

# **A Next-Generation Vaccine Candidate Using Alternative Epitopes to Protect against Wuhan and All Significant Mutant Variants of SARS-CoV-2: an Immunoinformatics Approach**

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# SUPPLEMENTARY DATA

**Supplementary Table 1.** Antigenicity, allergenicity, solubility, and physicochemical property assessments of the primary sequence of multi-epitope-based vaccine construct against SARS-CoV-2.

| Sl. No. | Features                                | Assessment   |
|---------|---|--|
| 1.      | Antigenicity                            | 0.6679 (Probable ANTIGEN) by VaxiJen v2.0  |
| 2.      | Allergenicity                           | Probable non-allergen (AllerTOP v.2.0) and Probable non-allergen (AllergenFP v.1.0)  |
| 3.      | Solubility                              | 0.316 (Soluble)  |
| 4.      | Number of amino acids                   | 479  |
| 5.      | Molecular weight                        | 52306.41 dalton  |
| 6.      | Theoretical Isoelectric point (pI)      | 8.98   |
| 7.      | Total number of atoms                   | 7318   |
| 8.      | Formula                                 | C <sub>2387</sub> H <sub>3617</sub> N <sub>615</sub> O <sub>687</sub> S <sub>12</sub>  |
| 9.      | Estimated half-life                     | 30 hours (mammalian reticulocytes, <i>in vitro</i> )<br>>20 min (yeast, <i>in vivo</i> )<br>>10 hours ( <i>Escherichia coli</i> , <i>in vivo</i> ) |
| 10.     | Instability index                       | 23.36 (Stable)   |
| 11.     | Aliphatic index                         | 76.18  |
| 12.     | Grand average of hydropathicity (GRAVY) | -0.168   |

# SUPPLEMENTARY DATA

**Supplementary Table 2.** Molecular docking of TLR4/MD2 and vaccine construct showing the interface residues where they bind along with distance measurement.

| Receptor ligands interactions | Distance (Å <sup>0</sup> ) |
|-------------------------------|----------------------------|
| 361A - 311                    | 4.245                      |
| 362A - 311                    | 2.662                      |
| 362A - 327                    | 4.326                      |
| 363A - 311                    | 3.785                      |
| 363A - 313                    | 4.991                      |
| 365A - 311                    | 3.416                      |
| 365A - 313                    | 4.068                      |
| 383A - 311                    | 4.537                      |
| 384A - 310                    | 4.210                      |
| 386A - 315                    | 4.875                      |
| 408A - 306                    | 4.657                      |
| 408A - 308                    | 3.654                      |
| 409A - 310                    | 4.535                      |
| 431A - 303                    | 4.997                      |
| 431A - 304                    | 3.815                      |
| 431A - 305                    | 4.731                      |
| 431A - 306                    | 2.132                      |
| 456A - 303                    | 2.503                      |
| 456A - 304                    | 1.964                      |
| 456A - 306                    | 4.253                      |
| 456A - 370                    | 4.316                      |
| 458A - 306                    | 4.974                      |
| 458A - 368                    | 4.847                      |
| 458A - 369                    | 2.145                      |
| 458A - 370                    | 3.761                      |
| 458A - 371                    | 4.300                      |
| 459A - 369                    | 4.363                      |
| 480A - 304                    | 3.957                      |
| 480A - 369                    | 2.142                      |
| 480A - 370                    | 3.763                      |
| 481A - 369                    | 3.416                      |
| 482A - 369                    | 3.925                      |
| 504A - 303                    | 4.366                      |
| 505A - 302                    | 3.619                      |
| 505A - 303                    | 2.539                      |
| 505A - 304                    | 2.842                      |
| 505A - 369                    | 4.758                      |
| 505A - 372                    | 4.566                      |
| 507A - 368                    | 4.067                      |
| 507A - 369                    | 4.090                      |

# SUPPLEMENTARY DATA

**Supplementary Table 3.** Molecular docking of TLR4/MD2 and C1 control shows the interface residues where they bind along with distance measurement.

| Receptor ligands interactions | Distance (Å <sup>0</sup> ) |
|-------------------------------|----------------------------|
| 34A - 115                     | 4.762                      |
| 34A - 117                     | 4.190                      |
| 35A - 114                     | 4.980                      |
| 35A - 115                     | 4.927                      |
| 35A - 117                     | 2.123                      |
| 35A - 225                     | 3.539                      |
| 35A - 226                     | 4.340                      |
| 36A - 225                     | 4.820                      |
| 36A - 226                     | 2.971                      |
| 54A - 281                     | 3.767                      |
| 54A - 282                     | 2.365                      |
| 55A - 224                     | 3.382                      |
| 55A - 226                     | 4.176                      |
| 55A - 282                     | 2.966                      |
| 57A - 226                     | 4.486                      |
| 57A - 227                     | 2.222                      |
| 57A - 228                     | 3.980                      |
| 57A - 229                     | 4.570                      |
| 57A - 230                     | 2.268                      |
| 78A - 278                     | 4.119                      |
| 78A - 282                     | 3.964                      |
| 79A - 227                     | 4.369                      |
| 79A - 228                     | 3.276                      |
| 79A - 229                     | 4.917                      |
| 79A - 278                     | 3.174                      |
| 79A - 282                     | 3.517                      |
| 81A - 227                     | 4.943                      |
| 81A - 229                     | 4.869                      |
| 81A - 230                     | 2.948                      |
| 102A - 240                    | 4.689                      |
| 102A - 243                    | 1.784                      |
| 102A - 274                    | 4.964                      |
| 102A - 278                    | 4.217                      |
| 103A - 22                     | 3.521                      |
| 103A - 229                    | 4.623                      |
| 103A - 236                    | 4.270                      |
| 103A - 240                    | 2.848                      |
| 103A - 241                    | 3.470                      |
| 103A - 244                    | 4.741                      |
| 103A - 278                    | 1.446                      |
| 105A - 232                    | 3.820                      |
| 105A - 236                    | 3.431                      |
| 126A - 239                    | 4.736                      |
| 126A - 243                    | 2.637                      |
| 126A - 271                    | 3.294                      |

# SUPPLEMENTARY DATA

## Supplementary files

**Table S1.** The B cell epitopes of the Wuhan variant of SARS-CoV-2 S protein along with their length predicted by ABCPred server.

| Rank | Sequence              | Start position | Score |
|------|-----------------------|----------------|-------|
| 1    | VTLADAGFIKQYGDCLGDIA  | 826            | 0.90  |
| 1    | IGAEHVNNSEYCDPIGAGI   | 651            | 0.90  |
| 1    | TNVYADSFVIRGDEVQRQIAP | 393            | 0.90  |
| 1    | VYYHKNNKSWMESEFRVYSS  | 143            | 0.90  |
| 2    | IHVSGTNGTKRFDNPVLPFN  | 68             | 0.89  |
| 2    | DVNCTEVPVAIHADQLTPTW  | 614            | 0.89  |
| 2    | SYLTPGDSSSGWTAGAAAYY  | 247            | 0.89  |
| 3    | KHTPINLVRDLPQGFSALEP  | 206            | 0.88  |
| 3    | VVIKVCCEQFCNDPFLGVYY  | 126            | 0.88  |
| 4    | DRLITGRLQSLQTYVTQQLI  | 994            | 0.87  |
| 4    | PFGEVFNATRFASVYAWNRK  | 337            | 0.87  |
| 4    | VTQQLIRAAEIRASANLAAT  | 1008           | 0.87  |
| 5    | DNTFVSGNCDVVIGIVNNTV  | 1118           | 0.86  |
| 5    | TTLDSKTQSLLVNNTATNVV  | 108            | 0.86  |
| 6    | YQPYRVVVLSEFLLHAPATV  | 505            | 0.85  |
| 6    | RSSVLHSTQDLFLPFFSNVT  | 44             | 0.85  |
| 6    | KRISNCVADYSVLYNSASFS  | 356            | 0.85  |
| 6    | IWLGFIAGLIAIVMVTIMLC  | 1216           | 0.85  |
| 7    | NVLYENQKLIANQFNQAIGK  | 914            | 0.84  |
| 7    | RGVYYPDKVFRSSVLHSTQD  | 34             | 0.84  |
| 8    | ISSVLNDILSRLDKVEAEVQ  | 973            | 0.83  |
| 8    | AGTITSGWTFGAGAALQIPF  | 879            | 0.83  |
| 8    | ISVTTEILPVSMTKTSVDCT  | 720            | 0.83  |
| 8    | PCSFQGVSVITPGTNTSNQV  | 589            | 0.83  |
| 9    | QDKNTQEVFAQVKQIYKTPP  | 774            | 0.82  |
| 9    | QQFGRDIADTTDAVRDPQTL  | 563            | 0.82  |
| 9    | KNKCVNFNFNGLTGTGVLTE  | 535            | 0.82  |
| 9    | SNLKPFERDISTEIQAGST   | 459            | 0.82  |
| 9    | DCALDPLSEKCTLKSFTVE   | 290            | 0.82  |
| 9    | DLEGKQGNFKNLREFVFKNI  | 178            | 0.82  |
| 9    | VSQPFLMDLEGKQGNFKNLR  | 171            | 0.82  |
| 9    | YSSANNCTFEYVSQPFLMDL  | 160            | 0.82  |
| 10   | PVAIHADQLTPTWRVYSTGS  | 621            | 0.81  |
| 10   | GCVIAWNSNNLDSKVGGNYN  | 431            | 0.81  |
| 11   | ECSNLLQYGSFCTQLNRAL   | 748            | 0.80  |
| 11   | GVSPTKLNLCFTNVYADSF   | 381            | 0.80  |
| 12   | LVKQLSSNFGAISSVLNDIL  | 962            | 0.79  |
| 12   | GVYFASTEKSNIIRGWIFGT  | 89             | 0.79  |
| 12   | CGKGYHLSFPQSAPHGVVF   | 1043           | 0.79  |
| 13   | ASQSIIAYTMSLGAENSVAY  | 688            | 0.78  |
| 13   | NSPRRARSVASQSIIAYTMS  | 679            | 0.78  |
| 13   | NIDGYFKIYSKHTPINLVRD  | 196            | 0.78  |
| 14   | GDIAARDLCAQKFNGLTVL   | 842            | 0.77  |
| 14   | DPSKPSKRSFIEDLLFNKVT  | 808            | 0.77  |
| 14   | SVDCTMYICGDSTECNLLL   | 735            | 0.77  |
| 15   | VVNQNAQALNTLVKQLSSNF  | 951            | 0.76  |
| 15   | KQYGDCLGDIAARDLCAQK   | 835            | 0.76  |
| 15   | LLHAPATVCGPKKSTNLVKN  | 517            | 0.76  |
| 15   | LLKYNENGTITDAVDCALDP  | 276            | 0.76  |
| 15   | GLIAIVMVTIMLCCMTSCCS  | 1223           | 0.76  |
| 15   | SGINASVVNIQKEIDRLNEV  | 1170           | 0.76  |

# SUPPLEMENTARY DATA

|    |                        |      |      |
|----|------------------------|------|------|
| 16 | RQIAPGQTGKIADYNYKLPD   | 408  | 0.75 |
| 16 | ITRFQTLALHRSYLTPGDS    | 235  | 0.75 |
| 16 | SQCVNLTRTQLPPAYTNSF    | 13   | 0.75 |
| 17 | ITPGTNTSNQVAVLYQDVNC   | 598  | 0.74 |
| 17 | LTGTGVLTESNKKFLPFQQF   | 546  | 0.74 |
| 17 | LYNSASFSTFKCYGVSPTKL   | 368  | 0.74 |
| 17 | KSFTVEKGIYQTSNFRVQPT   | 304  | 0.74 |
| 17 | LIVNNAATNVVIVKVECFQFCN | 118  | 0.74 |
| 17 | VVIGIVNNTVYDPLQPELDS   | 1128 | 0.74 |
| 18 | CTQLNRALTGIAVEQDKNTQ   | 760  | 0.73 |
| 18 | YFPLQSYGFQPTNGVGYQPY   | 489  | 0.73 |
| 18 | FSALEPLVDLPIGINITRFQ   | 220  | 0.73 |
| 18 | KSWMESEFRVYSSANNCTFE   | 150  | 0.73 |
| 18 | CSCGSCCKFDEDDSEPVKLG   | 1248 | 0.73 |
| 19 | GSNVFQTRAGCLIGAEHVNN   | 639  | 0.72 |
| 19 | VTIMLCCMTSCCCLKGCCS    | 1230 | 0.72 |
| 19 | FPREGVFVSNGTHWFVTQRN   | 1089 | 0.72 |
| 20 | TPTWRVYSTGSNVFQTRAGC   | 630  | 0.71 |
| 20 | GKIADYNYKLPDDFTGCVIA   | 416  | 0.71 |
| 20 | GTITDAVDCALDPLSETKCT   | 283  | 0.71 |
| 20 | KEELDKYFKNHTSPDVLGD    | 1149 | 0.71 |
| 21 | SALGKLQDVVNQNAQALNTL   | 943  | 0.70 |
| 21 | QIYKTPPIKDFGGFNFSQIL   | 787  | 0.70 |
| 21 | SKVGGNYNYLYRFRKSNLK    | 443  | 0.70 |
| 21 | TSCCCLKGCCSCGSCCKFD    | 1238 | 0.70 |
| 22 | QPTESIVRFPNITNLCPFGE   | 321  | 0.69 |
| 22 | FKNHTSPDVLGDISGINAS    | 1156 | 0.69 |
| 22 | NTVYDPLQPELDSFKEELDK   | 1135 | 0.69 |
| 22 | HWFVTQRNFYEPQIITDNT    | 1101 | 0.69 |
| 23 | SSGWTAGAAAYYVGYLQPR    | 255  | 0.68 |
| 23 | GQSKRVDFCGKGYHLSFPQ    | 1035 | 0.68 |
| 24 | SNKKFLPFQQFGRDIADTTD   | 555  | 0.66 |
| 25 | PKKSTNLVKNKCVNFNFNGL   | 527  | 0.65 |
| 25 | QELGKYEQYIKWPWYIWLGF   | 1201 | 0.65 |
| 26 | FNSAIGKIQDSLSTASALG    | 927  | 0.64 |
| 26 | WTFGAGAALQIPFAMQMA YR  | 886  | 0.64 |
| 27 | IDRLNEVAKNLNESLIDLQE   | 1183 | 0.63 |
| 28 | QKFNGLTVLPPLLTDEMIAQ   | 853  | 0.62 |
| 29 | IKDFGGFNFSQILPDPKPS    | 794  | 0.61 |
| 29 | VPAQEKNF T TAPAICHGKA  | 1068 | 0.61 |
| 30 | EIQAGSTPCNGVEGFNCYF    | 471  | 0.60 |
| 30 | ICHDGKAHFPREGVFVSNGT   | 1081 | 0.60 |
| 31 | AYSNNSIAIPTNFTISVTTE   | 706  | 0.59 |
| 32 | ECDIPGAGICASYQTQNS     | 661  | 0.58 |
| 32 | FPQSAPHGVVFLHVTVYVPAQ  | 1052 | 0.58 |
| 33 | KMSECVLQSKRVDFCGKGY    | 1028 | 0.57 |
| 34 | EIRASANLAATKMSECVLGQ   | 1017 | 0.56 |
| 35 | IQDSLSTASALGKLQDVVN    | 934  | 0.54 |

## SUPPLEMENTARY DATA

**Table S2.** The B cell epitopes of the newly emerging variant (B.1.135) of SARS-CoV-2 along S protein with their length predicted by ABCPred server.

| Rank | Sequence              | Start position | score |
|------|-----------------------|----------------|-------|
| 1    | VTLADAGFIKQYGDCLGDIA  | 826            | 0.90  |
| 1    | IGAEHVNNSYECDIPIGAGI  | 651            | 0.90  |
| 1    | TNVYADSFVIRGDEVQRQIAP | 393            | 0.90  |
| 1    | VYYHKNNKSWMESEFRVYSS  | 143            | 0.90  |
| 2    | IHVSGTNGTKRFANPVLPFN  | 68             | 0.89  |
| 3    | KHTPINLVRGLPQGFSALEP  | 206            | 0.88  |
| 3    | VVIKVCEFQFCNDPFLGVYY  | 126            | 0.88  |
| 4    | DRLITGRLQSLQTYVTQQLI  | 994            | 0.87  |
| 4    | GVNCTEVPVAIHADQLTPTW  | 614            | 0.87  |
| 4    | PCSFGGVSVITPGTNTSNQV  | 589            | 0.87  |
| 4    | PFGEVFNATRFASVYAWNRK  | 337            | 0.87  |
| 4    | VTQQLIRAAEIRASANLAAT  | 1008           | 0.87  |
| 5    | SYLTPGDSSSGWTAGAAAAYY | 247            | 0.86  |
| 5    | DNTFVSGNCDVVIGIVNNTV  | 1118           | 0.86  |
| 5    | TTLDSKTQSLIVNNAATNVV  | 108            | 0.86  |
| 6    | KQYGDCLGDIAARDLICAQK  | 835            | 0.85  |
| 6    | RSSVLHSTQDLFLPFFSNVT  | 44             | 0.85  |
| 6    | KRISNCVADYSVLYNSASFS  | 356            | 0.85  |
| 6    | APRDGQAYVRKDGWVLLST   | 1216           | 0.85  |
| 7    | NVLYENQKLIANQFNSAIGK  | 914            | 0.84  |
| 7    | RGVYYPDKVFRSSVLHSTQD  | 34             | 0.84  |
| 8    | ISSVLNDILSRLDKVEAEVQ  | 973            | 0.83  |
| 8    | AGTITSGWTFGAGAAALQIPF | 879            | 0.83  |
| 8    | ISVTTEILPVSMTKTSVDCT  | 720            | 0.83  |
| 8    | PVAIHADQLTPTWRVYSTGS  | 621            | 0.83  |
| 9    | QDKNTQEVFAQVKQIYKTPP  | 774            | 0.82  |
| 9    | ITPGTNTSNQVAVLYQGVNC  | 598            | 0.82  |
| 9    | QQFGRDIADTTDAVRDPQTL  | 563            | 0.82  |
| 9    | KNKCVNFNENGLTGTGVLTE  | 535            | 0.82  |
| 9    | SNLKPFERDISTEIQAGST   | 459            | 0.82  |
| 9    | DLEGKQGNFKNLREFVFKNI  | 178            | 0.82  |
| 9    | VSQPFLMDLEGKQGNFKNLR  | 171            | 0.82  |
| 9    | YSSANNCTFEYVSQPFLMDL  | 160            | 0.82  |
| 10   | GVYFASTEKSNIRGWIFGT   | 89             | 0.81  |
| 10   | YQPYRVVLSFELLHAPATV   | 505            | 0.81  |
| 10   | GCVIAWNSNNLDSKVGGNYN  | 431            | 0.81  |
| 11   | ECSNLLLQYGSFCTQLNRAL  | 748            | 0.80  |
| 11   | GVSPTKLNDLCFTNVYADSF  | 381            | 0.80  |
| 12   | LVKQLSSNFGAISSVLNDIL  | 962            | 0.79  |
| 12   | CGKGYHLMSFPQSAPHGVVF  | 1043           | 0.79  |
| 13   | ASQSIIAYTMSLGVENSVAY  | 688            | 0.78  |
| 13   | NSPGSASSVASQSIIAYTMS  | 679            | 0.78  |
| 13   | NIDGYFKIYSKHTPINLVRG  | 196            | 0.78  |
| 14   | DPSKPSKRFSIEDLLFNKVT  | 808            | 0.77  |
| 14   | SVDCTMYICGDSTECNLLL   | 735            | 0.77  |
| 14   | SHPQFEKGGGSGGGSGGSA   | 1261           | 0.77  |
| 15   | VVNQNAQALNTLVKQLSSNF  | 951            | 0.76  |
| 15   | KSFTVEKGIYQTSNFRVQPT  | 304            | 0.76  |
| 15   | DCALDPLSETKCTLKSFTVE  | 290            | 0.76  |
| 15   | LLKYNENGTITDAVDCALDP  | 276            | 0.76  |
| 15   | YVRKDGWVLLSTFLGRSLE   | 1223           | 0.76  |

# SUPPLEMENTARY DATA

|    |                        |      |      |
|----|------------------------|------|------|
| 15 | SGINASVVNIQKEIDRLNEV   | 1170 | 0.76 |
| 16 | ARDLICAQKFNGLTVLPPLL   | 846  | 0.75 |
| 16 | RQIAPGQTGNIADYNYKLPD   | 408  | 0.75 |
| 16 | ITRFQTLALHISYLTPGDS    | 235  | 0.75 |
| 17 | LTGTGVLTESNKKFLPFQQF   | 546  | 0.74 |
| 17 | LYNSASFSTFKCYGVSPTKL   | 368  | 0.74 |
| 17 | LIVNNATNVVIKVFCEFCN    | 118  | 0.74 |
| 17 | VVIGIVNNTVYDPLPELDS    | 1128 | 0.74 |
| 18 | LLHAPATVCGPKKSTNLVKN   | 517  | 0.73 |
| 18 | YFPLQSYGFQPTYGVGYQPY   | 489  | 0.73 |
| 18 | FSALEPLVDLPIGINITRFQ   | 220  | 0.73 |
| 18 | KSWMESEFRVYSSANNCTFE   | 150  | 0.73 |
| 18 | SQCVNFTTRTQLPPAYTNSF   | 13   | 0.73 |
| 18 | PGHHHHHHHSAWSHPQFEK    | 1248 | 0.73 |
| 19 | CTQLNRALTGIAVEQDKNTQ   | 760  | 0.72 |
| 19 | GSNVFQTRAGCLIGAEHVNN   | 639  | 0.72 |
| 19 | WVLLSTFLGRSLEVLFGQPG   | 1230 | 0.72 |
| 19 | FPREGVFSNGTHWFVTQRN    | 1089 | 0.72 |
| 20 | GLTVLPPLLTDEMI AQY TSA | 857  | 0.71 |
| 20 | TPTWRVYSTGSNVFQTRAGC   | 630  | 0.71 |
| 20 | QPTYGVGYQPYRVVLSFEL    | 498  | 0.71 |
| 20 | GNIADYNYKLPDDFTGCVIA   | 416  | 0.71 |
| 20 | GTITDAVDCALDPLSETKCT   | 283  | 0.71 |
| 20 | SSGWTAGAAAYVGYLQPR T   | 255  | 0.71 |
| 20 | KEELDKYFKNHTSPDVLGD    | 1149 | 0.71 |
| 21 | SALGKLQDVVNQNAQALNTL   | 943  | 0.70 |
| 21 | QIYKTPPIKDFGGFNFSQIL   | 787  | 0.70 |
| 21 | SKVGGNYNYLYRFRKSNLK    | 443  | 0.70 |
| 21 | GRSLEVLFGQPGHHHHHHHH   | 1238 | 0.70 |
| 22 | DEMI AQY TSALLAGTITSGW | 867  | 0.69 |
| 22 | QPTESIVRFPNITNLCPFGE   | 321  | 0.69 |
| 22 | FKNHTSPDVDLGDISGINAS   | 1156 | 0.69 |
| 22 | NTVYDPLQPELDSFKEELDK   | 1135 | 0.69 |
| 22 | HWFVTQRNFYEQIITDNT     | 1101 | 0.69 |
| 23 | GQSKRVDFCGKGYHLMSPQ    | 1035 | 0.68 |
| 24 | SNKKFLPFQQFGRDIADTTD   | 555  | 0.66 |
| 25 | PKKSTNLVKNKCVNFNFNGL   | 527  | 0.65 |
| 25 | QELGKYEQGSYIPEAPRDG    | 1201 | 0.65 |
| 26 | FNSAIGKIQDLSSTASALG    | 927  | 0.64 |
| 26 | WTFGAGAALQIPFAMQMAYR   | 886  | 0.64 |
| 26 | SNQVAVLYQGVNCTEVPVAI   | 605  | 0.64 |
| 27 | IDRLNEVAKNLNESLIDLQE   | 1183 | 0.63 |
| 28 | IKDFGGFNFSQILPDPSKPS   | 794  | 0.61 |
| 28 | TRTQLPPAYTNSFTRGVYYP   | 20   | 0.61 |
| 28 | VPAQEKNFTTAPAICHGDKA   | 1068 | 0.61 |
| 29 | EIQAGSTPCNGVKGFNCYF    | 471  | 0.60 |
| 29 | ICHDGKAHFPREGVFSNGT    | 1081 | 0.60 |
| 30 | AYSNNSIAIPTNFTISVTTE   | 706  | 0.59 |
| 31 | ECDIPIGAGICASYQTQNS    | 661  | 0.58 |
| 31 | FPQSAPHGVVFLHVTVPAQ    | 1052 | 0.58 |
| 32 | KMSECVLGQSKRVDFCGKGY   | 1028 | 0.57 |
| 33 | EIRASANLAATKMSECVLGQ   | 1017 | 0.56 |
| 34 | IQDLSSTASALGKLQDVVN    | 934  | 0.54 |

# SUPPLEMENTARY DATA

**Table S3.** The B cell epitopes of the newly emerging variant (B.1.1.1.7) of SARS-CoV-2 S protein along with their length predicted by ABCPred server.

| Rank | Sequence              | Start position | Score |
|------|-----------------------|----------------|-------|
| 1    | KVTLADAGFIKQYGDCLGDI  | 822            | 0.93  |
| 1    | ADSFVIRGDEVQRQIAPGQTG | 394            | 0.93  |
| 1    | PGDSSSGWTAGAAAYVGYL   | 248            | 0.93  |
| 2    | SLLVNNAATNVVIVKCEVQF  | 114            | 0.91  |
| 3    | TKLNDLCFTNVYADSFVIRG  | 382            | 0.90  |
| 4    | LNDILARLDKVEAEVQIDRL  | 974            | 0.88  |
| 4    | SSNFGAISSVLNDILARLDK  | 964            | 0.88  |
| 4    | IIAYTMSLGAENSVAYSNS   | 689            | 0.88  |
| 4    | VFNATRFASVYAWNRKRISN  | 338            | 0.88  |
| 5    | QIDRLITGRLQSLQTYVTQQ  | 989            | 0.87  |
| 5    | DCLGDIAARDLCAQKFNGL   | 836            | 0.87  |
| 6    | VLTESNKKFLPFQQFGRDID  | 548            | 0.86  |
| 6    | LVDLPIGINITRFQTLALH   | 223            | 0.86  |
| 6    | INLVRDLPQGFSALEPLVDL  | 207            | 0.86  |
| 6    | EFVFKNIDGYFKIYSKHTPI  | 188            | 0.86  |
| 6    | YVSQPFLMDLEGKQGNFKNL  | 167            | 0.86  |
| 6    | RVYSSANNCTFEYVSQPFLM  | 155            | 0.86  |
| 6    | VNNTVYDPLQPELDSFKEEL  | 1130           | 0.86  |
| 7    | PSKRSEFIEDLLFNKVTLADA | 809            | 0.85  |
| 7    | EVPVAIHADQLTPTWRVYST  | 616            | 0.85  |
| 7    | RVVVLSFELLHAPATVCGPK  | 506            | 0.85  |
| 7    | RSSVLHSTQDLFLPFFSNVT  | 44             | 0.85  |
| 8    | RGVYYPDKVFRSSVLHSTQD  | 34             | 0.84  |
| 9    | SVDCTMYICGDSTECNLLL   | 732            | 0.83  |
| 9    | TEILPVSMTKTSVDCTMYIC  | 721            | 0.83  |
| 9    | TNLVKNKCVNFNFNGLTGTG  | 528            | 0.83  |
| 10   | TLEILDITPCSFQGGVSVITP | 578            | 0.82  |
| 10   | VNFNFNGLTGTGVLTESNKK  | 536            | 0.82  |
| 10   | DPLSETKCTLKSFTVEKGIY  | 291            | 0.82  |
| 11   | SNIIRGWIFGTTLDLSTQSL  | 96             | 0.81  |
| 11   | TPPIKDFGGFNFSQILPDPS  | 788            | 0.81  |
| 11   | NTQEVFAQVKQIYKTPPIKD  | 774            | 0.81  |
| 11   | HVNNSYECDIPIGAGICASY  | 652            | 0.81  |
| 11   | TRFQTLALHRSYLTPGDSS   | 233            | 0.81  |
| 12   | FAMQMAYRFNGIGVTQNVLY  | 895            | 0.80  |
| 12   | RDIDDTTDAVRDPQLEILD   | 564            | 0.80  |
| 12   | HHHHHHSASWHPQFEKGGGS  | 1249           | 0.80  |
| 13   | TPGTNTSNQVAVLYQGVNCT  | 596            | 0.79  |
| 13   | SVLYNSASFSTFKCYGVSP   | 363            | 0.79  |
| 13   | DKYFKNHTSPDVLGDISGI   | 1150           | 0.79  |
| 14   | TQLNRALTGIAVEQDKNTQE  | 758            | 0.78  |
| 14   | TLDSKTQSLLVNNAATNVVI  | 107            | 0.78  |
| 15   | AQYTSALLAGTITSGWTFGA  | 868            | 0.77  |
| 15   | PLLTDEMIAQYTSALLAGTI  | 860            | 0.77  |
| 15   | GGFNFSQILPDPSKPSKRSF  | 795            | 0.77  |
| 15   | SNLLLQYGSFCTQLNRALTG  | 747            | 0.77  |
| 15   | LQSYGFQPTYGVGYQPVRVV  | 489            | 0.77  |
| 15   | PFERDISTEIQAGSTPCNG   | 460            | 0.77  |
| 15   | VEKGIYQTSNFRVQPTESIV  | 305            | 0.77  |
| 16   | NQKLIANQFNSAIGKIQDSL  | 916            | 0.76  |
| 16   | TFGAGAALQIPFAMQMAYRF  | 884            | 0.76  |
| 16   | NSIAIPINFITISVTTEILPV | 707            | 0.76  |

# SUPPLEMENTARY DATA

|    |                       |      |      |
|----|-----------------------|------|------|
| 16 | ISGTNGTKRFDNPVLPFNDG  | 68   | 0.76 |
| 16 | LPDDFTGCVIAWNSNNLDSK  | 422  | 0.76 |
| 16 | DISGINASVVNIQKEIDRLN  | 1165 | 0.76 |
| 17 | QKFNGLTVLPPLLTDEMAIQ  | 850  | 0.75 |
| 17 | AENSVAYSNNIAIPINFTI   | 698  | 0.75 |
| 17 | HAPATVCGPKKSTNLVKNKC  | 516  | 0.75 |
| 17 | VQPTESIVRFPNITNLCPFG  | 317  | 0.75 |
| 17 | KQGNFKNLREFVFKNIDGYF  | 179  | 0.75 |
| 17 | SQCVNLTTRTQLPPAYTNSF  | 13   | 0.75 |
| 17 | YEPQIITHTNTFVSGNCDVV  | 1107 | 0.75 |
| 17 | SNGTHWFVTQRNFYEPQIT   | 1094 | 0.75 |
| 18 | KCYGVSPTKLNLCFTNVYA   | 375  | 0.74 |
| 18 | QPRTFLLKYNENGTITDAVD  | 268  | 0.74 |
| 18 | QGSYIPEAPRDGQAYVRKD   | 1205 | 0.74 |
| 19 | KRISNCVADYSVLYNSASF   | 353  | 0.73 |
| 19 | AICHDGKAHFREGVVFVSN   | 1077 | 0.73 |
| 20 | ALNTLVKQLSSNFGAISSVL  | 955  | 0.72 |
| 20 | NYLYRFRKSNLKPFRDIS    | 447  | 0.72 |
| 20 | PGQTGKIADYNYKLPDDFTG  | 409  | 0.72 |
| 20 | LSTFLGRSLEVLFGQPGHHH  | 1230 | 0.72 |
| 21 | FDNPVLPFNDGVYFASTEKS  | 77   | 0.71 |
| 21 | RVYSTGSNVVFQTRAGCLIGA | 631  | 0.71 |
| 21 | DAVDCALDPLSETKCTLKS   | 284  | 0.71 |
| 21 | TFVSGNCDVVIGIVNNTVYD  | 1117 | 0.71 |
| 21 | CVLGQSKRVDFCGKGYHLMS  | 1029 | 0.71 |
| 22 | FQFCNDPFLGVYHKNNKSWM  | 131  | 0.70 |
| 22 | SLEVLFGQPGHHHHHHHSA   | 1237 | 0.70 |
| 22 | VPAQEKNFTTAPAICHDGKA  | 1065 | 0.70 |
| 23 | TEIYQAGSTPCNGVEGFNCY  | 467  | 0.69 |
| 23 | PQSAPHGVVFLHVTYVPAQE  | 1050 | 0.69 |
| 23 | CGKGYHLMSFPQSAPHGVVF  | 1040 | 0.69 |
| 24 | TAGAAAYVGYLQPRTFLLK   | 256  | 0.68 |
| 24 | QQLIRAAEIRASANLAATKM  | 1007 | 0.68 |
| 25 | PIGAGICASYQTQTNHSGSA  | 662  | 0.67 |
| 25 | QTRAGCLIGAEHVNNSECD   | 641  | 0.67 |
| 26 | SALGKLQDVVNQNAQALNTL  | 940  | 0.66 |
| 26 | FLPFQQFGRDIDDTDAVRD   | 556  | 0.66 |
| 27 | AWNSNNLDSKVGGNYNLYR   | 432  | 0.65 |
| 28 | KYNENGTITDAVDCALDPLS  | 275  | 0.64 |
| 28 | AWSHPQFEKGGSGGGGSGG   | 1256 | 0.64 |
| 28 | QKEIDRLNEVAKNLNESLID  | 1177 | 0.64 |
| 29 | PNITNLCPFGVEVFNATRFAS | 327  | 0.61 |
| 30 | QSLQTYVTQQLIRAAEIRAS  | 999  | 0.60 |
| 31 | NEVAKNLNESLIDLQELGKY  | 1184 | 0.59 |
| 32 | NSAIGKIQDLSSTASALGK   | 925  | 0.57 |
| 32 | VFLHVTYVPAQEKNFTTAPA  | 1058 | 0.57 |
| 32 | SANLAATKMSECVLGQSKRV  | 1018 | 0.57 |
| 33 | DSLSTASALGKLQDVVNQN   | 933  | 0.54 |
| 34 | STPCNGVEGFNCYFPLQSYG  | 474  | 0.52 |

# SUPPLEMENTARY DATA

**Table S4.** The B cell epitopes of the newly emerging variant (B.1.1.28) of SARS-CoV-2 S protein along with their length predicted by ABCPred server.

| Rank | Sequence              | Start position | Score |
|------|-----------------------|----------------|-------|
| 1    | VTLADAGFIKQYGDCLGDIA  | 826            | 0.90  |
| 1    | IGAEHVNNSYECDIPIGAGI  | 651            | 0.90  |
| 1    | TNVYADSFVIRGDEVQRQIAP | 393            | 0.90  |
| 1    | VYYHKNNKSWMESEFRVYSS  | 143            | 0.90  |
| 2    | IHVSGTNGTKRFDNPVLPFN  | 68             | 0.89  |
| 2    | SYLTPGDSSSGWTAGAAAYY  | 247            | 0.89  |
| 3    | KHTPINLVRDLPQGFSALEP  | 206            | 0.88  |
| 3    | VVIKVCDFQFCNDPFLGVYY  | 126            | 0.88  |
| 4    | DRLITGRQLSLOTQYVTQQLI | 994            | 0.87  |
| 4    | GVNCTEVPVAIHADQLTPTW  | 614            | 0.87  |
| 4    | PCSFGGVSVITPGTNTSNQV  | 589            | 0.87  |
| 4    | PFGEVFNATRFASVYAWNRRK | 337            | 0.87  |
| 4    | VTQQLIRAAEIRASANLAAT  | 1008           | 0.87  |
| 5    | DNTFVSGNCDVVIGIVNNTV  | 1118           | 0.86  |
| 5    | TTLDSKTQSLIVNNAATNVV  | 108            | 0.86  |
| 6    | KQYGDCLGDIAARDLICAQK  | 835            | 0.85  |
| 6    | RSSVLHSTQDLFLPFFSNVT  | 44             | 0.85  |
| 6    | KRISNCVADYSVLVNSASFS  | 356            | 0.85  |
| 6    | APRDGQAYVRKDGWVLLST   | 1216           | 0.85  |
| 7    | NVLYENQKLIANQFNSAIGK  | 914            | 0.84  |
| 7    | RGVYYDPKVRSSVLHSTQD   | 34             | 0.84  |
| 8    | ISSVLNDILSRDKVEAEVQ   | 973            | 0.83  |
| 8    | AGTITSGWTFGAGAALQIPF  | 879            | 0.83  |
| 8    | ISVTTEILPVSMTKTSVDCT  | 720            | 0.83  |
| 8    | PVAIHADQLTPTWRVYSTGS  | 621            | 0.83  |
| 9    | QDKNTQEVFAQVKQIYKTPP  | 774            | 0.82  |
| 9    | QQFGRDIADTTDAVRDPQTL  | 563            | 0.82  |
| 9    | KNKCVNFNFNGLTGTGVLTE  | 535            | 0.82  |
| 9    | SNLKPFERDISTEIQAGST   | 459            | 0.82  |
| 9    | DCALDPLSEKTKLKSFTVE   | 290            | 0.82  |
| 9    | DLEGKQGNFKNLREFVFKNI  | 178            | 0.82  |
| 9    | VSQPFLMDLEGKQGNFKNLR  | 171            | 0.82  |
| 9    | YSSANNCTFEYVSQPFLMDL  | 160            | 0.82  |
| 10   | YQPYRVVLSFELLHAPATV   | 505            | 0.81  |
| 10   | GCVIAWNSNNLDSKVGGNYN  | 431            | 0.81  |
| 11   | ECSNLLLQYGSFCTQLNRAL  | 748            | 0.80  |
| 11   | GVSPTKLNLDLFTNVYADSF  | 381            | 0.80  |
| 12   | LVKQLSSNFGAISSVLNDIL  | 962            | 0.79  |
| 12   | GVYFASTEKSNIIRGWIFGT  | 89             | 0.79  |
| 12   | CGKGYHLMSFPQSAPHGVVF  | 1043           | 0.79  |
| 13   | ASQSIIAYTMSLGAENSVAY  | 688            | 0.78  |
| 13   | NSPGSASSVASQSIIAYTMS  | 679            | 0.78  |
| 13   | NIDGYFKIYSKHPTINLVRD  | 196            | 0.78  |
| 14   | DPSKPSKRSFIEDLLFNKVT  | 808            | 0.77  |
| 14   | SVDCTMYICGDSTECNLLL   | 735            | 0.77  |
| 14   | SHPQFEKGGGSGGGGSGGSA  | 1261           | 0.77  |
| 15   | VVNQNAQALNTLVKQLSSNF  | 951            | 0.76  |
| 15   | LLKYNENGTITDAVDCALDP  | 276            | 0.76  |
| 15   | YVRKDGWVLLSTFLGRSLE   | 1223           | 0.76  |
| 15   | SGINASVVNIQKEIDRLNEV  | 1170           | 0.76  |
| 16   | ARDLICAQKFNGLTVLPPLL  | 846            | 0.75  |
| 16   | RQIAPGQTGNIADYNYKLPD  | 408            | 0.75  |

# SUPPLEMENTARY DATA

|    |                       |      |      |
|----|-----------------------|------|------|
| 16 | ITRFQTLALHRSYLTPGDS   | 235  | 0.75 |
| 16 | SQCVNLTRTQLPPAYTNSF   | 13   | 0.75 |
| 17 | LTGTGVLTESNKKFLPFQQF  | 546  | 0.74 |
| 17 | LYNSASFSTFKCYGVSPTKL  | 368  | 0.74 |
| 17 | KSFTVEKGIYQTSNFRVQPT  | 304  | 0.74 |
| 17 | LIVNNATNVVIKVEFQFCN   | 118  | 0.74 |
| 17 | VVIGIVNNTVYDPLQPELDS  | 1128 | 0.74 |
| 18 | LLHAPATVCGPKKSTNLVKN  | 517  | 0.73 |
| 18 | YFPLQSYGFQPTYGVGYQPY  | 489  | 0.73 |
| 18 | FSALEPLVDLPIGINITRFQ  | 220  | 0.73 |
| 18 | KSWMESEFRVYSSANNCTFE  | 150  | 0.73 |
| 18 | PGHHHHHHHSAWSHPQFEK   | 1248 | 0.73 |
| 19 | CTQLNRALTGIAVEQDKNTQ  | 760  | 0.72 |
| 19 | GSNVFQTRAGCLIGAHEVNN  | 639  | 0.72 |
| 19 | WVLLSTFLGRSLEVLFGQPG  | 1230 | 0.72 |
| 19 | FPREGVVFVSNQTHWVFTQRN | 1089 | 0.72 |
| 20 | TPTWRVYSTGSNVFOQRAGC  | 630  | 0.71 |
| 20 | QPTYGVGYQPYRVVLSFEL   | 498  | 0.71 |
| 20 | GNIADYNYKLPDDFTGCVIA  | 416  | 0.71 |
| 20 | GTITDAVDCALDPLSETKCT  | 283  | 0.71 |
| 20 | KEELDKYFKNHTSPDVLGD   | 1149 | 0.71 |
| 21 | SALGKLQDVVNQNAQALNTL  | 943  | 0.70 |
| 21 | QIYKTPPIKDFGGFNFSQIL  | 787  | 0.70 |
| 21 | SKVGGNYNYLYRFRKSNLK   | 443  | 0.70 |
| 21 | GRSLEVLFGQPGHHHHHHHH  | 1238 | 0.70 |
| 22 | QPTESIVRFPNITNLCPFGE  | 321  | 0.69 |
| 22 | FKNHTSPDVLGDISGINAS   | 1156 | 0.69 |
| 22 | NTVYDPLQPELDSFKEELDK  | 1135 | 0.69 |
| 22 | HWFVTQRNFYEPQIITDNT   | 1101 | 0.69 |
| 23 | SSGWTAGAAAYYVGYLQPR   | 255  | 0.68 |
| 23 | GQSKRVDFCGKGYHLMSFPQ  | 1035 | 0.68 |
| 24 | SNKKFLPFQFGRDIADTTD   | 555  | 0.66 |
| 25 | PKKSTNLVKNKCVNFNFNGL  | 527  | 0.65 |
| 25 | QELGKYEQGSYIPEAPRDG   | 1201 | 0.65 |
| 26 | FNSAIGKIQDLSSTASALG   | 927  | 0.64 |
| 26 | WTFGAGAALQIPFAMQMAYR  | 886  | 0.64 |
| 26 | SNQVAVLYQGVNCTEVPVAI  | 605  | 0.64 |
| 27 | IDRLNEVAKNLNESLIDLQE  | 1183 | 0.63 |
| 28 | IKDFGGFNFSQILPDPKPS   | 794  | 0.61 |
| 28 | VPAQEKNFTTAPAICHDGKA  | 1068 | 0.61 |
| 29 | GLTVLPLLTDemiaQY TSA  | 706  | 0.59 |
| 29 | EIYQAGSTPCNGVKGFNCYF  | 857  | 0.60 |
| 29 | ICHDGKAHPREGVVSNGT    | 471  | 0.60 |
| 30 | AYSNNIAIPTNFTISVTTE   | 1081 | 0.60 |
| 31 | ECDIPIGAGICASYQTQNS   | 661  | 0.58 |
| 31 | FPQSAPHGVVFLHVTVVPAQ  | 1052 | 0.58 |
| 32 | KMSECVLQSKRVDFCGKGY   | 1028 | 0.57 |
| 33 | EIRASANLAATKMSECVLGQ  | 1017 | 0.56 |
| 34 | IQDLSSTASALGKLQDVVN   | 934  | 0.54 |