

C-IMMSIM simulation results

December 14, 2025

Abstract

This document includes the plots relative to the simulation and the outcome of the epitope/peptide prediction used.

Produced by the C-IMMSIM Online server available at
<http://c-immsim.iac.rm.cnr.it> (alias to <http://kraken.iac.rm.cnr.it/C-IMMSIM>)

CITATIONS: For publication of results, please cite the following:

Nicolas Rapin, Ole Lund, Massimo Bernaschi, Filippo Castiglione. Computational Immunology Meets Bioinformatics: The Use of Prediction Tools for Molecular Binding in the Simulation of the Immune System. PLoS ONE 5(4): e9862
tt doi:10.1371/journal.pone.0009862, 2010

A retrospective validation

In-silico evaluation of adenoviral COVID-19 vaccination protocols: Assessment of immunological memory up to 6 months after the third dose. P. Stolfi, F. Castiglione, E. Mastrostefano, I. Di Biase, S. Di Biase, G. Palmieri, A. Prisco. Frontiers in Immunology, 13 (2022) doi: 10.3389/fimmu.2022.998262
<https://www.frontiersin.org/articles/10.3389/fimmu.2022.998262i>

An in vivo validation

Identification and validation of viral antigens sharing sequence and structural homology with tumor associated antigens (TAAs). C. Ragone, C. Manolio, B. Cavalluzzo, A. Petrizzo, A. Mauriello, M-L. Tornesello, F. M. Buonaguro, F. Castiglione, L. Vitagliano, M. Ruvo, M. Tagliamonte, L. Buonaguro. Journal for ImmunoTherapy of Cancer. 9:e002694 (2021)
<https://jitz.bmjjournals.com/content/9/5/e002694>

Original C-IMMSIM model: www.iac.cnr.it/~filippo/c-immsim

GETTING HELP:

Scientific problems: Filippo Castiglione (filippo dot castiglione at cnr dot it)

Technical problems: Ilaria Gonnella (ilaria dot gonnella at cnr dot it)

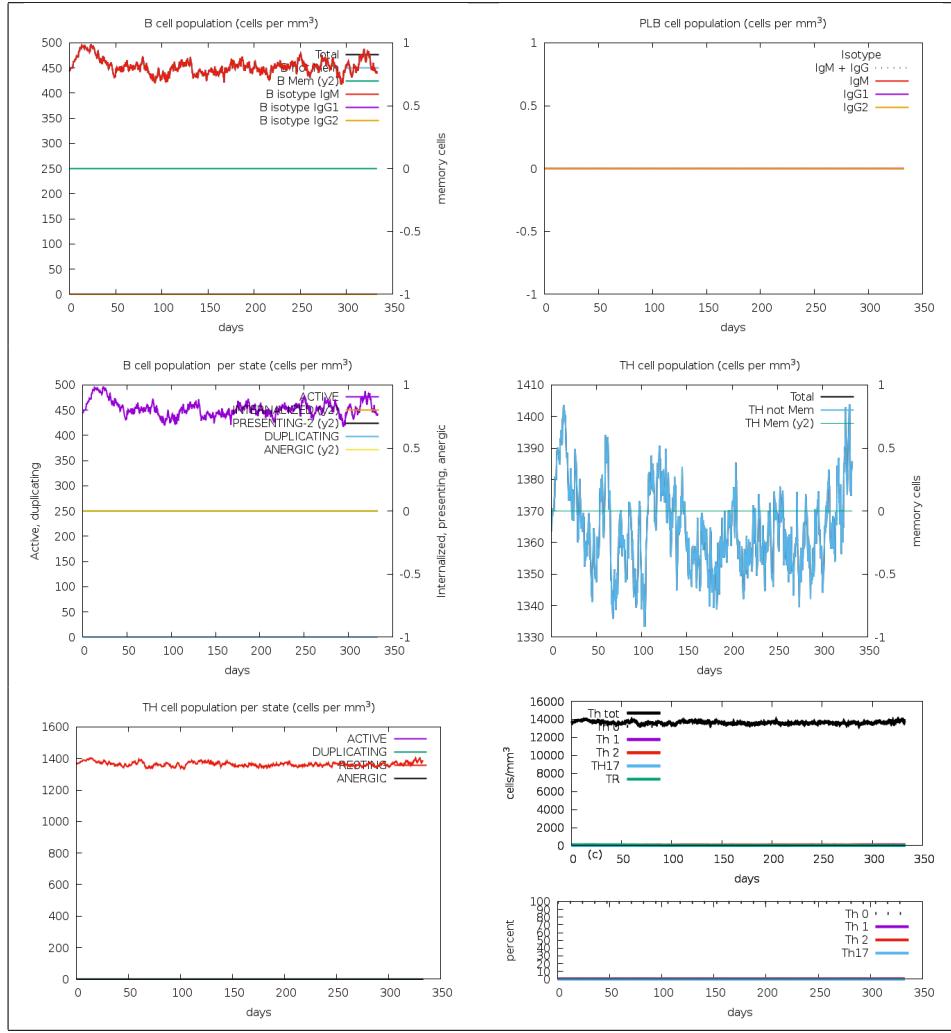


Figure 1: Cell counts shown. Legend: Act=active, Intern=internalized the Ag, Pres II = presenting on MHC II, Dup = in the mitotic cycle, Anergic = anergic, Resting = not active.

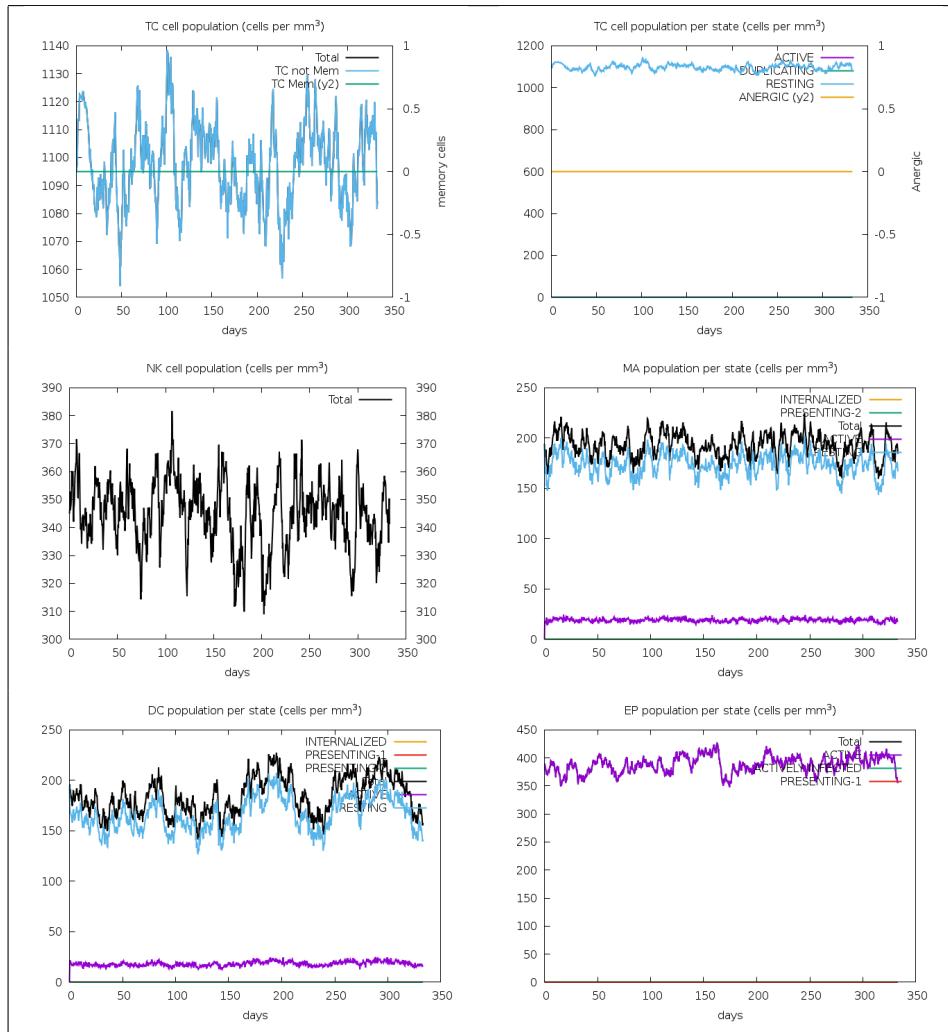


Figure 2: Legend: symbols as figure above.

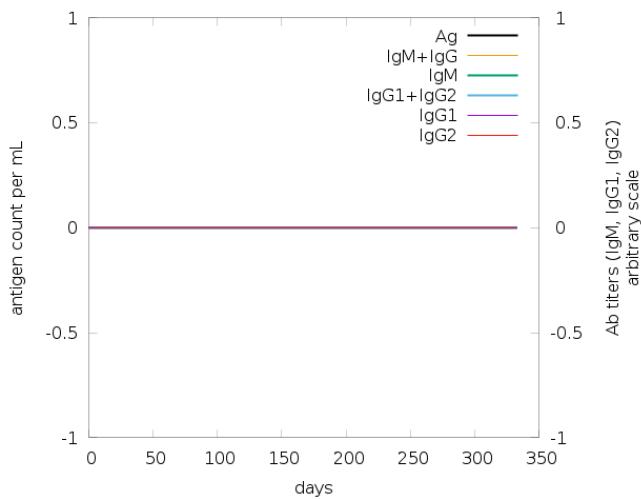


Figure 3: The virus, the immunoglobulins and the immunocomplexes.

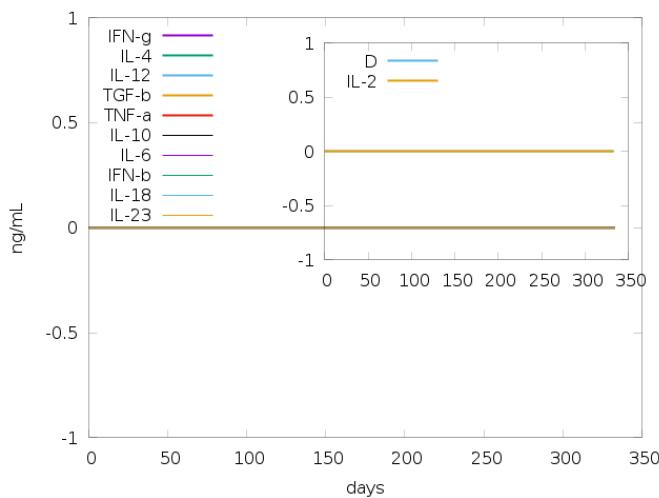


Figure 4: Concentration of cytokines and interleukins. Inset plot shows danger signal together with leukocyte growth factor IL-2.

Parker_B_scale_epitope_find
Use Parker's propensity scale, takes an antigen block as input,
and creates a list of residues that are possible epitopes.

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044_20251214-070025_5_bqisBajAVGmm.FSA_1_001

GIINTLQKYCYCRVRRGRCAVSLSCPKEEQIGKCSTRGKCCRRAKAYYQSFSFWFLAYYMLNQVTIAYYVLYDEFVT
IAYYILSDENYLLGPGPAGYYISLNSMYTRGPGPGIAGAKSKFPRSMSLISGPGPVGVIAGAKSKFPRSMSLGPGPVGFLDP
NNEVMPLIINGPGPGINFRQGSSPILCIFETKKPSFVRDFTTENIVNSVLQTGDGK

Epitopes of protein 0 -----

- ```
1] pos=27 len=4 EQIG
2] pos=33 len=9 STRGRKCCR
3] pos=212 len=4 GDGK
```

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044\_20251214-070025\_5\_bqiSbAJAVGmm.FSA\_1\_002

GIINTLQKYKYYCRVRRGRCAVSLCPKEEQIGKCSTRGRKCRRKKAYYYIITSYLQKAYYYLAKILCLKGPGPGLLQRGR  
LPLVSEFSDGPGLQRGRLPLVSEFSDEKKIILFQNNDINAQQKFANVISKIYTLIYRQLTSNVDVGCLLTDTIESTKTK  
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISEEYLSKEDRIITILQNIIVNEHDIKYDNKLLNMRDLYLTVFRERYS

### Epitopes of protein 1 -----

- |    |               |           |
|----|---------------|-----------|
| 1] | pos=27 len=4  | EQIG      |
| 2] | pos=33 len=9  | STRGRKCCR |
| 3] | pos=153 len=6 | IESTKT    |
| 4] | pos=183 len=4 | NKKE      |

## DoPeptideList\_I:

Given the antigen injected creates the list of peptides for all the NumAgProts proteins and for all i.e., 4 MHC I molecules

Read class I peptide list from file? NO

Allele: A0201  
Pseudo sequence: KAAHVEQRKAQTRTV  
Threshold: 9.523800  
Max score: 27.437000

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044\_20251214-070025\_5\_bqiSbAJAVGmm.FSA\_1\_001

GIINTLQKYYCRVRRGRCAVLSCLPKEEQIGKCSTRGRKCCRRKKAYYYQSFSFWFLAYYMLNVQTLIAYYVLYDEFVT  
IAYYILSDENYLLGPGPAYYISLNSMYTRGPGPVIAGAKSKFPRSMSLSIGPGPGVIAGAKSKFPRSMSLGPGPGYFLDP  
NNEVMPPLIINGPGPGIFRQGSSPILCIFETKKPSFVRLDTTETNIVNSVLQTGDGK

Epitopes of protein 0 -----

|    |                                                    |                   |
|----|----------------------------------------------------|-------------------|
| 0] | pos= 48 score=0.018963 unnormalised=2.1192000000   | YQSFSFWFL         |
| 1] | pos= 60 score=0.012440 unnormalised=1.3902000000   | MLLNVQTLI         |
| 2] | pos= 72 score=0.006928 unnormalised=0.7742000000   | VLYDEFVTI         |
| 3] | pos= 84 score=0.006838 unnormalised=0.7642000000   | ILSDENYLL         |
| 4] | pos= 90 score=0.016708 unnormalised=1.8672000000   | YLLGPGPGA         |
| 5] | pos= -1 score=0.938124 unnormalised=104.8410000000 | non-binding event |

-----  
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044\_20251214-070025\_5\_bqiSbAJAVGmm.FSA\_1\_002  
-----

GIINTLQKYYCRVRRGRCAVLSCLPKEEQIGKCSTRGRKCCRRKKAYYYIITSYLQKAYYYLAKILCLKGPGLLQRGR  
LPLVSEFSDEKQGPGLQRGRPLVSEFSDEKKIILFQNNDINAQQFANVISKIYRQLTSNVVGCLLTDTIESTTK  
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISEEYLSKEDRIITILQNIVNEHDIKYDNKLLNMRDLIVTFRERYS

Epitopes of protein 1 -----

|    |                                                    |                   |
|----|----------------------------------------------------|-------------------|
| 0] | pos= 53 score=0.043842 unnormalised=4.8072000000   | YLQKAYYYL         |
| 1] | pos= -1 score=0.956158 unnormalised=104.8410000000 | non-binding event |

=====

Allele: A0301

Pseudo sequence: KAAHVEQRKAQTRRV

Threshold: 8.185000

Max score: 23.064000

-----  
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044\_20251214-070025\_5\_bqiSbAJAVGmm.FSA\_1\_001  
-----

GIINTLQKYYCRVRRGRCAVLSCLPKEEQIGKCSTRGRKCCRRKKAYYYQSFSFWFLAYYMLNVQTLIAYYVLYDEFVT  
IAYYILSDENYLLGPGPAYYISLNSMYTRGPGPVIAGAKSKFPRSMSLSIGPGPGVIAGAKSKFPRSMSLGPGPGYFLDP  
NNEVMPPLIINGPGPGIFRQGSSPILCIFETKKPSFVRLDTTETNIVNSVLQTGDGK

Epitopes of protein 0 -----

|    |                                                    |                   |
|----|----------------------------------------------------|-------------------|
| 0] | pos= 1 score=0.001020 unnormalised=0.1070000000    | IINTLQKYY         |
| 1] | pos= -1 score=0.998980 unnormalised=104.8410000000 | non-binding event |

-----  
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044\_20251214-070025\_5\_bqiSbAJAVGmm.FSA\_1\_002  
-----

GIINTLQKYYCRVRRGRCAVLSCLPKEEQIGKCSTRGRKCCRRKKAYYYIITSYLQKAYYYLAKILCLKGPGLLQRGR  
LPLVSEFSDEKQGPGLQRGRPLVSEFSDEKKIILFQNNDINAQQFANVISKIYRQLTSNVVGCLLTDTIESTTK  
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISEEYLSKEDRIITILQNIVNEHDIKYDNKLLNMRDLIVTFRERYS

Epitopes of protein 1 -----

|    |                                                    |                   |
|----|----------------------------------------------------|-------------------|
| 0] | pos= 1 score=0.000911 unnormalised=0.1070000000    | IINTLQKYY         |
| 1] | pos= 48 score=0.038857 unnormalised=4.5620000000   | IIITSYLQK         |
| 2] | pos= 60 score=0.002087 unnormalised=0.2450000000   | YLAKILCLK         |
| 3] | pos= 101 score=0.007972 unnormalised=0.9360000000  | LVSEFSDEK         |
| 4] | pos= 122 score=0.010545 unnormalised=1.2380000000  | QQFANVISK         |
| 5] | pos= 176 score=0.002121 unnormalised=0.2490000000  | LIKFISDNK         |
| 6] | pos= 190 score=0.044529 unnormalised=5.2280000000  | IISEEYLSK         |
| 7] | pos= -1 score=0.892978 unnormalised=104.8410000000 | non-binding event |

=====

Allele: B0702  
Pseudo sequence: KAAREEQQIKAQTRE  
Threshold: 8.702800  
Max score: 28.406000

-----  
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044\_20251214-070025\_5\_bqiSbAJAVGmm.FSA\_1\_001  
-----

GIINTLQKYYCRVRRGRCAVLSCLPKEEQIGKCSTRGRKCCRKKAYYYQSFSFWFLAYYMLNVQTLIAYYVLYDEFVT  
IAYYILSDENYLLGPGLQPGAYYISLNSMYTRGPGLQPGIAGAKSKFPRSMSLSIGPGPGVIAGAKSKFPRSMSLSGPGLQPGYFLDP  
NNEVMPLIINGPGPGIFRQGSSPILCIFETKKPSFVRDFTETNIVNSVLQTGDGK

Epitopes of protein 0 -----

0] pos= -1 score=1.000000 unnormalised=104.8410000000 non-binding event

-----  
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044\_20251214-070025\_5\_bqiSbAJAVGmm.FSA\_1\_002  
-----

GIINTLQKYYCRVRRGRCAVLSCLPKEEQIGKCSTRGRKCCRKKAYYYITSYLQKAYYYLAKILCLKGPGPGLLQRGR  
LPLVSEFSDFGPGLQPGRLPVSEFSDEKKIILFQNNDINAQQFANVISKIYTLIYRQLTSNVDVGCLLTDTESTTK  
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISEEYLSKEDRIITILQNIVNEHDIKYDNKLLNMRDLIVTFRERYS

Epitopes of protein 1 -----

0] pos= 91 score=0.007302 unnormalised=0.7712000000 GPGLQRGRL  
1] pos= -1 score=0.992698 unnormalised=104.8410000000 non-binding event

=====

Allele: B3501  
Pseudo sequence: KAARVEQQIKAQTRE  
Threshold: 9.376400  
Max score: 27.550000

-----  
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044\_20251214-070025\_5\_bqiSbAJAVGmm.FSA\_1\_001  
-----

GIINTLQKYYCRVRRGRCAVLSCLPKEEQIGKCSTRGRKCCRKKAYYYQSFSFWFLAYYMLNVQTLIAYYVLYDEFVT  
IAYYILSDENYLLGPGLQPGAYYISLNSMYTRGPGLQPGIAGAKSKFPRSMSLSIGPGPGVIAGAKSKFPRSMSLSGPGLQPGYFLDP  
NNEVMPLIINGPGPGIFRQGSSPILCIFETKKPSFVRDFTETNIVNSVLQTGDGK

Epitopes of protein 0 -----

0] pos= 51 score=0.018026 unnormalised=1.9246000000 FSFWFLAYY  
1] pos= -1 score=0.981974 unnormalised=104.8410000000 non-binding event

-----  
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044\_20251214-070025\_5\_bqiSbAJAVGmm.FSA\_1\_002  
-----

GIINTLQKYYCRVRRGRCAVLSCLPKEEQIGKCSTRGRKCCRKKAYYYITSYLQKAYYYLAKILCLKGPGPGLLQRGR  
LPLVSEFSDFGPGLQPGRLPVSEFSDEKKIILFQNNDINAQQFANVISKIYTLIYRQLTSNVDVGCLLTDTESTTK  
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISEEYLSKEDRIITILQNIVNEHDIKYDNKLLNMRDLIVTFRERYS

Epitopes of protein 1 -----

0] pos= 124 score=0.009313 unnormalised=0.9856000000 FANVISKIY  
1] pos= -1 score=0.990687 unnormalised=104.8410000000 non-binding event

---



---

```

DoPeptideList_II:
 Given the antigen injected creates the list of peptides for all the
 NumAgProts proteins and for all i.e., 2 MHCII molecules

 Read class II peptide list from file? NO

=====
Allele: DRB1_0301
Pseudo sequence: RVTLCRDAYW
Threshold: 2.237910
Max score: 30.179000

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044_20251214-070025_5_bqiSbAJAVGmm.FSA_1_001

GIINTLQKYYCRVRGGRCAVLSCLPKEEQIGKCSTRGRKCCRKKAYYYQSFSFWFLAYYMLNVQTLIAYYVLYDEFVT

IAYYILSDENYLLPGPGAYYISLNSMYTRGPGPVIAGAKSKFPRSMSLSIGPGPGVIAGAKSKFPRSMSLGPGPGYFLDP

NNEVMPLINGPGPGIFRQGSSPILCIFETKKPSFVRLDTETNIVNSVLQTDGDK

Epitopes of protein 0 -----
0] pos= 1 score=0.014606 unnormalised=1.5140900000 IINTLQKYY
1] pos= 60 score=0.035357 unnormalised=3.6650900000 MLLNVQTLL
2] pos= 62 score=0.005480 unnormalised=0.5680900000 LNVQTLIAY
3] pos= 72 score=0.021639 unnormalised=2.2430900000 VLYDEFVTI
4] pos= 83 score=0.019999 unnormalised=2.0730900000 YILSDENYL
5] pos= 84 score=0.098235 unnormalised=10.1830900000 IILSDENYLL
6] pos= 99 score=0.073665 unnormalised=7.6360900000 YYISLNSMY
7] pos= 100 score=0.005625 unnormalised=0.5830900000 YISLNSMYT
8] pos= 101 score=0.012561 unnormalised=1.3020900000 ISLNSMYTR
9] pos= 147 score=0.001969 unnormalised=0.2040900000 MLSGPGPGY
10] pos= 155 score=0.031585 unnormalised=3.2740900000 YFLDPNNEV
11] pos= 186 score=0.019439 unnormalised=2.0150900000 IFETKKPSF
12] pos= 195 score=0.021523 unnormalised=2.2310900000 VRLDTTETN
13] pos= -1 score=0.638317 unnormalised=66.1680000000 non-binding event

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044_20251214-070025_5_bqiSbAJAVGmm.FSA_1_002

GIINTLQKYYCRVRGGRCAVLSCLPKEEQIGKCSTRGRKCCRKKAYYYIITSYLQKAYYYLAKILCLKGPGPGLLQRGR

LPLVSEFSDGPGPGLQRGRRLPVSEFSDEKKIILFQNNDINAQQFANVISKIYTLIYRQLTSNVDVGCLLTDTESTKTK

ISIEKIKQTGGINNVQSLIKFISDNKKEYTIISEEYLSKEDRIITILQNI
VNEHDIKYDNKLLNMRD
LIVTFRERYS

Epitopes of protein 1 -----
0] pos= 1 score=0.011164 unnormalised=1.5140900000 IINTLQKYY
1] pos= 48 score=0.000133 unnormalised=0.0180900000 IIITSYLNQK
2] pos= 49 score=0.048635 unnormalised=6.5960900000 IIITSYLNQKA
3] pos= 74 score=0.029206 unnormalised=3.9610900000 LLQRGRRLPL
4] pos= 75 score=0.003776 unnormalised=0.5120900000 LQRGRRLPLV
5] pos= 94 score=0.003776 unnormalised=0.5120900000 LQRGRRLPLV
6] pos= 101 score=0.014416 unnormalised=1.9550900000 LVSEFSDEK
7] pos= 148 score=0.043555 unnormalised=5.9070900000 LLTDTEST
8] pos= 152 score=0.001910 unnormalised=0.2590900000 TIESTKTKI
9] pos= 179 score=0.101303 unnormalised=13.7390900000 FISDNKKEY
10] pos= 190 score=0.015205 unnormalised=2.0620900000 IIISEEYLSK
11] pos= 196 score=0.007507 unnormalised=1.0180900000 LSKEDRIIT
12] pos= 205 score=0.020867 unnormalised=2.8300900000 ILQNI
VNEH

```

```

13] pos= 209 score=0.035761 unnormalised=4.8500900000 IVNEHDIKY
14] pos= 215 score=0.104245 unnormalised=14.1380900000 IKYDNKLLN
15] pos= 217 score=0.000686 unnormalised=0.0930900000 YDNKLLNMR
16] pos= 221 score=0.000952 unnormalised=0.1290900000 LLNMRDLIV
17] pos= 227 score=0.069023 unnormalised=9.3610900000 LIVTFRERY
18] pos= -1 score=0.487880 unnormalised=66.1680000000 non-binding event
=====
```

Allele: DRB1\_1501  
Pseudo sequence: RVTLGRDASW  
Threshold: 3.125180  
Max score: 28.118000

```

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044_20251214-070025_5_bqiSbAJAVGmm.FSA_1_001

```

GIINTLQKYYCRVRRGRCAVLSCLPKEEQIGKCSTRGRKCCRKKAYYYQSFSFWFLAYYMLNVQTLIAYYVLYDEFVT  
IAYYILSDENYLLGPGPYAYYISLNSMYTRGPGPYAGAKSKFPRSMSLSIGPGPVIAGAKSKFPRSMSLSGPYPGYFLDP  
NNEVMPLIINGPGPGLFRQGSSPILCIFETKKPSFVRLDTETTNIVNSVLQTDGDK

Epitopes of protein 0 -----  
0] pos= 5 score=0.005722 unnormalised=0.5428200000 LQKYYCRVR  
1] pos= 45 score=0.008473 unnormalised=0.8038200000 AYYYQSFSF  
2] pos= 55 score=0.006555 unnormalised=0.6218200000 FLAYYMLLN  
3] pos= 56 score=0.031865 unnormalised=3.0228200000 LAYYMLNV  
4] pos= 58 score=0.025530 unnormalised=2.4218200000 YYMLLNQ  
5] pos= 64 score=0.055942 unnormalised=5.3068200000 VQTLIAYYV  
6] pos= 100 score=0.060464 unnormalised=5.7358200000 YISLNSMYT  
7] pos= 101 score=0.014377 unnormalised=1.3638200000 ISLNSMYTR  
8] pos= 127 score=0.025909 unnormalised=2.4578200000 LSIGPGPGV  
9] pos= 175 score=0.028745 unnormalised=2.7268200000 IFRQGSSPI  
10] pos= 176 score=0.038907 unnormalised=3.6908200000 FRQGSSPIL  
11] pos= -1 score=0.697511 unnormalised=66.1680000000 non-binding event

```

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/43044_20251214-070025_5_bqiSbAJAVGmm.FSA_1_002

```

GIINTLQKYYCRVRRGRCAVLSCLPKEEQIGKCSTRGRKCCRKKAYYYITSYLQKAYYYLAKILCLKGPGPGLLQRGR  
LPLVSEFSDFGPGLQRGRPLVSEFSDEKKIILFQNNDINAQQFANVISKIYTLIYRQLTSNVVGCLLTDTIESTTK  
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISEEYLSKEDRIITILQNIVNEHDIKYDNKLLNMRDLIVTFRERYS

Epitopes of protein 1 -----  
0] pos= 5 score=0.004629 unnormalised=0.5428200000 LQKYYCRVR  
1] pos= 40 score=0.003981 unnormalised=0.4668200000 CRRKKAYYI  
2] pos= 46 score=0.022026 unnormalised=2.5828200000 YYIIITSYL  
3] pos= 47 score=0.045930 unnormalised=5.3858200000 YIIITSYQ  
4] pos= 75 score=0.043048 unnormalised=5.0478200000 LQRGRLPLV  
5] pos= 94 score=0.043048 unnormalised=5.0478200000 LQRGRLPLV  
6] pos= 111 score=0.053691 unnormalised=6.2958200000 IILFQNNDI  
7] pos= 121 score=0.017353 unnormalised=2.0348200000 AQQFANVIS  
8] pos= 135 score=0.009686 unnormalised=1.1358200000 IYRQLTSNV  
9] pos= 136 score=0.011682 unnormalised=1.3698200000 YRQLTSNV  
10] pos= 170 score=0.028115 unnormalised=3.2968200000 INNVQSLIK  
11] pos= 176 score=0.012057 unnormalised=1.4138200000 LIKFISDNK  
12] pos= 177 score=0.020167 unnormalised=2.3648200000 IKFISDNKK  
13] pos= 203 score=0.108987 unnormalised=12.7798200000 ITILQNIVN  
14] pos= 221 score=0.011315 unnormalised=1.3268200000 LLNMRDLIV  
15] pos= -1 score=0.564283 unnormalised=66.1680000000 non-binding event

