

Table S1 CTL Epitopes predicted by IEDB Consensus Method

| Protein | | | | |
|-----------------|----------|---|--------------|----------------|
| Calcium Binding | | | | |
| Epitopes | Position | Alleles | Antigenicity | Immunogenicity |
| EVEAVIEAY | 285-293 | HLA-A*26:01 HLA-A*25:01 HLA-A*01:01 HLA-B*35:01 | 0.7113 | 0.34471 |
| FSPRRYRKL | 152-160 | HLA-B*14:02 HLA-C*07:02 HLA-E*01:01 HLA-B*08:01 HLA-C*06:02 | 1.0381 | 0.01308 |
| YLDEDYLHS | 387-395 | HLA-C*05:01 | 0.8030 | 0.13561 |
| DSDHDGIPN | 267-275 | HLA-C*08:02 HLA-C*05:01 | 0.5176 | 0.19909 |
| LEDEDHDMI | 318-326 | HLA-B*40:01 HLA-C*05:01 | 0.9741 | 0.19852 |
| IPDHLEGDI | 32-40 | HLA-C*08:02 HLA-B*51:01 HLA-B*53:01 | 1.3173 | 0.16476 |
| KQDNRLRL | 332-340 | HLA-B*48:01 HLA-A*02:06 | 0.8049 | 0.06153 |
| VEVEAVIEA | 284-292 | HLA-B*40:02 HLA-B*18:01 | 0.7580 | 0.36193 |
| DSDGDGVLD | 498-506 | HLA-C*05:01 HLA-C*08:02 | 1.7229 | 0.17921 |
| DKDTNNNGM | 294-302 | HLA-C*05:01 | 1.2454 | 0.04821 |
| ESDDDDDDD | 685-693 | HLA-C*05:01 | 2.2082 | 0.10368 |
| DSDGDGILD | 181-189 | HLA-C*08:02 HLA-C*05:01 | 1.4040 | 0.20064 |
| DTDDDETNN | 700-708 | HLA-C*05:01 | 1.3095 | 0.17435 |
| EGDINHNGI | 37-45 | HLA-C*05:01 | 2.0346 | 0.17961 |
| EDDLDGNGI | 364-372 | HLA-C*05:01 HLA-C*08:02 | 2.2002 | 0.06388 |
| QFSPRRYRK | 151-159 | HLA-A*31:01 | 1.2006 | 0.06138 |

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|---------------------------------|---------|---|--------|---------|
| | | HLA-C*04:01 | | |
| YDDDDDDNDG | 474-482 | HLA-C*05:01 | 1.7125 | 0.0795 |
| FYDDDDDDND | 473-481 | HLA-C*08:02 | 1.1230 | 0.08694 |
| KQDRRHKKI | 604-612 | HLA-A*32:01 | 1.5880 | 0.04143 |
| AKDTDGDGI | 514-522 | HLA-C*08:02 HLA-C*05:01 | 1.3628 | 0.13828 |
| DDDIDHAHY | 736-744 | HLA-C*05:01 | 0.7508 | 0.24509 |
| DRRHKKIAN | 606-614 | HLA-B*14:02 | 1.0397 | 0.01303 |
| DIHEDENKN | 550-558 | HLA-A*25:01 | 1.4391 | 0.09564 |
| Mycosubtilin synthase subunit C | | | | |
| RQLGFNVNL | 514-522 | HLA-B*48:01 HLA-A*32:01 HLA-B*40:01 HLA-A*02:06 HLA-B*27:05 HLA-B*39:01 HLA-B*40:02 | 1.5715 | 0.16947 |
| FIDPHTNHL | 262-270 | HLA-C*08:02 HLA-A*02:06 HLA-B*39:01 HLA-C*06:02 HLA-C*05:01 HLA-C*07:02 HLA-C*07:02 | 0.5218 | 0.07752 |
| RSRERARKV | 463-471 | HLA-C*15:02 HLA-C*06:02 HLA-A*30:01 HLA-C*07:01 | 1.9596 | 0.12246 |
| IVLTARYYY | 661-669 | HLA-A*29:02 HLA-A*30:02 HLA-A*11:01 HLA-B*57:01 | 1.1714 | 0.117 |
| YENPYEHTF | 669-677 | HLA-B*18:01 HLA-B*44:02 HLA-B*40:01 HLA-C*07:02 HLA-B*40:02 HLA-B*40:02 HLA-B*38:01 | 1.1243 | 0.12737 |

| | | | | |
|-----------|---------|--|--------|---------|
| | | HLA-A*23:01 | | |
| RYYYENPYE | 666-674 | HLA-C*14:02 HLA-A*30:01 | 0.5529 | 0.07497 |
| FMAVFSHYI | 373-381 | HLA-A*02:01 HLA-A*02:06 HLA-A*68:02 HLA-A*29:02 HLA-B*39:01 HLA-A*32:01 HLA-A*24:02 HLA-B*46:01 | 1.1695 | 0.03765 |
| DPHTNHLYI | 264-272 | HLA-B*51:01 HLA-B*53:01 | 0.7871 | 0.06219 |
| VNGIRFHAS | 282-290 | HLA-B*08:01 HLA-B*08:01 | 0.5288 | 0.35568 |
| YYENPYEHT | 668-676 | HLA-C*14:02 HLA-C*07:02 | 1.0707 | 0.11511 |
| KLVGVLISL | 681-689 | HLA-A*02:06 HLA-A*02:01 HLA-B*48:01 HLA-A*32:01 | 1.1142 | 0.09292 |
| VLVNAFIEK | 622-630 | HLA-A*11:01 HLA-A*03:01 | 0.9063 | 0.32601 |
| SRERARKVL | 464-472 | HLA-B*14:02 HLA-C*07:02 HLA-B*39:01 HLA-C*06:02 | 1.2369 | 0.01352 |
| HMNENRNTM | 346-354 | HLA-C*07:02 HLA-B*39:01 HLA-B*35:01 | 0.9323 | 0.15829 |
| LLSTQIVAI | 727-735 | HLA-A*32:01 HLA-A*02:01 | 0.5295 | 0.05554 |
| TVLATEQLR | 506-514 | HLA-A*68:01 | 0.9125 | 0.06358 |
| NVNLDVFTK | 519-527 | HLA-A*68:01 HLA-A*11:01 | 1.4741 | 0.16868 |
| KYFQITHIT | 19-27 | HLA-C*14:02 HLA-A*23:01 | 0.6024 | 0.19264 |
| YICGRTNEL | 271-279 | HLA-A*25:01 HLA-C*06:02 HLA-B*08:01 HLA-B*39:01 | 0.5753 | 0.15658 |
| IIDVLVNAF | 619-627 | HLA-A*32:01 HLA-B*46:01 HLA-A*01:01 | 0.9993 | 0.0942 |
| PKDDEDFYL | 490-498 | HLA-B*38:01 | 0.5501 | 0.24454 |

| | | | | |
|------------|---------|---|--------|---------|
| | | HLA-E*01:03 | | |
| QQLINLTKY | 12-20 | HLA-A*30:02 | 0.5046 | 0.02034 |
| EPNDNHEKI | 357-365 | HLA-B*51:01 HLA-B*53:01 | 0.9947 | 0.00287 |
| KNDDFMAVF | 369-377 | HLA-C*05:01 HLA-B*58:02 HLA-C*04:01 | 0.6749 | 0.03536 |
| GFNVNLDVF | 517-525 | HLA-A*23:01 HLA-C*04:01 HLA-B*46:01 | 1.7873 | 0.06554 |
| IQGTAICIV | 137-145 | HLA-A*02:06 | 0.5705 | 0.2457 |
| MEDEWYLSS | 583-591 | HLA-B*18:01 | 1.1215 | 0.21415 |
| QTVHGRDLK | 330-338 | HLA-A*68:01 HLA-A*11:01 | 1.3044 | 0.13991 |
| VLSVGTPIQ | 130-138 | HLA-E*01:01 | 1.2292 | 0.12578 |
| AKQGYAAVV | 774-782 | HLA-B*39:01 | 0.5217 | 0.08687 |
| KVNGIRFHA | 281-289 | HLA-A*30:01 | 1.3148 | 0.32802 |
| DLKLVCIFYV | 336-344 | HLA-E*01:03 | 0.7469 | 0.00493 |
| QYLSPTFIN | 383-391 | HLA-E*01:03 HLA-A*23:01 | 0.9109 | 0.03223 |
| TGKIGSILK | 528-536 | HLA-A*30:01 | 1.0987 | 0.04703 |
| LTEVIESYL | 644-652 | HLA-A*01:01 | 0.7447 | 0.15611 |
| NPYEHTFVK | 671-679 | HLA-B*53:01 HLA-A*68:01 | 1.4480 | 0.29051 |
| TNHLYICGR | 267-275 | HLA-A*68:01 | 1.6066 | 0.09532 |
| CSREELLVN | 311-319 | HLA-C*15:02 | 1.0726 | 0.21937 |
| CGRTNELIK | 273-281 | HLA-A*30:01 | 0.8446 | 0.21221 |
| LIRSRRERAR | 461-469 | HLA-A*31:01 HLA-B*14:02 | 1.3840 | 0.06152 |
| YEIFIEQWN | 599-607 | HLA-B*40:01 | 1.3698 | 0.41651 |
| IDPHTNHLY | 263-271 | HLA-A*29:02 | 0.8416 | 0.08148 |

| | | | | |
|-----------|---------|-------------|--------|---------|
| LYICGRTNE | 270-278 | HLA-C*14:02 | 1.5607 | 0.09965 |
|-----------|---------|-------------|--------|---------|

Table S2 HTL Epitopes predicted by IEDB Consensus Method

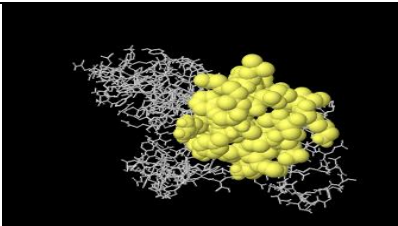
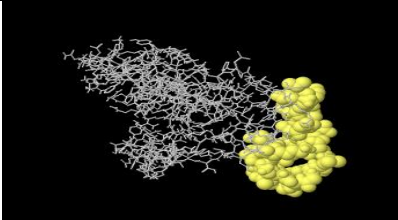
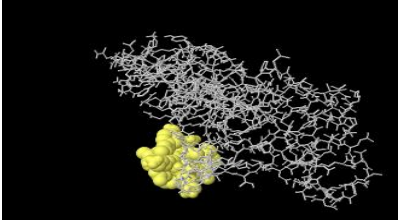
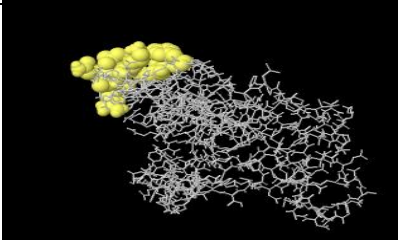
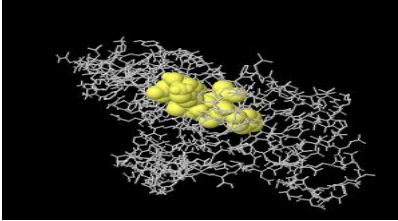
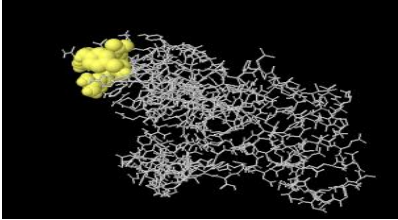
| Protein | | | | | | |
|---------------------------------|----------|--|--------------|---------------|-------------|--------------|
| Calcium binding | | | | | | |
| HTL epitopes | Position | alleles | Antigenicity | IFN- γ | IL-4 | IL-10 |
| KQDNRLRLSKNKKS | 332-346 | HLA-DRB1*04:26 HLA-DRB1*04:21 HLA-DRB1*11:01 HLA-DRB1*04:02 | 0.9238 | Positive | IL4-inducer | IL10-inducer |
| QDNRLRLSKNKKSK | 333-347 | HLA-DRB1*04:26 HLA-DRB1*11:01 HLA-DRB1*04:21 HLA-DRB5*01:01 HLA-DRB1*04:02 | 1.1906 | Positive | IL4-inducer | IL10-inducer |
| Mycosubtilin synthase subunit C | | | | | | |
| KCSRNFKLIRSRERA | 454-468 | HLA-DRB5*01:01 HLA-DRB5*01:05 | 0.4332 | Positive | IL4-inducer | IL10-inducer |
| RNFKLIRSRERARKV | 457-471 | HLA-DRB5*01:01 HLA-DRB5*01:05 HLA-DRB1*08:04 HLA-DRB1*11:01 HLA-DRB1*08:13 HLA-DRB1*08:06 | 1.0836 | Positive | IL4-inducer | IL10-inducer |
| SRNFKLIRSRERARK | 456-470 | HLA-DRB5*01:01 HLA-DRB5*01:05 HLA-DRB1*08:04 HLA-DRB1*11:01 HLA-DRB1*08:13 HLA-DRB1*08:06 | 1.0114 | Positive | IL4-inducer | IL10-inducer |
| GKCSRNFKLIRSRER | 453-467 | HLA-DRB5*01:01 HLA-DRB5*01:05 | 0.7614 | Positive | IL4-inducer | IL10-inducer |
| FKLIRSRERARKVLA | 459-473 | HLA-DRB5*01:01 HLA-DRB5*01:05 HLA-DRB1*08:04 HLA-DRB1*08:13 HLA-DRB1*08:06 | 0.8807 | Positive | IL4-inducer | IL10-inducer |
| NKLVGVLISLPAKHV | 680-694 | HLA-DRB1*01:01 HLA-DRB1*04:04 HLA-DRB1*09:01 | 0.8180 | Positive | IL4-inducer | IL10-inducer |

| | | | | | | |
|------------------|---------|--|--------|----------|-------------|--------------|
| | | HLA-DRB5*01:01 HLA-DRB1*15:01 HLA-DRB1*12:01 | | | | |
| VGVLISLPAKHVPSR | 683-697 | HLA-DRB1*01:01 HLA-DRB1*15:01 HLA-DRB1*09:01 HLA-DRB1*11:01 HLA-DRB1*12:01 | 0.6887 | Positive | IL4-inducer | IL10-inducer |
| EHTFVKNKLVGV LIS | 674-688 | HLA-DRB1*08:06 HLA-DRB1*13:02 | 1.4159 | Positive | IL4-inducer | IL10-inducer |

Table S3 LBL Epitopes predicted by ABCPred

| Peptide | Protein | Score | Antigenicity | Immunogenicity |
|-----------------|---------------------------------|-------|--------------|----------------|
| FIPDYVEDDLDGNG | calcium binding | 0.89 | 1.6532 | 0.23092 |
| DDQDDDDDNNGIKD | calcium binding | 0.86 | 1.2587 | 0.07674 |
| KSDNDGIIDFYDD | calcium binding | 0.85 | 0.6044 | 0.41776 |
| DSDGDGIPDYLNN | calcium binding | 0.85 | 0.8382 | 0.21302 |
| DGIIDFYDDDDND | calcium binding | 0.83 | 0.5183 | 0.40974 |
| GDGVPDYLEDANS | calcium binding | 0.83 | 0.5520 | 0.21816 |
| SDGDGIPDYQEDSD | calcium binding | 0.82 | 0.8082 | 0.10663 |
| DGDGIPDYLD DDD | calcium binding | 0.81 | 0.5581 | 0.24146 |
| LEGDINHNGIIDYL | calcium binding | 0.80 | 1.3728 | 0.48626 |
| VPDHLEEDSDGDI | calcium binding | 0.79 | 1.1378 | 0.17647 |
| DDDNDDIPDHLDSD | calcium binding | 0.78 | 0.8840 | 0.12741 |
| NDGIPDDQDDDDDN | calcium binding | 0.68 | 1.6097 | 0.16028 |
| DDDDDGILDIHEDE | calcium binding | 0.66 | 0.8358 | 0.48203 |
| DSDGDGILDFLEDS | calcium binding | 0.66 | 0.7632 | 0.43732 |
| DHLETDDTDGDGII | calcium binding | 0.65 | 0.7522 | 0.39779 |
| DCDDDDDDDDGILD | calcium binding | 0.61 | 1.7767 | 0.29686 |
| GDSVPEDKVADR NH | calcium binding | 0.61 | 0.8812 | 0.02522 |
| DFLEDSGDGIPDY | calcium binding | 0.58 | 0.5002 | 0.19573 |
| DVTGIVFHNELDVK | Mycosubtilin synthase subunit C | 0.84 | 1.1856 | 0.4856 |
| IDVLVNAFIEKDRL | Mycosubtilin synthase subunit C | 0.82 | 0.6455 | 0.2613 |
| FMPGDLGFIDPHTN | Mycosubtilin synthase subunit C | 0.73 | 0.6452 | 0.37904 |
| EQLRQLGFNVNLDV | Mycosubtilin synthase subunit C | 0.72 | 1.5411 | 0.10329 |
| LTEVIESYLN AHKY | Mycosubtilin synthase subunit C | 0.66 | 0.8240 | 0.05747 |

Table S4 Conformational B cell epitopes in the vaccine predicted by ElliPro Server

| Sr.No | Residues | No. of residues | Score | 3D structure |
|-------|--|-----------------|-------|---|
| | _:A1, _:P2, _:P3, _:H4, _:A5, _:L6, _:S7, _:E8, _:A9, _:A10, _:A11, _:K12, _:I13, _:P14, _:D15, _:H16, _:L17, _:E18, _:G19, _:D20, _:I21, _:A22, _:A23, _:Y24, _:F25, _:S26, _:P27, _:R28, _:R29, _:R31 | 30 | 0.904 |  |
| | _:H152, _:V153, _:K154, _:K155, _:I157, _:P158, _:D159, _:V161, _:E162, _:D163, _:D164, _:L165, _:D166, _:G167, _:N168, _:G169, _:K170, _:K171, _:D172, _:C173, _:D174, _:D175, _:D176, _:D177, _:D178, _:D179, _:D180, _:D181, _:G182, _:D185, _:K186 | 31 | 0.732 |  |
| | _:K202, _:K203, _:T205, _:E206, _:V207, _:I208, _:E209, _:S210, _:Y211, _:L212, _:N213, _:A214, _:H215, _:K216, _:Y217 | 15 | 0.704 |  |
| | _:K68, _:A70, _:A71, _:Y72, _:R73, _:Q74, _:L75, _:G76, _:V79, _:A82, _:A83, _:Y85 | 12 | 0.644 |  |
| | _:Y30, _:K32, _:L33, _:A34, _:A35, _:Y36, _:E39 | 7 | 0.641 |  |
| | _:Y60, _:R63, _:E64, _:R67 | 4 | 0.593 |  |

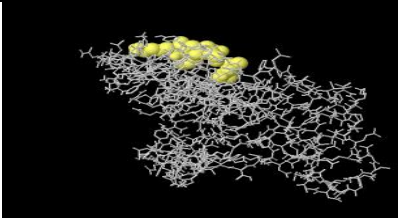
| | | | | |
|--|---|---|-------|---|
| | _:L106, _:S112, _:K113, _:G114, _:P115, _:G116 | 6 | 0.508 |  |
|--|---|---|-------|---|

Table S5 Linear B cell epitopes predicted in vaccine by ABCPred server

| Sr.No | Peptide | Position | Score | Antigenicity |
|-------|-----------------|----------|-------|--------------|
| 1. | VGVLISLPAKHVKK | 142 | 0.83 | 0.7008 |
| 2. | DDLDGNGKKDCDDD | 163 | 0.81 | 1.4896 |
| 3. | KKSKGPGPGRNFKL | 110 | 0.81 | 0.5205 |
| 4. | AKIPDHLEGDIAAY | 11 | 0.80 | 0.9291 |
| 5. | PRRYRKLAAYEVEA | 27 | 0.79 | 0.5366 |
| 6. | NLAAYYENPYEHTF | 80 | 0.77 | 0.7856 |
| 7. | YRSRERARKVAAYR | 60 | 0.77 | 1.0773 |
| 8. | IPDYVEDDLDGNGK | 157 | 0.76 | 1.5153 |
| 9. | LGFNVNLAAYYENP | 75 | 0.74 | 1.1876 |
| 10. | PGRNFKLIRSRERA | 117 | 0.73 | 0.5278 |
| 11. | EGDIAAYFSPRRYR | 18 | 0.69 | 1.1236 |
| 12. | EAYAAAYFMAVFSHY | 43 | 0.64 | 0.9670 |
| 13. | DDDDDDDDGILDKKD | 175 | 0.60 | 0.9661 |
| 14. | LRLSKNKKSKGPGP | 104 | 0.60 | 1.3415 |
| 15. | SHYIAAYRSRERAR | 54 | 0.57 | 0.8101 |
| 16. | KKDCDDDDDDDDGI | 170 | 0.56 | 1.2584 |