of T-cell epitopes from S protein.

Peptide	Allergenicity	Toxicity	Hydrophobicity	Hydropathicity	Hydrophilicity	Charge	pI	Mol wt
MHC class I binding peptides								
IPFAMQMAYR	A	NT	-0.01	0.38	-0.7	1	9.1	1227.6
VVFLHVTYV	A	NT	0.3	2.02	-1.5	0.5	7.09	1076.4
FPNITNLCPF	A	NT	0.09	0.55	-0.96	0	5.85	1165.5
KWPWYIWLGF	A	NT	0.2	0.12	-1.56	1	8.94	1385.8
LPIGINITRF	NA	NT	0.08	0.94	-0.69	1	10.11	1143.6
IAIVMVTIM	NA	NT	0.43	2.98	-1.32	0	5.88	990.47
ESNKKFLPF	A	NT	-0.23	-0.87	0.3	1	8.94	1109.4
LPFFSNVTW	A	NT	0.17	0.68	-1.29	0	5.88	1110.4
FAMQMAYRF	A	NT	-0.02	0.41	-0.86	1	9.1	1164.5
MHC class II binding peptides								
VGYQPYRVVVLSFEL	NA	NT	0.04	0.69	-0.68	0	6.35	1769.3
FAMQMAYRFNGIGVT	NA	NT	0.04	0.49	-0.75	1	9.1	1706.23
IPFAMQMAYRFNGIG	A	NT	0.06	0.45	-0.74	1	9.1	1716.27
NFTISVTTEILPVSM	NA	NT	0.1	0.91	-0.64	-1	4	1652.16
LVLLPLVSSQCVNLT	NA	NT	0.15	1.55	-0.93	0	5.85	1599.2
VVFLHVTYVPAQEKN	NA	NT	-0.01	0.27	-0.51	0.5	7.1	1744.25
TNFTISVTTEILPVS	NA	NT	0.07	0.73	-0.58	-1	4	1622.07
QYIKWPWYIWLGFIA	A	NT	0.2	0.48	-1.45	1	8.83	1984.61
PTNFTISVTTEILPV	NA	NT	0.09	0.68	-0.6	-1	4	1632.11
GVVFLHVTYVPAQEK	A	NT	0.04	0.47	-0.52	0.5	7.1	1687.2
GYQPYRVVVLSFELL	NA	NT	0.04	0.66	-0.7	0	6.35	1783.33
VFLHVTYVPAQEKNF	A	NT	0	0.17	-0.57	0.5	7.1	1792.29
ALQIPFAMQMAYRFN	NA	NT	-0.01	0.35	-0.76	1	9.1	1801.37

NA non-allergic, A allergic, NT non-toxic.

Supplementary Table 8B. Allergenicity, toxicity, hydro and physiochemical properties of T-cell epitopes in M protein.

Peptide	Allergenity	Toxicity	Hydrophobicity	Hydropathicity	Hydrophilicity	Charge	pI	Mol wt
MHC class I binding peptides (NA non-allergic, A allergic, NT non-toxic, T toxic)								
EQWNLVIGF	NA	NT	0.11	0.39	-0.84	-1	4	1105.4
LVIGAVILR	NA	NT	0.25	2.43	-0.86	1	10.11	953.38
RTRSMWSF	A	NT	-0.37	-0.94	-0.13	2	12.01	1070.33
LAAVYRINW	A	NT	0.03	0.66	-0.96	1	9.1	1105.43
VIGFLFLTW	A	NT	0.43	2.21	-1.74	0	5.88	1095.49
GTITVEELK	A	NT	-0.08	-0.02	0.34	-1	4.54	989.27
LEQWNLVIGF	A	NT	0.15	0.73	-0.94	-1	4	1218.58
VLAAVYRINW	A	NT	0.08	1.01	-1.01	1	9.1	1204.58
DSGFAAYSRY	NA	NT	-0.17	-0.62	-0.15	0	6.18	1136.3
MHC class II binding peptides (NA non-allergic, A allergic, NT non-toxic, T toxic)								
LACFVLAAVYRINWI	NA	NT	0.2	1.7	-1.18	1	8.57	1752.37
TLACFVLAAVYRINW	A	NT	0.14	1.35	-1.09	1	8.57	1740.31
VTLACFVLAAVYRIN	NA	NT	0.15	1.69	-0.96	1	8.57	1653.23
ACFVLAAVYRINWIT	NA	NT	0.15	1.4	-1.09	1	8.57	1740.31
CFVLAAVYRINWITG	A	NT	0.15	1.25	-1.05	1	8.57	1726.29
IGFLFLTWICLLQFA	NA	NT	0.36	2.09	-1.56	0	5.85	1785.46
YRINWITGGIAIAMA	NA	NT	0.14	0.91	-0.86	1	9.1	1650.2
FVLAAVYRINWITGG	NA	NT	0.15	1.06	-0.99	1	9.1	1680.21
NLVIGFLFLTWICLL	NA	NT	0.37	2.32	-1.58	0	5.85	1765.48
LVIGFLFLTWICLLQ	NA	T	0.37	2.32	-1.58	0	5.85	1779.51
WNLVIGFLFLTWICL	NA	NT	0.36	2.01	-1.69	0	5.85	1838.53
LTWICLLQFAYANRN	NA	T	0	0.46	-0.95	1	8.57	1826.37
LEQWNLVIGFLFLTW	NA	NT	0.23	1.07	-1.29	-1	4	1879.48

Supplementary Table 8C. Allergenicity, toxicity, hydro and physiochemical properties of T-cell epitopes in N protein.

Peptide	Allergenity	Toxicity	Hydrophobicity	Hydropathicity	Hydrophilicity	Charge	pI	Mol wt
MHC class I binding peptides								
KMKDLSPRW	A	NT	-0.43	-1.49	0.64	2	10.01	1160.52
KLDDKDPNF	A	NT	-0.44	-1.87	1.21	-1	4.43	1091.3
KMKDLSPRWY	A	NT	-0.38	-1.47	0.35	2	9.72	1323.71
DLSPRWYFY	A	NT	-0.14	-0.81	-0.67	0	6.18	1246.5
SSRGTSPAR	A	NT	-0.46	-1.37	0.67	2	12.01	918.08
GKMKDLSPRW	NA	NT	-0.37	-1.38	0.58	2	10.01	1217.59
SSRSRNSSR	NA	NT	-0.8	-2.33	1.19	3	12.31	1036.17
NFKDQVILL	A	NT	-0.02	0.52	-0.33	0	6.19	1089.44
DPNFKDQVI	A	NT	-0.23	-0.89	0.4	-1	4.21	1075.31

NA non-allergic, A allergic, NT non-toxic, T toxic.

Supplementary Table 9A. Non-digesting enzymes of T-cell epitopes from S protein.

Peptide	Non-digesting enzymes
MHC class I binding peptides	
IPFAMQMAYR	Trypsin, Clostripain, IodosoBenzoate, Staph_Protease, Trypsin_K, Trypsin_R, AspN
VVFLHVTYV	Trypsin, Clostripain, Cyanogen_Bromide, IodosoBenzoate, Proline_Endopept, Staph_Protease, Trypsin_K, Trypsin_R, AspN
FPNITNLCPF	Trypsin, Clostripain, Cyanogen_Bromide, IodosoBenzoate, Staph_Protease, Trypsin_K, Trypsin_R, AspN
KWPWYIWLGF	Clostripain, Cyanogen_Bromide, Staph_Protease, Trypsin_R, AspN
LPIGINITRF	Chymotrypsin, Cyanogen_Bromide, IodosoBenzoate, Staph_Protease,Trypsin_K, AspN, Chymotrypsin(modified)
IAIVMVTIM	Trypsin, Chymotrypsin, Clostripain, Cyanogen_Bromide, IodosoBenzoate, Proline_Endopept, Staph_Protease, Trypsin_K, Trypsin_R, AspN, Chymotrypsin(modified)
ESNKKFLPF	Clostripain, Cyanogen_Bromide, IodosoBenzoate, Trypsin_R , AspN, Elastase
LPFFSNVTW	Trypsin, Clostripain, Cyanogen_Bromide, IodosoBenzoate, Staph_Protease, Trypsin_K, Trypsin_R, AspN
FAMQMAYRF	IodosoBenzoate, Proline_Endopept, Staph_Protease, Trypsin_K, AspN
MHC class II binding peptides	
VGYQPYRVVVLSFEL	Cyanogen_Bromide, IodosoBenzoate, Trypsin_K, AspN
FAMQMAYRFNGIGVT	IodosoBenzoate, Proline_Endopept, Staph_Protease, Trypsin_K, AspN
IPFAMQMAYRFNGIG	IodosoBenzoate, Staph_Protease, Trypsin_K, AspN
NFTISVTTEILPVSM	Trypsin, Clostripain, Cyanogen_Bromide, IodosoBenzoate, Trypsin_K, Trypsin_R, AspN
LVLLPLVSSQCVNLT	Trypsin, Chymotrypsin, Clostripain, Cyanogen_Bromide, IodosoBenzoate, Staph_Protease, Trypsin_K, Trypsin_R, AspN
VVFLHVTYVPAQEKN	Clostripain, Cyanogen_Bromide, IodosoBenzoate, Trypsin_R, AspN
TNFTISVTTEILPVS	Trypsin, Clostripain, Cyanogen_Bromide, IodosoBenzoate, Trypsin_K, Trypsin_R, AspN
QYIKWPWYIWLGFIA	Clostripain, Cyanogen_Bromide, Staph_Protease, Trypsin_R, AspN
PTNFTISVTTEILPV	Trypsin, Clostripain, Cyanogen_Bromide, IodosoBenzoate, Trypsin_K, Trypsin_R, AspN
GVVFLHVTYVPAQEK	Trypsin, Clostripain, Cyanogen_Bromide, IodosoBenzoate, Trypsin_K, Trypsin_R, AspN
GYQPYRVVVLSFELL	Cyanogen_Bromide, IodosoBenzoate, Trypsin_K, AspN
VFLHVTYVPAQEKNF	Clostripain, Cyanogen_Bromide, IodosoBenzoate, Trypsin_R, AspN
ALQIPFAMQMAYRFN	IodosoBenzoate, Staph_Protease, Trypsin_K, AspN

Supplementary Table 9B. Non-digesting enzymes of T-cell epitopes in M protein.

Peptide	Non-digesting enzymes
MHC class I binding peptides	
EQWNLVIGF	Proline_Endopept, Trypsin, Cyanogen_Bromide, Trypsin_K, AspN, Clostripain, Trypsin_R
LVIGAVILR	Proline_Endopept, Chymotrypsin, Trypsin, Cyanogen_Bromide, Trypsin_K, AspN, Clostripain, Staph_Protease, Trypsin_R, IodosoBenzoate
RTRSMWSF	Proline_Endopept, Trypsin_K, AspN, Staph_Protease, Elastase
LAAVYRINW	Proline_Endopept, Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease, IodosoBenzoate
VIGFLFLTW	Proline_Endopept, Trypsin, Cyanogen_Bromide, Trypsin_K, AspN, Clostripain, Staph_Protease, Trypsin_R, IodosoBenzoate
GTITVEELK	Proline_Endopept, Chymotrypsin, Trypsin, Cyanogen_Bromide, Trypsin_K, AspN, Clostripain, Trypsin_R, IodosoBenzoate
LEQWNLVIGF	Proline_Endopept, Trypsin, Cyanogen_Bromide, Trypsin_K, AspN, Clostripain, Trypsin_R
VLAAVYRINW	Proline_Endopept, Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease, IodosoBenzoate
DSGFAAYSRY	Proline_Endopept, Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease, IodosoBenzoate
MHC class II binding peptides	
LACFVLAAVYRINWI	Proline_Endopept, Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease
TLACFVLAAVYRINW	Proline_Endopept, Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease, IodosoBenzoate
VTLACFVLAAVYRIN	Proline_Endopept, Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease, IodosoBenzoate
ACFVLAAVYRINWIT	Proline_Endopept, Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease
CFVLAAVYRINWITG	Proline_Endopept, Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease
IGFLFLTWICLLQFA	Proline_Endopept, Trypsin, Cyanogen_Bromide, Trypsin_K, AspN, Clostripain, Staph_Protease, Trypsin_R
YRINWITGGIAIAMA	Proline_Endopept, Trypsin_K, AspN, Staph_Protease
FVLAAVYRINWITGG	Proline_Endopept, Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease
NLVIGFLFLTWICLL	Proline_Endopept, Trypsin, Cyanogen_Bromide, Trypsin_K, AspN, Clostripain, Staph_Protease, Trypsin_R
LVIGFLFLTWICLLQ	Proline_Endopept, Trypsin, Cyanogen_Bromide, Trypsin_K, AspN, Clostripain, Staph_Protease, Trypsin_R
WNLVIGFLFLTWICL	Proline_Endopept, Trypsin, Cyanogen_Bromide, Trypsin_K, AspN, Clostripain, Staph_Protease, Trypsin_R
LTWICLLQFAYANRN	Proline_Endopept, Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease
LEQWNLVIGFLFLTW	Proline_Endopept, Trypsin, Cyanogen_Bromide, Trypsin_K, AspN, Clostripain, Trypsin_R

Supplementary Table 9C. Non-digesting enzymes of T-cell epitopes in N protein.

Peptide	Non-digesting enzymes
MHC class I binding peptides	
KMKDLSPRW	Chymotrypsin, Staph_Protease, IodosoBenzoate
KLDDKDPNF	Chymotrypsin, Cyanogen_Bromide, Clostripain, Staph_Protease, Trypsin_R, IodosoBenzoate
KMKDLSPRWY	Staph_Protease
DLSPRWYFY	Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease
SSRGTSPAR	Chymotrypsin, Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease, Chymotrypsin(modified), IodosoBenzoate
GKMKDLSPRW	Chymotrypsin, Staph_Protease, IodosoBenzoate
SSRSRNSSR	Proline_Endopept, Chymotrypsin, Cyanogen_Bromide, Trypsin_K, AspN, Staph_Protease, Elastase, Chymotrypsin(modified), IodosoBenzoate
NFKDQVILL	Proline_Endopept, Cyanogen_Bromide, Clostripain, Staph_Protease, Trypsin_R, IodosoBenzoate
DPNFKDQVI	Cyanogen_Bromide, Clostripain, Staph_Protease, Trypsin_R, IodosoBenzoate

Supplementary Table 10. Mutations observed in the 34 non-allergenic and non-toxic linear B-cell epitopes.

start	end	peptide	antigenicity	method	server	Protein	Peptide Length	RBD	Topology	Allergenicity	Toxicity	Mutations
34	41	RGVYYPDK	1.0191	Kolaskar and Tongaonkar antigenicity	IEDB	S	8	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
65	70	FHAIHV	1.6766	Kolaskar and Tongaonkar antigenicity	IEDB	S	6	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	65-72FHAIHVSG>X
70	78	VSGTNGTKR	0.9855	Hydrophilicity	BcePred	S	9	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	65-72FHAIHVSG>X
90	97	VYFASTEK	0.9206	Flexibility	BcePred	S	8	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
108	116	TTLDSKTQS	1.0106	Karplus and Schulz flexibility	IEDB	S	9	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	110L>*
108	117	TTLDSKTQSL	0.99	Accessibility	BcePred	S	10	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	110L>*
108	115	TTLDSKTQ	1.0912	Flexibility	BcePred	S	8	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	110L>*
109	115	TLDSKTQ	1.2584	Parker hydrophilicity	IEDB	S	7	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	110L>*
109	115	TLDSKTQ	1.2584	Chou and Fasman beta turn	IEDB	S	7	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	110L>*
177	189	MDLEGKQGNFKNL	1.2592	Bepipred2.0	IEDB	S	13	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
180	188	EGKQGNFKN	1.1232	Parker hydrophilicity	IEDB	S	9	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
265	273	YYVGYLQPR	1.4692	Antigenic_Propensity	BcePred	S	9	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
278	287	KYNENGTITD	0.9589	Hydrophilicity	BcePred	S	10	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
294	305	DPLSETKCTLKS	0.9204	Karplus and Schulz flexibility	IEDB	S	12	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
295	302	PLSETKCT	1.2573	Parker hydrophilicity	IEDB	S	8	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
333	339	TNLCPFG	1.1812	Kolaskar and Tongaonkar antigenicity	IEDB	S	7	RBD	Outside	Non-Toxin	NON-ALLERGEN	No
369	393	YNSASFSTFKCYGVSPTKLNDLCFT	1.4031	Bepipred2.0	IEDB	S	25	RBD	Outside	Non-Toxin	NON-ALLERGEN	No
380	389	YGVSPTKLND	1.4531	Chou and Fasman beta turn	IEDB	S	10	RBD	Outside	Non-Toxin	NON-ALLERGEN	No
404	426	GDEVRQIAPGQTGKIADYNYKLP	1.1017	Bepipred2.0	IEDB	S	23	RBD	Outside	Non-Toxin	NON-ALLERGEN	408R>*;414-415QT>P; 414Q>K; 414Q>*; 414-; 414Q>E;417K>*
407	420	VRQIAPGQTGKIAD	1.2606	Bepipred	IEDB	S	14	RBD	Outside	Non-Toxin	NON-ALLERGEN	408R>*;414-415QT>P; 414Q>K; 414Q>*; 414-; 414Q>E； 417K>*
411	425	APGQTGKIADYNYKL	1.4441	Parker hydrophilicity	IEDB	S	15	RBD	Outside	Non-Toxin	NON-ALLERGEN	414-415QT>P; 414Q>K; 414Q>*; 414-; 414Q>E;417K>*
411	430	APGQTGKIADYNYKLPDDFT	1.0425	Chou and Fasman beta turn	IEDB	S	20	RBD	Outside	Non-Toxin	NON-ALLERGEN	414-415QT>P; 414Q>K; 414Q>*; 414-; 414Q>E;417K>*
417	430	KIADYNYKLPDDFT	0.9567	Accessibility	BcePred	S	14	RBD	Outside	Non-Toxin	NON-ALLERGEN	417K>*
505	519	YQPYRVVVLSFELLH	0.9711	Antigenic_Propensity	BcePred	S	15	RBD	Outside	Non-Toxin	NON-ALLERGEN	No
537	548	KCVNFNFNGLTG	1.6969	Chou and Fasman beta turn	IEDB	S	12	RBD	Outside	Non-Toxin	NON-ALLERGEN	No
545	558	GLTGTGVLTESNKK	1.0227	Karplus and Schulz flexibility	IEDB	S	14	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
584	601	ILDITPCSFGGVSVITPG	1.1031	Antigenic_Propensity	BcePred	S	18	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
614	620	DVNCTEV	2.2015	Parker hydrophilicity	IEDB	S	7	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
654	662	EHVNNSYEC	1.068	Parker hydrophilicity	IEDB	S	9	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
705	714	VAYSNNSIAI	1.0545	Chou and Fasman beta turn	IEDB	S	10	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
1031	1039	ECVLGQSKR	0.9377	Flexibility	BcePred	S	9	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
1033	1046	VLGQSKRVDFCGKG	1.3582	Parker hydrophilicity	IEDB	S	14	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	No
1156	1168	FKNHTSPDVDLGD	1.0616	Parker hydrophilicity	IEDB	S	13	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	1157-;1157K>*
1157	1167	KNHTSPDVDLG	1.4039	Bepipred	IEDB	S	11	nonRBD	Outside	Non-Toxin	NON-ALLERGEN	1157-; 1157K>*