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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Predicting 9 -mer- epitope binding HLA-A\*0201 peptides (wild type and mutant)** | | | | | | | | | | | | | | | | | |
| **Count** | | | | | | | **Motif** | | | | | | | **Enzyme** | | | |
| 12 | | | | | | | Wild type | | | | | | |  | | | |
| 11 | | | | | | | AGC | | | | | | | AID | | | |
| 13 | | | | | | | GCT | | | | | | | AID | | | |
| 13 | | | | | | | GTA | | | | | | | AID | | | |
| 12 | | | | | | | TAC | | | | | | | AID | | | |
| 13 | | | | | | | GCA | | | | | | | AID | | | |
| 14 | | | | | | | TGC | | | | | | | AID | | | |
| 15 | | | | | | | GA/G>C | | | | | | | A3A/A3B | | | |
| 13 | | | | | | | GA | | | | | | | A3A/A3B | | | |
| 17 | | | | | | | TC /C >G | | | | | | | A3A/A3B | | | |
| 14 | | | | | | | TC | | | | | | | A3A/A3B | | | |
| 12 | | | | | | | GAA | | | | | | | A3A/A3B | | | |
| 13 | | | | | | | TTC | | | | | | | A3A/A3B | | | |
| **Experimentally Known Epitopes** | | | | | | | | | | | | | | | | | |
| **Position** | **wt Peptide** | **Affinity (nM)** | **Rank** |
| 605 | YLSGANLNL | 18.8 | 0.25 |
| 694 | GVLVGVALI | 901 | 3.854 |
| 61 | HLFGYSWYK | 247.9 | 1.88 |
| 691 | IMIGVLVGV | 4.6 | 0.03 |
| **Stop codon gained** | | | | | | | | | | | | | | | | | |
| **Position** | **Sequence** | | | | | | **Enzyme** | | | | | **Consist with existent mutations** | | | | | |
| 277 | FQQSTQEL  FQ\*STQEF | | | | | | AID | | | | |  | | | | | |
| 17 | RLLLTASLL  RLLLTA\*L | | | | | | A3A/A3B | | | | |  | | | | | |
| 18 | LLLTASLLT  LLLTA\*LVT | | | | | | A3A/A3B | | | | |  | | | | | |
| 569 | YVCGIQNSV  YVCGMQN\*V | | | | | | A3A/A3B | | | | |  | | | | | |
| 176 | YLWWVNNQS  YLWWVNN\*S | | | | | | A3A/A3B | | | | |  | | | | | |
| 354 | WVNNQSLPV  WVNN\*SLPV | | | | | | A3A/A3B | | | | |  | | | | | |
| 535 | WVNGQSLPV  WVNG\*SLPV | | | | | | A3A/A3B | | | | |  | | | | | |
| **Novel Epitopes** | | | | | | | | | | | | | | | | | |
| **mt Peptide** | **Affinity (nM)** | **Rank** | **Binding level** | **wt Peptide** | | | **Enzyme** | | **Consist with existent mutations** | | | | | | | |
| GQFR**I**YPEL | 304.4 | 2.00 | WB | GQFRVYPEL | | | AID | |  | | | | | | | |
| YLFGYSWYK | 31.3 | 0.50 | SB | HLFGYSWYK | | | AID | |  | | | | | | | |
| NLNLSCHA**V** | 282.5 | 2.00 | SB | NLNLSCHAA | | | AID | |  | | | | | | | |
| NLSLSCHA**V** | 213.5 | 1.70 | WB | NLSLSCHAA | | | AID | |  | | | | | | | |
| HLF**D**Y**N**WYK | 214.9 | 1.70 | WB | HLFGYSWYK | | | AID | |  | | | | | | | |
| **H**T**A**FYTLHV | 267.5 | 1.90 | WB | DTGFYTLHV | | | A3A/A3B | |  | | | | | | | |
| **Q**LFIPNITV | 103.6 | 1.10 | WB | ELFIPNITV | | | A3A/A3B | |  | | | | | | | |
| LLSVT**S**N**H**V | 91.7 | 1.00 | WB | LLSVTRNDV | | | A3A/A3B | |  | | | | | | | |
| **K**LFIPNITV | 40.8 | 0.60 | WB | ELFIPNITV | | | A3A/A3B | |  | | | | | | | |
| T**L**WNPPTTA | 239.1 | 1.80 | WB | TFWNPPTTA | | | A3A/A3B | |  | | | | | | | |
| IIYPNA**C**LL | 259.0 | 1.90 | WB | IIYPNASLL | | | A3A/A3B | |  | | | | | | | |
| ELF**M**PN**M**TV | 226.1 | 1.70 | WB | ELFIPNITV | | | A3A/A3B | |  | | | | | | | |
| **M**TSNN**C**NPV | 290.5 | 2.00 | WB | ITSNNSNPV | | | A3A/A3B | |  | | | | | | | |
| YLWWVNN**E**S | 69.0 | 0.80 | WB | YLWWVNNQ | | | A3A/A3B | |  | | | | | | | |
| KT**M**TV**C**AEL | 184.8 | 1.60 | WB | VKTITVSAEL | | | A3A/A3B | |  | | | | | | | |
| YLWWVNG**E**S | 213.8 | 1.70 | WB | YLWWVNGQS | | | A3A/A3B | |  | | | | | | | |
| VNG**E**SLPVS | 163.9 | 1.40 | WB | VNGQSLPVS | | | A3A/A3B | |  | | | | | | | |
| YLWGANLNL | 4.9 | 0.04 | SB | YLSGANLNL | | | A3A/A3B | | ---- | | | | | | | |
| IIYPNA**F**LL | 25.6 | 0.40 | SB | IIYPNASLL | | | A3A/A3B | |  | | | | | | | |
| ITSNN**F**NPV | 245.9 | 1.80 | WB | ITSNNSNPV | | | A3A/A3B | |  | | | | | | | |
| NLSL**F**CHAA | 245.8 | 1.80 | WB | NLSLSCHAA | | | A3A/A3B | | c.1262C>T p.S421F COSM3736772 Substitution - Missense | | | | | | | |
| KTITV**F**AEL | 242.7 | 1.80 | WB | KTITVSAEL | | | A3A/A3B | |  | | | | | | | |
| NLNL**F**CH**L**A | 248.4 | 1.80 | WB | NLNLSCHSA | | | A3A/A3B | |  | | | | | | | |
| **FL**AGATVGI | 5.4 | 0.04 | SB | LSAGATVGI | | | A3A/A3B | |  | | | | | | | |
| YLLGANLNL | 7.6 | 0.08 | SB | YLSGANLNL | | | A3A/A3B | | ---- | | | | | | | |
| IIYPN**T**SLL | 209.5 | 1.70 | WB | IIYPNASLL | | | AID | |  | | | | | | | |
| IIYPN**V**SLL | 202.5 | 1.60 | WB | IIYPNASLL | | | AID | |  | | | | | | | |
| TVTTITVY**V** | 133.2 | 1.30 | WB | TVTTITVYA | | | AID | |  | | | | | | | |
| P**L**AQY**F**WLI | 244.0 | 1.80 | WB | PPAQYSWLI | | | 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** |
| YLWW**I**NNQS | 109.2 | 1.1 | WB | YLWWVNNQS | | | 134.3 | 1.3 | | WB | | 25.1 | | | AID | |  |
| W**I**NNQSLPV | 97.7 | 1.0 | WB | WVNNQSLPV | | | 245.4 | 1.8 | | WB | | 147.7 | | | AID | | c.538G>A p.V180I COSM3534470 Substitution - Missense |
| RLLLT**V**SLL | 94.5 | 1.00 | WB | RLLLTASLL | | | 202.1 | 1.6 | | WB | | 107.6 | | | AID | |  |
| LLLT**V**SLLT | 141.2 | 1.30 | WB | LLLTASLLT | | | 251.6 | 1.8 | | WB | | 110.4 | | | AID | |  |
| YLSG**V**NLNL | 8.8 | 0.10 | SB | YLSGANLNL | | | 18.8 | 0.25 | | SB | | 10 | | | AID | | c.1826C>T p.A609V COSM4140678 Substitution - Missense |
| YLWW**I**NNQS | 109.2 | 1.10 | WB | YLWWVNNQS | | | 134.3 | 1.3 | | WB | | 25.1 | | | AID | |  |
| W**I**NNQSLPV | 97.7 | 1.00 | WB | WVNNQSLPV | | | 245.4 | 1.8 | | WB | | 147.7 | | | AID | |  |
| W**I**NGQSLPV | 83.6 | 0.90 | WB | WVNGQSLPV | | | 197.6 | 1.6 | | WB | | 114 | | | AID | |  |
| YLWWVNN**H**S | 121.9 | 1.20 | WB | YLWWVNNQS | | | 134.3 | 1.3 | | WB | | 12.4 | | | AID | |  |
| WVNN**H**SLPV | 115.2 | 1.10 | WB | WVNNQSLPV | | | 245.4 | 1.8 | | WB | | 130.2 | | | A3A/A3B | |  |
| YLWWVNN**H**S | 121.9 | 1.20 | WB | YLWWVNNQS | | | 134.3 | 1.3 | | WB | | 12.4 | | | A3A/A3B | |  |
| WVNN**H**SLPV | 115.2 | 1.10 | WB | WVNNQSLPV | | | 245.4 | 1.8 | | WB | | 130.2 | | | A3A/A3B | |  |
| WVNG**H**SLPV | 97.6 | 1.00 | WB | WVNGQSLPV | | | 197.6 | 1.6 | | WB | | 100 | | | A3A/A3B | |  |
| YVCAI**H**NSV | 146.3 | 1.30 | WB | YVCGIQNSV | | | 225.0 | 1.7 | | WB | | 78.7 | | | A3A/A3B | |  |
| VLYGP**H**TPI | 101.6 | 1.10 | WB | VLYGPDTPI | | | 109.5 | 1.1 | | WB | | 7.9 | | | A3A/A3B | |  |
| YLS**A**ANLNL | 11.8 | 0.15 | SB | YLSGANLNL | | | 18.8 | 0.25 | | SB | | 7 | | | A3A/A3B | |  |
| YVC**E**IQNSV | 53.6 | 0.70 | WB | YVCGIQNSV | | | 225.0 | 1.7 | | WB | | 171.4 | | | A3A/A3B | |  |
| VLYGP**N**TPI | 81.4 | 0.90 | WB | VLYGPDTPI | | | 109.5 | 1.1 | | WB | | 28.1 | | | A3A/A3B | | c.1762G>A p.D588N COSM6337024 Substitution - Missense |
| YLS**E**ANLNL | 5.4 | 0.04 | SB | YLSGANLNL | | | 18.8 | 0.25 | | SB | | 13.4 | | | A3A/A3B | |  |
| YLWWVNN**E**S | 69.0 | 0.80 | WB | YLWWVNNQS | | | 134.3 | 1.3 | | WB | | 65.3 | | | A3A/A3B | |  |
| WVNN**E**SLPV | 199.6 | 1.60 | WB | WVNNQSLPV | | | 245.4 | 1.8 | | WB | | 45.8 | | | A3A/A3B | |  |
| WVNN**E**SLPV | 199.6 | 1.60 | WB | WVNNQSLPV | | | 245.4 | 1.8 | | WB | | 45.8 | | | A3A/A3B | |  |
| **M**MIGVLVGV | 3.2 | 0.01 | SB | IMIGVLVGV | | | 4.6 | 0.03 | | SB | | 1.4 | | | A3A/A3B | |  |
| RLLLTA**L**LL | 85.9 | 0.90 | WB | RLLLTASLL | | | 202.1 | 1.6 | | WB | | 116.2 | | | A3A/A3B | |  |
| LLLTA**L**LLT | 98.8 | 1.00 | WB | LLLTASLLT | | | 251.6 | 1.8 | | WB | | 152.8 | | | A3A/A3B | |  |
| ATV**D**IMIGV | 13.0 | 0.17 | SB | ATVGIMIGV | | | 25.7 | 0.4 | | SB | | 12.7 | | | AID | |  |
| RLL**F**TASLL | 125.4 | 1.20 | WB | RLLLTASLL | | | 202.1 | 1.6 | | WB | | 76.7 | | | AID | |  |
| LL**F**TASLLT | 86.9 | 1.00 | WB | LLLTASLLT | | | 251.6 | 1.8 | | WB | | 164.7 | | | AID | |  |
| YL**L**GANLNL | 7.6 | 0.08 | SB | YLSGANLNL | | | 18.8 | 0.25 | | SB | | 11.2 | | | AID | | c.1808C>T p.S603L COSM7587056 Substitution - Missense |
| YVC**E**IQNSV | 53.6 | 0.70 | WB | YVCGIQNSV | | | 225.0 | 1.70 | | WB | | 171.4 | | | AID | | c.1715G>A p.G572E COSM5389880 Substitution - Missense |
| YLWWVNN**E**S | 57 | 0.73 |  | YLWWVNNQS | | | 134.3 | 1.3 | | WB | | 77 | | | A3A/A3B | |  |
| WVNG**E**SLPV | 169 | 1.51 |  | WVNGQSLPV | | | 197.6 | 1.60 | |  | | 28.6 | | | A3A/A3B | |  |
| YL**L**GANLNL | 4.75 | 0.027 |  | YLSGANLNL | | | 18.8 | 0.25 | |  | | 14 | | | A3A/A3B | | c.1820C>T p.S607L COSM226824 Substitution - Missense |
| **Reduced HLA Affinity** | | | | | | | | | | | | | | | | | |
| **mt Peptide** | **Affinity (nM)** | **Rank** | **Binding level** | **wt Peptide** | | **Affinity (nM)** | | **Rank** | | | **Binding level** | | **Delta nM** | | **Enzyme** | **Consist with existent mutations** | |
| ATVGI**I**IAV | 44.7 | 0.60 | WB | ATVGIMIGV | | 25.7 | | 0.40 | | | SB | | -19 | | A3A/A3B |  | |
| I**I**IAVLVGV | 10.8 | 0.12 | SB | IMIGVLVGV | | 4.6 | | 0.03 | | | SB | | -6.2 | | A3A/A3B |  | |
| ATVGI**I**I**E**V | 49.1 | 0.60 | WB | ATVGIMIGV | | 25.7 | | 0.40 | | | SB | | -23.4 | | A3A/A3B |  | |
| I**I**I**E**VLVGV | 4.9 | 0.04 | SB | IMIGVLVGV | | 4.6 | | 0.03 | | | SB | | -0.3 | | A3A/A3B |  | |
| ATVG**M**MIGV | 35.3 | 0.50 | SB | ATVGIMIGV | | 25.7 | | 0.40 | | | SB | | -9.6 | | A3A/A3B |  | |
| VLYGPDTP**M** | 254 | 1.94 | WB | VLYGPDTPI | | 109.5 | | 1.10 | | | WB | | -144.5 | | A3A/A3B |  | |
| **Abrogated Epitopes** | | | | | | | | | | | | | | | | | |
| **Position** | **wt Peptide** | **Affinity (nM)** | **Rank** | **Binding level** | **Enzyme** | | | | | | **Consist with existent mutations** | | | | | | |
| 569 | YVCGIQNLV | 225.0 | 1.70 | WB | A3A/A3B | | | | | | c.1727C>T p.S576L COSM1525174  Substitution - Missense | | | | | | |