**Table S1:** Physico-Chemical parameters of spike (S) protein computed through ExPASy ProtParam server**.**

|  |  |
| --- | --- |
| Parameters | S protein |
| Mol. Weight | 149368.04 Dalton |
| No. of amino acids | 1353 |
| Theoretical *pI* | 5.70 |
| Instability index (II) | 36.60 (stable) |
| No. of Negatively Charged Residues (Asp + Glu) | 112 |
| No. of Positively Charged Residues (Arg + Lys) | 95 |
| Aliphatic Index | 82.71 |
| Grand average of Hydropathicity (GRAVY) | -0.074 |
| Atomic Composition | |  |  | | --- | --- | | Carbon | 6682 | | Hydrogen | 10245 | | Nitrogen | 1735 | | Oxygen | 2029 | | Sulfur |  | |
| Amino Acid Composition | |  |  |  | | --- | --- | --- | | Ala (A) | 88 | 6.5% | | Arg (R) | 44 | 3.3% | | Asn (N) | 77 | 5.7% | | Asp (D) | 66 | 4.9% | | Cys (C) | 42 | 3.1% | | Gln (Q) | 72 | 5.3% | | Glu (E) | 46 | 3.4% | | Gly (G) | 92 | 6.8% | | His (H) | 20 | 1.5% | | Ile (I) | 73 | 5.4% | | Leu (L) | 120 | 8.9% | | Lys (K) | 51 | 3.8% | | Met (M) | 21 | 1.6% | | Phe (F) | 71 | 5.2% | | Pro (P) | 62 | 4.6% | | Ser (S) | 134 | 9.9% | | Thr (T) | 92 | 6.8% | | Trp (W) | 10 | 0.7% | | Tyr (Y) | 76 | 5.6% | | Val (V) | 96 | 7.1% | | Pyl (O) | 0 | 0% | | Sec (U) | 0 | 0% | |

**Table S2:** Predicteddisulphide bonds within residues of spike protein via DiANNA 1.1 web

Server. The bonds with lowest Score indicated as red colours are weak bonds.

|  |
| --- |
| Serial no positions peptide bonds scores |
| 1 30-1106 SVKSACIEVDI-DKVNECVKAQS 0.96107 |
| 2 176-1319 LLPDGCGTLLR-VFFILCCTGCG 0.0104 |
| 3 185-817 LRAFYCILEPR-NGFQKCEQLLR 0.01042 |
| 4 195-237 RSGNHCPAGNS-FNLRNCTFMYT 0.72506 |
| 5 214-713 TPATDCSDGNY-QTPVGCVLGLV 0.99878 |
| 6 339-650 RRAIDCGFNDL-DGNYYCLRACV 0.98513 |
| 7 349-383 LSQLHCSYESF-AEGVECDFSPL 0.99964 |
| 8 407-1320 LVFTNCNYNLT-FFILCCTGCGT 0.01176 |
| 9 425-828 VNDFTCSQISP-EYGQFCSKINQ 0.95301 |
| 10 437-503 AIASNCYSSLI-SYINKCSRLLS 0.85147 |
| 11 478-620 FSNPTCLILAT-GVFQNCTAVGV 0.95997 |
| 12 526-654 NQYSPCVSILP-YCLRACVSVPV 0.9526 |
| 13 585-736 DTNSVCPKLEF-LGQSLCALPDT 0.98408 |
| 14 603-1117 SQLGNCVEYSL-KRSGFCGQGTH 0.99715 |
| 15 679-727 FGSVACEHISS-LFVEDCKLPLG 0.88581 |
| 16 806-811 KVTVDCKQYVC-CKQYVCNGFQK 0.99595 |
| 17 912-1164 QGYDDCMQQGP-ANPTNCIAPVN 0.43292 |
| 18 925-1337 ARDLICAQYVA-KCNRCCDRYEE 0.99536 |
| 19 1156-1336 SAYGLCDAANP-LKCNRCCDRYE 0.98674 |
| 20 1313-1327 VALALCVFFIL-GCGTNCMGKLK 0.01058 |
| 21 1323-1333 LCCTGCGTNCM-MGKLKCNRCCD 0.99851 |

**Table S3:** Emini surface accessibility prediction results computed through IEDB Analysis Resource**.**

|  |
| --- |
| Position Residue Start End Peptide Score |
| 306 D 304 309 QSDRKA 4.076 |
| 468 N 466 471 QFNYKQ 3.478 |
| 510 D 508 513 SDDRTE 4.862 |
| 540 Y 538 543 GDYYRK 4.224 |
| 541 Y 539 544 DYYRKQ 7.392 |
| 542 R 540 545 YYRKQL 3.65 |
| 665 K 663 668 YDKETK 6.951 |
| 666 E 664 669 DKETKT 6.403 |
| 667 T 665 670 KETKTH 5.217 |
| 690 S 688 693 QYSRST 3.661 |
| 691 R 689 694 YSRSTR 4.14 |
| 692 S 690 695 SRSTRS 3.541 |
| 699 R 697 702 LKRRDS 3.763 |
| 700 R 698 703 KRRDST 6.585 |
| 701 D 699 704 RRDSTY 5.16 |
| 1102 K 1100 1105 KDKVNE 3.669 |
| 1110 Q 1108 1113 KAQSKR 4.881 |
| 1176 N 1174 1179 KTNNTR 5.607 |
| 1290 T 1288 1293 NYTYYN 3.816 |
| 1291 Y 1289 1294 YTYYNK 4.745 |
| 1340 Y 1338 1343 DRYEEY 6.401 |
| 1341 E 1339 1344 RYEEYD 6.401 |

**Table S4:** Conservancy results of B-cells and T-cells (MHC Class-I and II) epitopes among all 8 MERS-CoV isolates of different countries (Saudi Arabia, Abu Dhabi, Jordan, Qatar, South Korea, Thailand, USA and UK) have been shown. The analyses were done using the IEDB Analysis Resource.

|  |  |  |  |
| --- | --- | --- | --- |
| Sr# | Sequences | Epitope length | Identity (8/8) |
| B-Cells peptides | | | |
| 1 | TPTESYVDVGPDSV | 14 | 100% |
| 2 | TPATDCSDGNYNRN | 14 | 100% |
| 3 | LEWFGITQTAQGVH | 14 | 100% |
| 4 | QLQMGFGITVQYGT | 14 | 100% |
| 5 | GNYTYYNKWPWYIW | 14 | 100% |
| 6 | RYEEYDLEPHKVHV | 14 | 100% |
| MHC class-I binding peptides | | | |
| 1 | YKLQPLTFL | 9 | 100% |
| 2 | LTLLEPVSI | 9 | 100% |
| 3 | ESAALSAQL | 9 | 100% |
| 4 | IAGLVALAL | 9 | 100% |
| 5 | AGYKVLPPL | 9 | 100% |
| 6 | WPRPIDVSK | 9 | 100% |
| MHC class-II binding peptides | | | |
| 1 | YCILEPRSG | 9 | 100% |
| 2 | LYFMHVGYY | 9 | 100% |
| 3 | MRLASIAFN | 9 | 100% |
| 4 | FGITQTAQG | 9 | 100% |
| 5 | VRIGAAANS | 9 | 100% |
| 6 | VYKLQPLTF | 9 | 100% |