|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Predicting 9 mer- epitope binding HLA-A0201 peptides (wild type and mutant)** | | | | | | | | | | | | | | | | | | | | |
|  | **Count** | | | | | | | | | | | | **Motif** | | | | | | | |  |
|  | 9 | | | | | | | | | | | | Wild type | | | | | | | |  |
|  | 8 | | | | | | | | | | | | GCA | | | | | | | | AID |
|  | 9 | | | | | | | | | | | | GCT | | | | | | | | AID |
|  | 8 | | | | | | | | | | | | AGC | | | | | | | | AID |
|  | 9 | | | | | | | | | | | | GTA | | | | | | | | AID |
|  | 9 | | | | | | | | | | | | TAC | | | | | | | | AID |
|  | 7 | | | | | | | | | | | | GA | | | | | | | | A3A/A3B |
|  | 11 | | | | | | | | | | | | GA/G>C | | | | | | | | A3A/A3B |
|  | 18 | | | | | | | | | | | | TC | | | | | | | | A3A/A3B |
|  | 12 | | | | | | | | | | | | TC/C >G | | | | | | | | A3A/A3B |
|  | 9 | | | | | | | | | | | | GAA | | | | | | | | A3A/A3B |
|  | 8 | | | | | | | | | | | | TTC | | | | | | | | A3A/A3B |
| **Experimentally Known Epitopes** | | | | | | | | | | | | | | | | | | | | | |
| **Position** | | **wt Peptide** | **Affinity (nM)** | | **Rank** |  | |
|  | | ……... | …….. | | ……... |  | |
|  | **Stop codon gained** | | | | | | | | | | | | | | | | | | | | |
| **Position** | |  | | **Sequence** | | | | | | | | **Enzyme** | | | | | | | **Consist with existent mutations** | | |
|  | |  | | CMWSGFSAA  CM\*SGFSAAA | | | | | | | | A3A/A3B | | | | | | |  | | |
| **Novel Epitopes** | | | | | | | | | | | | | | | | | | | | | |
| **mt Peptide** | | **Affinity (nM)** | **Rank** | | **Binding level** |  | | **Enzyme** | | | | | | **Consist with existent mutations** | | | | | | | |
| **MMM**QDCMWS | | 139 | 1.3 | | WB | IIIQDCMWS | | A3A/A3B | | | | | | c.420C>G p.I140M COSM9214310  Substitution - Missense | | | | | | | |
| ATMPLNVS**L** | | 219 | 1.764 | | WB | ATMPLNVSF | | A3A/A3B | | | | | |  | | | | | | | |
| **MM**QDCMWSG | | 263 | 1.9 | | WB | IIQDCMWSG | | A3A/A3B | | | | | |  | | | | | | | |
| **M**QDCMWSGL | | 224 | 1.77 | | WB | IQDCMWSGF | | A3A/A3B | | | | | |  | | | | | | | |
| G**LW**AAAKLV | | 31.8 | 0.50 | | WB | GFSAAAKLV | | A3A/A3B | | | | | |  | | | | | | | |
| GL**Y**SPSYVA | | 105.5 | 1.10 | | WB | GLCSPSYVA | | AID | | | | | |  | | | | | | | |
| KLKRSFFAL | | 98.6 | 1.00 | | WB | ELKRSFFAL | | A3A/A3B | | | | | | c.1105G>A p.E369K COSM3645024  Substitution - Missense | | | | | | | |
| FQLLPTPPL | | 24.5 | 0.40 | | SB | FELLPTPPL | | A3A/A3B | | | | | |  | | | | | | | |
| HMVTQLLAA | | 169.5 | 1.50 | | WB | EMVTELLGG | | A3A/A3B | | | | | |  | | | | | | | |
| **F**GLC**L**P**F**YV | | 42.2 | 0.60 | | WB | SGLCSPSYV | | A3A/A3B | | | | | | c.245C>T p.S82F COSM3645019  Substitution - Missense | | | | | | | |
| F**L**AAAKLV**L** | | 37.2 | 0.50 | | SB | FSAAAKLVS | | A3A/A3B | | | | | | c.461C>T p.S154L COSM5763068  Substitution - Missense | | | | | | | |
| A**L**ECIDP**L**V | | 50.3 | 0.70 | | WB | ASECIDPSV | | A3A/A3B | | | | | |  | | | | | | | |
| F**FSFL**D**F**LL | | 128.5 | 1.20 | | WB | FSPSSDSLL | | A3A/A3B | | | | | |  | | | | | | | |
| **SFL**D**F**LL**FL** | | 231.6 | 1.80 | | WB | PSSDSLLSS | | A3A/A3B | | | | | |  | | | | | | | |
| **FL**D**F**LL**FL**T | | 25.0 | 0.40 | | SB | SSDSLLSST | | A3A/A3B | | | | | |  | | | | | | | |
| **F**LL**FL**TE**FF** | | 136.8 | 1.30 | | WB | SLLSSTESS | | A3A/A3B | | | | | | c.710C>T p.S237F COSM4171783  Substitution - Missense | | | | | | | |
| **FL**TE**FF**PQG | | 168.1 | 1.50 | | WB | SSTESSPQG | | A3A/A3B | | | | | | c.722C>T p.S241L COSM6549727  Substitution - Missense | | | | | | | |
| R**L**E**F**G**L**P**F**A | | 143.8 | 1.30 | | WB | RSESGSPSA | | A3A/A3B | | | | | | c.875C>T p.S292L COSM8643452  Substitution - Missense | | | | | | | |
| **F**T**W**KDY**S**AA | | 261.7 | 1.9 | | WB | STRKDYPAA | | A3A/A3B | | | | | | c.986C>T p.S329F COSM4847953  Substitution - Missense | | | | | | | |
| **Increased HLA Affinity** | | | | | | | | | | | | | | | | | | | | | |
| **mt Peptide** | | **Affinity (nM)** | **Rank** | | **Binding level** | **wt Peptide** | | | **Affinity (nM)** | | **Rank** | | | | **Binding level** | **Delta nM** | **Enzyme** | | | **Consist with existent mutations** | |
| CMWSG**LW**AA | | 5.0 | 0.04 | | SB | CMWSGFSAA | | | 22.2 | | 0.30 | | | | SB | 17.2 | A3A/A3B | | |  | |
| YLQD**V**SAAA | | 12.4 | 0.15 | | SB | YLQDLSAAA | | | 15.9 | | 0.20 | | | | SB | 3.5 | A3A/A3B | | | c.577C>G p.L193V COSM3316941  Substitution - Missense | |
| ILKK**V**T**V**YI | | 99.8 | 1.00 | | WB | ILKKATAYI | | | 177.7 | | 1.5 | | | | WB | 77.9 | AID | | | c.1215C>T p.A405= COSM9505916  Substitution - coding silent | |
| K**V**T**V**YILSV | | 82.0 | 0.90 | | WB | KATAYILSV | | | 185.7 | | 1.6 | | | | WB | 103.7 | AGC | | |  | |
| **Y**MWSGFSAA | | 3.8 | 0.02 | | SB | CMWSGFSAA | | | 22.2 | | 0.30 | | | | SB | 18.4 | AID | | |  | |
| SLYLQ**N**LSA | | 171.5 | 1.50 | | WB | SLYLQDLSA | | | 211.3 | | 1.7 | | | | WB | 39.8 | A3A/A3B | | | C.538G>A p.D180N COSM5873903  Substitution - Missense | |
| SLYLQ**H**LSA | | 201.0 | 1.60 | | WB | SLYLQDLSA | | | 211.3 | | 1.7 | | | | WB | 10.3 | A3A/A3B | | |  | |
| KLIS**QQH**LL | | 30.9 | 0.40 | | SB | KLISEEDLL | | | 249.9 | | 1.8 | | | | WB | 219 | A3A/A3B | | |  | |
| KATAYIL**F**V | | 77.4 | 0.90 | | WB | KATAYILSV | | | 185.7 | | 1.6 | | | | WB | 108.3 | A3A/A3B | | | c.? p.S415F  COSM9213341  Substitution - Missense | |
| KLI**F**EEDLL | | 203.7 | 1.688 | |  | KLISEEDLL | | | 249.9 | | 1.8 | | | | WB | 47 | A3A/A3B | | |  | |
| **Reduced HLA Affinity** | | | | | | | | | | | | | | | | | | | | | |
| **mt Peptide** | | **Affinity (nM)** | **Rank** | | **Binding level** | **wt Peptide** | | | **Affinity (nM)** | | **Rank** | | | | **Binding level** | **Delta nM** | | **Enzyme** | | **Consist with existent mutations** | |
| SLYLQD**V**SA | | 232.4 | 1.80 | | wb | SLYLQDLSA | | | 211.3 | | 1.70 | | | | WB | -21.1 | | A3A/A3B | |  | |
| ALRDQ**M**PEL | | 91.37 | 1.021 | |  | ALRDQIPEL | | | 49.3 | | 0.60 | | | | WB | -66.99 | | A3A/A3B | |  | |
| CMWS**D**FSAA | | 33.7 | 0.50 | | SB | CMWSGFSAA | | | 22.2 | | 0.30 | | | | SB | -11.5 | | A3A/A3B | | c.455G>A p.G152D COSM3316927  Substitution - Missense | |
| YLQ**N**LSAAA | | 54.1 | 0.70 | | WB | YLQDLSAAA | | | 15.9 | | 0.20 | | | | SB | -38.2 | | A3A/A3B | |  | |
| CM**C**SGFSAA | | 215.6 | 1.70 | | WB | CMWSGFSAA | | | 22.2 | | 0.30 | | | | SB | -193.4 | | A3A/A3B | |  | |
| YLQ**H**LSAAA | | 44.9 | 0.60 | | WB | YLQDLSAAA | | | 15.9 | | 0.20 | | | | SB | -29 | | A3A/A3B | |  | |
| ALR**HH**IP**Q**L | | 191.9 | 1.60 | | WB | ALRDQIPEL | | | 49.3 | | 0.60 | | | | WB | -142.6 | | A3A/A3B | | c.1140G>C p.Q380H COSM1330322  Substitution - Missense | |
| ILKKAT**T**YI | | 280.5 | 2.00 | | WB | ILKKATAYI | | | 177.7 | | 1.50 | | | | WB | -102.8 | | AID | |  | |
| KLIS**K**EDLL | | 279.1 | 1.90 | | WB | KLISEEDLL | | | 249.9 | | 1.80 | | | | WB | -29.2 | | A3A/A3B | | c.1273G>A p.E425K COSM5727622 Substitution - Missense | |
| YVAVTPF**F**L | | 19.1 | 0.25 | | SB | YVAVTPFSL | | | 69.8 | | 0.80 | | | | WB | -50.7 | | A3A/A3B | |  | |
| **F**TADQLEMV | | 16.3 | 0.25 | | SB | STADQLEMV | | | 267.7 | | 1.90 | | | | WB | -251.4 | | A3A/A3B | |  | |
| CMWSGF**L**AA | | 24.8 | 0.40 | | SB | CMWSGFSAA | | | 22.2 | | 0.3 | | | | SB | -2.6 | | A3A/A3B | |  | |
| **M**LKKATAY**M** | | 289.5 | 2.00 | | WB | ILKKATAYI | | | 177.7 | | 1.5 | | | | WB | -111.8 | | A3A/A3B | |  | |
| ALR**N**QIPEL | | 126.3 | 1.256 | | WB | ALRDQIPEL | | | 49.3 | | 0.6 | | | | WB | -76 | | A3A/A3B | |  | |
| STA**H**QL**H**MV | | 406.5 | 2.497 | | WB | STADQLEMV | | | 267.7 | | 1.9 | | | | WB | -138 | | A3A/A3B | | c.294G>C p.Q98H COSM1159800  Substitution - Missense | |
|  | **Abrogated Epitopes** | | | | | | | | | | | | | | | | | | | | |
| **Position** | | **wt Peptide** | **Affinity (nM)** | | **Rank** | **Binding level** | **Enzyme** | | | **Consist with existent mutations** | | | | | | | | | | | |
| 89 | | YVAVTPFSL | 69.8 | | 0.80 | WB | A3A/A3B | | |
| 413 | | KATAYILSV | 185.7 | | 1.60 | WB | A3A/A3B | | |  | | | | | | | | | | | |
| 413 | | KATAYILSV | 185.7 | | 1.60 | WB | A3A/A3B | | |  | | | | | | | | | | | |
| 190 | | SLYLQDLSA | 211.3 | | 1.70 | WB | AID | | |  | | | | | | | | | | | |
| 427 | | KLISEEDLL | 249.9 | | 1.80 | WB | AID | | |  | | | | | | | | | | | |
| 109 | | STADQLEMV | 267.7 | | 1.90 | WB | A3A/A3B | | |  | | | | | | | | | | | |
| 427 | | KLISEEDLL | 249.9 | | 1.80 | WB | A3A/A3B | | | c.1228G>A p.E410K  COSM5727623  Substitution - Missense | | | | | | | | | | | |
| 109 | | STADQLEMV | 267.7 | | 1.90 | WB | A3A/A3B | | | c.294G>C p.Q98H  COSM1159800  Substitution - Missense | | | | | | | | | | | |
| 427 | | KLISEEDLL | 249.9 | | 1.80 | WB | A3A/A3B | | |  | | | | | | | | | | | |