|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Predicting 9 mer- epitope binding HLA-A0201 peptides (wild type and mutant)** | | | | | | | | | | | | | | |
| **Count** | | | | | | | **Motif** | | | | | **Enzyme** | | |
| 11 | | | | | | | Wild Type | | | | |  | | |
| 15 | | | | | | | TGC | | | | | AID | | |
| 10 | | | | | | | GCA | | | | | AID | | |
| 13 | | | | | | | AGC | | | | | AID | | |
| 12 | | | | | | | GCT | | | | | AID | | |
| 14 | | | | | | | TAC | | | | | AID | | |
| 11 | | | | | | | GTA | | | | | AID | | |
| 11 | | | | | | | TC | | | | | A3A/A3B | | |
| 20 | | | | | | | TC/ C >G | | | | | A3A/A3B | | |
| 14 | | | | | | | GA | | | | | A3A/A3B | | |
| 16 | | | | | | | GA/ G>C | | | | | A3A/A3B | | |
| 12 | | | | | | | TTC | | | | | A3A/A3B | | |
| 12 | | | | | | | GAA | | | | | A3A/A3B | | |
| **Experimentally Known Epitopes** | | | | | | | | | | | | | | |
| **Position** | **wt Peptide** | **Affinity (nM)** | **Rank** | **Binding level** |  | | | | | | | | | |
|  |  |  |  |  |  | | | | | | | | | |
|  |  |  |  |  |  | | | | | | | | | |
| **Stop codon gained** | | | | | | | | | | | | | | |
| **Position** | **Sequence** | | | | | | **Enzyme** | | | | | | **Consist with existent mutations** | |
| 326 | KAIKKIWLV  KAIKKI\*LV | | | | | | AID | | | | | |  | |
| **Novel Epitopes** | | | | | | | | | | | | | | |
| **mt Peptide** | **Affinity (nM)** | **Rank** | **Binding level** | **wt Peptide** | | **Affinity (nM)** | | **Rank** | **Binding level** | **Enzyme** | | | | **Consist with existent mutations** |
| VAVAGLLA**V** | 275.5 | 1.90 | WB | VAVAGLLAA | | 26986 | | 19.6 |  | AID | | | |  |
| FLTTAEVI**V** | 29.4 | 0.4 | SB | FLTTAEVIA | | 280 | | 2.3 |  | AID | | | |  |
| HLNKDLAF**I** | 54.2 | 0.70 | WB | HLNKDLAFT | | 959 | | 3.96 |  | AID | | | |  |
| F**I**LEERQQL | 242.3 | 1.80 | WB | FTLEERQQL | | 1435 | | 4.90 |  | AID | | | |  |
| KLALYTAC**A** | 74.0 | 0.90 | WB | KLALYTACG | | 3897 | | 8.21 |  | A3A/A3B | | | |  |
| YIALR**HTT**V | 272.8 | 1.90 | WB | YIGLRQRRV | | 9734.57 | | 14.5 |  | A3A/A3B | | | |  |
| CLIQFQ**H**FA | 66.7 | 0.80 | WB | CLIQFEDFA | | 353.3 | | 2.3 |  | A3A/A3B | | | |  |
| IQ**A**TASVAV | 174.0 | 1.50 | WB | IQGTASVAV | | 1067 | | 4.19 |  | A3A/A3B | | | |  |
| GLLAAL**P**IT | 123.6 | 1.20 | WB | GLLAALRIT | | 1995 | | 5.79 |  | A3A/A3B | | | |  |
| FQ**A**A**AQ**AAL | 102.1 | 1.10 | WB | FQGAGEAAL | | 560.8 | | 2.97 |  | A3A/A3B | | | |  |
| IIFA**F**SNPT | 192.4 | 1.60 | WB | IIFALSNPT | | 1301 | | 4.63 |  | A3A/A3B | | | |  |
| ALYTAC**E**G**I** | 47.7 | 0.60 | WB | ALYTACGGM | | 1163. | | 4.38 |  | A3A/A3B | | | | c.549G>A p.M183I  COSM8055262 |
| **K**LLK**N**PLYI | 25.0 | 0.40 | SB | ELLKDPLYI | | 497. | | 2.79 |  | A3A/A3B | | | | c.613G>A p.D205N  COSM3630187 |
| VLT**C**DIEK**L** | 305.6 | 2.00 | WB | VLTSDIEKF | | 10156 | | 4.86 |  | A3A/A3B | | | | c.275C>G p.S92C  COSM1312409 |
| IVYT**A**TVG**V** | 25.6 | 0.40 | SB | IVYTPTVGL | | 641.7 | | 3.20 |  | A3A/A3B | | | |  |
| FANVNAF**GV** | 63.7 | 0.80 | WB | FANVNAFRL | | 869.7 | | 3.77 |  | A3A/A3B | | | |  |
| KL**C**D**E**TIL**L** | 19.2 | 0.25 | SB | KLSDQTILF | | 1000 | | 4.0 |  | A3A/A3B | | | |  |
| V**L**PGVA**V**GV | 36.4 | 0.5 | SB | VFPGVALGV | | 5180 | | 9.73 |  | A3A/A3B | | | |  |
| I**L**LTTAEVI | 210.8 | 1.70 | WB | IFLTTAEVI | | 12009 | | 16.8 |  | A3A/A3B | | | |  |
| **Y**LNKDLAFT | 28.5 | 0.40 | SB | HLNKDLAFT | | 959.5 | | 3.96 |  | A3A/A3B | | | |  |
| IVYT**S**TVGL | 237.0 | 1.80 | WB | IVYTPTVGL | | 641.7 | | 3.20 |  | A3A/A3B | | | |  |
| WLVD**L**KGLI | 299.3 | 2.00 | WB | WLVDSKGLI | | 1761 | | 5.42 |  | A3A/A3B | | | |  |
| M**S**IVYTPTV | 142.5 | 1.30 | WB | MPIVYTPTV | | 4493 | | 9.0 |  | AID | | | |  |
| F**V**NVNVFRL | 67.9 | 0.80 | WB | FANVNAFRL | | 869 | | 3.77 |  | AID | | | |  |
| A**V**LGIVHLI | 78.6 | 0.90 | WB | AALGIAHLI | | 1940 | | 5.71 |  | AID | | | |  |
| ALYTACGG**I** | 211.7 | 1.70 | WB | ALYTACGGM | | 1163 | | 4.38 |  | A3A/A3B | | | | c.549G>A p.M183I  COSM8055262 |
| WLVD**L**KGLI | 299.3 | 2.00 | WB | WLVDSKGLI | | 1761 | | 5.42 |  | A3A/A3B | | | |  |
| **Increased HLA affinity** | | | | | | | | | | | | | | |
| **mt Peptide** | **Affinity (nM)** | **Rank** | **Binding level** | **wt Peptide** | | **Affinity (nM)** | | **Rank** | **Binding level** | **Delta nM** | **Enzyme** | | | **Consist with existent mutations** |
| ILFQG**V**GEA | 48.3 | 0.60 | WB | ILFQGAGEA | | 184.4 | | 1.50 | WB | 136 | AID | | |  |
| FMPIVY**I**PT | 140.0 | 1.30 | WB | FMPIVYTPT | | 150.2 | | 1.40 | WB | 10.2 | AID | | |  |
| EL**F**KDPLYI | 229.2 | 1.7 | WB | ELLKDPLYI | | 497 | | 2.9 | WB | 267 | AID | | |  |
| NIFLT**I**AEV | 95.1 | 1.00 | WB | NIFLTTAEV | | 161.7 | | 1.40 | WB | 66.6 | AID | | |  |
| VLNAWP**QH**V | 18.4 | 0.25 | SB | VLNAWPEDV | | 108.0 | | 1.10 | WB | 89.8 | A3A/A3B | | | c.424G>C p.E142Q  COSM6405114  Substitution - Missense |
| ILFQ**A**A**AQ**A | 110.0 | 1.10 | WB | ILFQGAGEA | | 184.4 | | 1.50 | WB | 74 | A3A/A3B | | |  |
| KAIK**N**IWLV | 19.5 | 0.30 | SB | KAIKKIWLV | | 36.4 | | 0.50 | SB | 17 | A3A/A3B | | |  |
| FLTTA**Q**VIA | 249.3 | 1.80 | WB | FLTTAEVIA | | 280.92 | | 2.013 | WB | 31.6 | A3A/A3B | | |  |
| ALGVVAC**E**L | 248.9 | 1.80 | WB | ALGVVACGL | | 374.13 | | 2.389 | WB | 125 | A3A/A3B | | |  |
| RQIT**N**NIFL | 267.8 | 1.90 | WB | RQITDNIFL | | 274.3 | | 1.987 | WB | 6.25 | A3A/A3B | | |  |
| CLI**E**FEDFA | 87.5 | 1.00 | WB | CLIQFEDFA | | 353.39 | | 2.314 | WB | 265 | A3A/A3B | | |  |
| AVAG**V**LAAV | 8.3 | 0.09 | SB | AVAGLLAAL | | 83.1 | | 0.90 | SB | 74 | A3A/A3B | | |  |
| KA**M**KKIWLV | 13.4 | 0.17 | SB | KAIKKIWLV | | 36.4 | | 0.50 | SB | 23 | A3A/A3B | | |  |
| RQ**M**TDNI**L**L | 178.7 | 1.50 | WB | RQITDNIFL | | 274.32 | | 1.987 | WB | 95 | A3A/A3B | | |  |
| **G**LY**AA**LNTI | 29.6 | 0.40 | SB | RLYPPLNTI | | 45.6 | | 0.60 | 29 | 16 | A3A/A3B | | |  |
| YLLTRNP**Y**L | 4.6 | 0.03 | SB | YLLTRNPHL | | 11.3 | | 0.15 | SB | 6.7 | A3A/A3B | | |  |
| L**I**FEDFANV | 9.2 | 0.10 | SB | IQFEDFANV | | 18.6 | | 0.25 | SB | 9.4 | A3A/A3B | | |  |
| **W**LY**SS**LNTI | 16.0 | 0.20 | SB | RLYPPLNTI | | 45.6 | | 0.60 | SB | 30 | A3A/A3B | | | c.1492C>T p.R498W COSM6304515  c.1504C>T p.P502S COSM4467718 |
| FM**S**IVYTPT | 48.1 | 0.60 | WB | FMPIVYTPT | | 150.2 | | 1.40 | WB | 102 | AID | | |  |
| **V**LGVVACGL | 289.0 | 2.00 | WB | ALGVVACGL | | 374.13 | | 2.389 | WB | 85 | AID | | |  |
| FLTT**V**EVIA | 118.6 | 1.20 | WB | FLTTAEVIA | | 280.92 | | 2.013 | WB | 162.32 | AID | | |  |
| NIFLTT**V**EV | 91.2 | 1.00 | WB | NIFLTTAEV | | 161.7 | | 1.40 | WB | 70.5 | AID | | |  |
| **LI**FEDFANV | 9.2 | 0.10 | SB | IQFEDFANV | | 18.6 | | 0.25 | SB | 9.4 | AID | | |  |
| CLIQFEDF**V** | 51.2 | 0.70 | WB | CLIQFEDFA | | 353 | | 2.31 | WB | AID |  | | |  |
| **Reduced HLA Affinity** | | | | | | | | | | | | | | |
|  |  |  |  |  | |  | |  |  |  |  | | |  |
| **mt Peptide** | **Affinity (nM)** | **Rank** | **Binding level** | **wt Peptide** | | **Affinity (nM)** | | **Rank** | **Binding level** | **Delta nM** | **Enzyme** | | | **Consist with existent mutations** |
| GL**T**CQQYSL | 150.2 | 1.40 | WB | FMPIVYTPT | | 150.2 | | 1.40 | WB | -71.1 | AID | | |  |
| AVAGLLA**T**L | 98.3 | 1.00 | WB | AVAGLLAAL | | 83.1 | | 0.90 | WB | -15.2 | AID | | |  |
| NIFLTT**T**EV | 180.7 | 1.50 | WB | NIFLTTAEV | | 161.7 | | 1.40 | WB | -19 | AID | | |  |
| AVAGLLA**V**L | 241.5 | 1.80 | WB | AVAGLLAAL | | 83.1 | | 0.90 | WB | -158 | AID | | |  |
| RLYPPLN**I**I | 115.1 | 1.10 | WB | RLYPPLNTI | | 45.6 | | 0.60 | WB | -69.5 | AID | | |  |
| IQF**QH**FANV | 49.4 | 0.60 | SB | IQFEDFANV | | 18.6 | | 0.25 | SB | -30.8 | A3A/A3B | | |  |
| NIFLTTA**Q**V | 244 | 1.875 | WB | NIFLTTAEV | | 161.7 | | 1.40 | WB | -82.3 | A3A/A3B | | |  |
| RLYPP**F**NTI | 65.9 | 0.80 | WB | RLYPPLNTI | | 45.6 | | 0.60 | SB | -20.3 | A3A/A3B | | |  |
| FL**NK**FMKAV | 10.6 | 0.12 | SB | FLDEFMEAV | | 2.0 | | 0.01 | SB | -8.6 | A3A/A3B | | | c.676G>A p.D226N  COSM237717 c.679G>A p.F227K COSM1214792 |
| IQF**K**NFANV | 104.2 | 1.10 | WB | IQFEDFANV | | 18.6 | | 0.25 | SB | -85.6 | A3A/A3B | | | c.733G>A p.E245K COSM5405890 |
| ILFQ**E**AE**KA** | 353.17 | 2.313 |  | ILFQGAGEA | | 184.4 | | 1.50 | WB | -186 | A3A/A3B | | | c.902G>A p.G301E COSM8118648 |
| YLLTRNP**D**L | 56.6 | 0.70 | WB | YLLTRNPHL | | 11.3 | | 0.15 | SB | -44 | A3A/A3B | | |  |
| KLFYRVLT**C** | 242.7 | 1.80 | WB | KLFYRVLTS | | 241.8 | | 1.86 | WB |  | A3A/A3B | | | c.275C>G p.S92C  COSM1312409 |
| NI**L**LTTAEV | 231.3 | 1.80 | WB | NIFLTTAEV | | 161.7 | | 1.40 | WB | -69 | A3A/A3B | | |  |
| VLN**T**WPEDV | 165.1 | 1.50 | WB | VLNAWPEDV | | 108.0 | | 1.10 | WB | -57 | AID | | |  |
| VLN**V**WPEDV | 200.8 | 1.60 | WB | VLNAWPEDV | | 108.0 | | 1.10 | WB | -92 | AID | | |  |
| **V**V**V**GLL**V**AL | 367.09 | 2.364 |  | AVAGLLAAL | | 83.1 | | 0.90 | WB | -283 | AID | | |  |
| FLD**K**FMEAV | 3.1 | 0.01 | SB | FLDEFMEAV | | 2.0 | | 0.01 | SB | -1.1 | A3A/A3B | | | c.676G>A p.E227K  COSM1214792 |
| **Abrogated Epitopes** | | | | | | | | | | | | | | |
| **Position** | **wt Peptide** | **Affinity (nM)** | **Rank** | **Binding level** | **Enzyme** |  | | | | | | | | |
|  | ILFQGAGEA | 184.4 | 1.50 | WB | AID |
|  | FMPIVYTPT | 150.2 | 1.40 | WB | A3A/A3B |  | | | | | | | | |
|  | GLACQQYSL | 28.0 | 0.40 | SB | A3A/A3B |  | | | | | | | | |
|  | VLNAWPEDV | 108.0 | 1.10 | WB | A3A/A3B |  | | | | | | | | |
|  | ILFQGAGEA | 184.4 | 1.50 | WB | A3A/A3B |  | | | | | | | | |
|  | FMPIVYTPT | 150.2 | 1.40 | WB | A3A/A3B |  | | | | | | | | |
|  | VLNAWPEDV | 108.0 | 1.10 | WB | A3A/A3B |  | | | | | | | | |
|  | AVAGLLAAL | 83.1 | 0.90 | WB | A3A/A3B |  | | | | | | | | |