

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
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.2022.998262>

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://jitc.bmj.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)

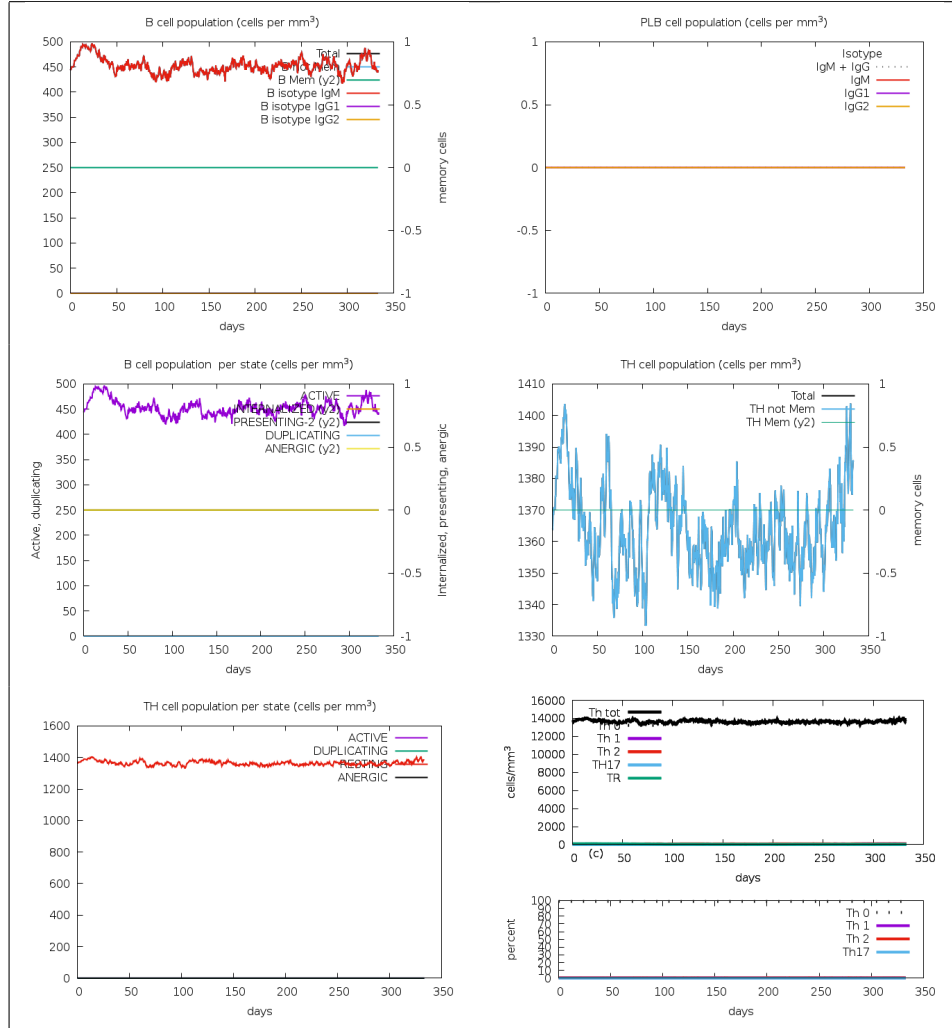


Figure 1: Cell counts shown. Legend: Act=active, Intern=internalized the Ag, Pres II = presenting on MHC II, Dup = in the mitotic cycle, Anergic = anergic, Resting = not active.

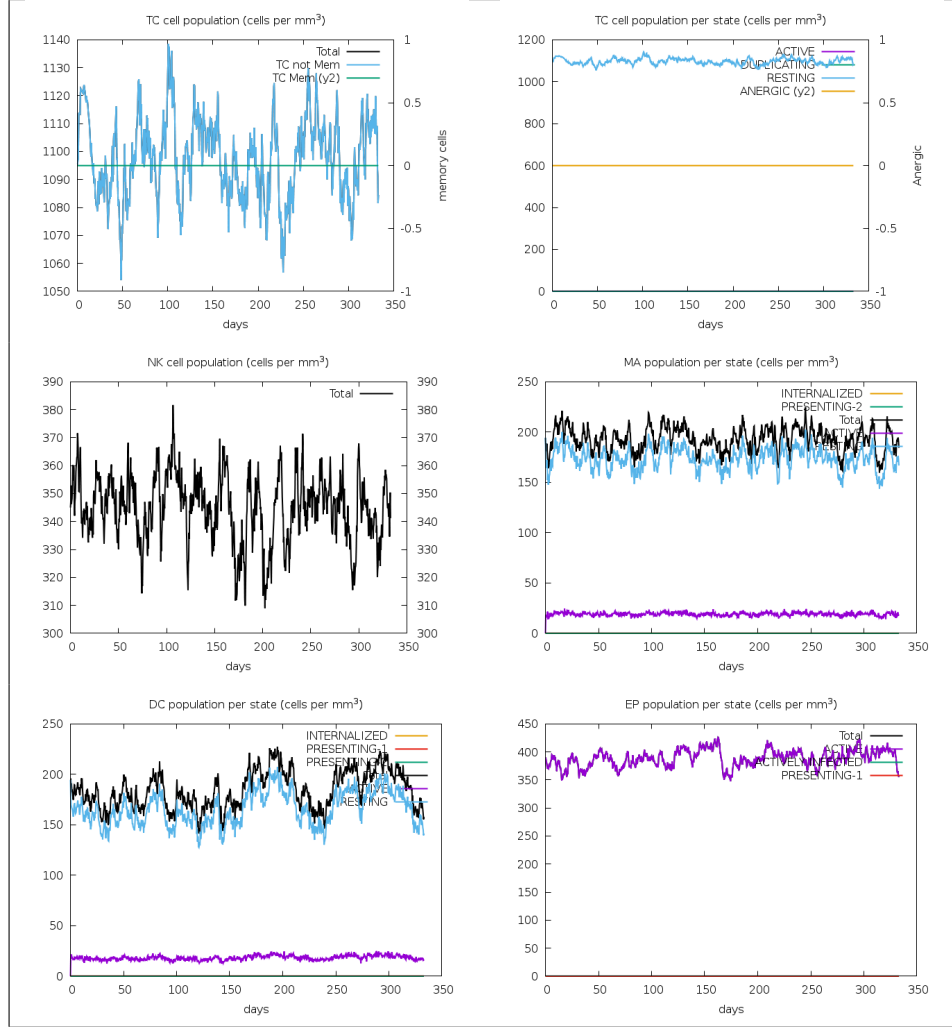


Figure 2: Legend: symbols as figure above.

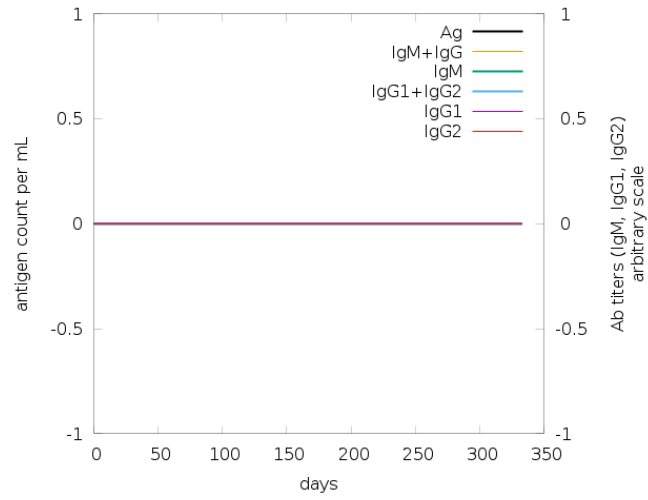


Figure 3: The virus, the immunoglobulins and the immunocomplexes.

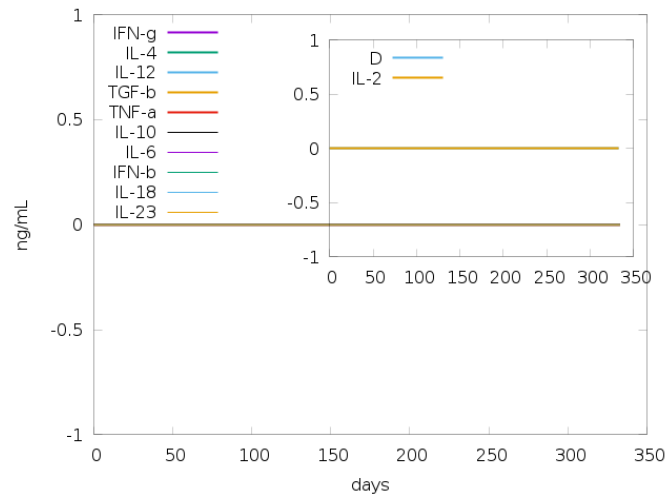


Figure 4: Concentration of cytokines and interleukins. Inset plot shows danger signal together with leukocyte growth factor IL-2.

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

GIINTLQKYYCRVRGGRCAVLSCLPKEEQIGKCKSTRGRKCCRRKKAYYYQSFSFWLAYMYLLNVQTLIAYVYLYDEFVT
IAYYILSDENYLLGPGPGAYYISLNSMYTRGPGPIAGAKSKFPRSMLSIGPGPGVIAGAKSKFPRSMLSGPGPGYFLDP
NNEVMPLIINPGPGPIFRQSSPILCIFETKKPSEVRLDTTETNIVNSVIQTGDGK

[illegible]

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

GIINTLQKYYCVRVGRGCAVLSCLPKEEQIGKCKSTRGRKCCRKKYAYIIITSYLQKAYYYLAKILCLKGPGGLLQGRG
LPLVSEFSDGPGPLQGRGLPLVSEFSDEKKIILFQNNIDNAQQFANVISKIYTYLIYRQLTSNVVDCGLLTDTIESTKTK
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISFEVY SKEDRIITTLQNVNEHDIKYDNKILNMRDIIVTRFRYS

[illegible]

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

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

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

5

GIINTLQKYYCRVGRGCAVLSCLPKEEQIGKCSTRGRKCCRKKAYYYQSFSFWFLAYYMLLNVTLIAYYVLYDEFVT
IAYYILSDENYLLGPGPGAYYISLNSMYTRGPGGIAGAKSKFPRSMLSIGPGPGVIAGAKSKFPRSMLSGPGPGYFLDP
NNEVMPLIINGPGPGIFRQGSSPILCIFETKKPSFVRLDTTETNIVNSVLQTGDGK

Epitopes of protein 0 -----

0]	pos=	48	score=0.018963	unnormalised=2.1192000000	YQSFSFWFL
1]	pos=	60	score=0.012440	unnormalised=1.3902000000	MLLNVTLI
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

GIINTLQKYYCRVGRGCAVLSCLPKEEQIGKCSTRGRKCCRKKAYYYIITSYLQKAYYLAAILCLKGPGLLQGR
LPLVSEFSDGPGPGLQGRPLVSEFSDEKKIILFQNDINAQQFANVISKIYTLIYRQLTSNVDVGCLLTDTIESTKTK
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISEEYLSKEDRIITILQNIVNEHDIKYNKLLNMRDLIVFRERY

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

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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

GIINTLQKYYCRVGRGCAVLSCLPKEEQIGKCSTRGRKCCRKKAYYYQSFSFWFLAYYMLLNVTLIAYYVLYDEFVT
IAYYILSDENYLLGPGPGAYYISLNSMYTRGPGGIAGAKSKFPRSMLSIGPGPGVIAGAKSKFPRSMLSGPGPGYFLDP
NNEVMPLIINGPGPGIFRQGSSPILCIFETKKPSFVRLDTTETNIVNSVLQTGDGK

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

GIINTLQKYYCRVGRGCAVLSCLPKEEQIGKCSTRGRKCCRKKAYYYIITSYLQKAYYLAAILCLKGPGLLQGR
LPLVSEFSDGPGPGLQGRPLVSEFSDEKKIILFQNDINAQQFANVISKIYTLIYRQLTSNVDVGCLLTDTIESTKTK
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISEEYLSKEDRIITILQNIVNEHDIKYNKLLNMRDLIVFRERY

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

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Allele: B0702
Pseudo sequence: KAAREEQIKAQTRE
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

GIINTLQKYYCRVRGGRC AVLSCLPKEEQIGKCSTRGRKCCRRKKAYYYQSFSFWFLAYYMLNVQTLIAYYVLYDEFVT
IAYYILSDENYLLGPGPGAYYISLNSMYTRGPGPGIAGAKSKFPRSMLSIGPGPGVIAGAKSKFPRSMLSGPGPGYFLDP
NNEVMPLIINGPGPGIFRQGSSPILCIFETKKPSFVRLDTTETNIVNSVLQTGDGK

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

GIINTLQKYYCRVRGGRC AVLSCLPKEEQIGKCSTRGRKCCRRKKAYYYIITSYLQKAYYLLAKILCLKGPGPGLLQRGR
LPLVSEFSDGPGPGLQRGLPLVSEFSDEKKIILFQNNNDINAQQFANVISKIYTLIYRQLTSNVDVGCLLTDTIESTTK
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISEEYLSKEDRIITILQNIVNEHDIKYDNKLLNMRDLIVTFRERY

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

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Allele: B3501
Pseudo sequence: KAARVEEQIKAQTRE
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

GIINTLQKYYCRVRGGRC AVLSCLPKEEQIGKCSTRGRKCCRRKKAYYYQSFSFWFLAYYMLNVQTLIAYYVLYDEFVT
IAYYILSDENYLLGPGPGAYYISLNSMYTRGPGPGIAGAKSKFPRSMLSIGPGPGVIAGAKSKFPRSMLSGPGPGYFLDP
NNEVMPLIINGPGPGIFRQGSSPILCIFETKKPSFVRLDTTETNIVNSVLQTGDGK

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

GIINTLQKYYCRVRGGRC AVLSCLPKEEQIGKCSTRGRKCCRRKKAYYYIITSYLQKAYYLLAKILCLKGPGPGLLQRGR
LPLVSEFSDGPGPGLQRGLPLVSEFSDEKKIILFQNNNDINAQQFANVISKIYTLIYRQLTSNVDVGCLLTDTIESTTK
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISEEYLSKEDRIITILQNIVNEHDIKYDNKLLNMRDLIVTFRERY

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: RVTLGRDAYW
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

GIINTLQKYYCRVRGGRCVLSCLPKEEQIGKCSTRGRKCCRRKKAYYYQSFSFWFLAYYMLLNVTLIAYYVLYDEFVT
IAYYILSDENYLLGPGPGAYYISLNSMYTRGPGPGIAGAKSKFPRSMLSIGPGPGVIAGAKSKFPRSMLSGPGPGYFLDP
NNEVMPLIINGPGPGIFRQGSSPILCIFETKKPSFVRLDTTETNIVNSVLQTGDGK

Epitopes of protein 0 -----

0]	pos=	1	score=0.014606	unnormalised=1.5140900000	IINTLQKYY
1]	pos=	60	score=0.035357	unnormalised=3.6650900000	MLLNVTLI
2]	pos=	62	score=0.005480	unnormalised=0.5680900000	LNVTLIAY
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	ILSDENYLL
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

GIINTLQKYYCRVRGGRCVLSCLPKEEQIGKCSTRGRKCCRRKKAYYIIITSYLQKAYYLAAILCLKGPGLLQGRGR
LPLVSEFSDGPGPLQGRPLPLVSEFSDEKKIILFQNNINAQQFANVISKIYTLIYRQLTSNVDVGCLLTDTIESTTKT
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISEEYLSKEDRIITILQNIIVNEHDIKYNKLLNMRDLIVFRERYYS

Epitopes of protein 1 -----

0]	pos=	1	score=0.011164	unnormalised=1.5140900000	IINTLQKYY
1]	pos=	48	score=0.000133	unnormalised=0.0180900000	IIITSYLQK
2]	pos=	49	score=0.048635	unnormalised=6.5960900000	IITSYLQKA
3]	pos=	74	score=0.029206	unnormalised=3.9610900000	LLQGRPLPL
4]	pos=	75	score=0.003776	unnormalised=0.5120900000	LQGRPLPLV
5]	pos=	94	score=0.003776	unnormalised=0.5120900000	LQGRPLPLV
6]	pos=	101	score=0.014416	unnormalised=1.9550900000	LVSEFSDEK
7]	pos=	148	score=0.043555	unnormalised=5.9070900000	LLTDTIEST
8]	pos=	152	score=0.001910	unnormalised=0.2590900000	TIESTTKTI
9]	pos=	179	score=0.101303	unnormalised=13.7390900000	FISDNKKEY
10]	pos=	190	score=0.015205	unnormalised=2.0620900000	IISEEYLSK
11]	pos=	196	score=0.007507	unnormalised=1.0180900000	LSKEDRIIT
12]	pos=	205	score=0.020867	unnormalised=2.8300900000	ILQNIIVNEH

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

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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

GIINTLQKYYCRVRGGRCVLSCLPKKEQIGKCSTRGRKCCRKKAYYYQSFSFWFLAYYMLLNVTLIAYYVLYDEFVT
IAYYILSDENYLLGPGPGAYYISLNSMYTRGPGPIAGAKSKFPRSMLSIGPGPGVIAGAKSKFPRSMLSGPGPGYFLDP
NNEVMPLIINGPGPGIFRQGSSPILCFETKKPSFVRLDTTETNIVNSVLQTGDGK

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	LAYYMLLN
4]	pos= 58	score=0.025530	unnormalised=2.4218200000	YYMLLNVT
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

GIINTLQKYYCRVRGGRCVLSCLPKKEQIGKCSTRGRKCCRKKAYYIIITSYLQKAYYLAAILCLKGPGLLQRGR
LPLVSEFSFGPGPLQRGRPLVSEFSDEKKIILFQNNINAQQFANVISKIYTLIRQLTSNVDVGCLLTDITESTKTK
ISIEKIKQTGINNVQSLIKFISDNKKEYKTIISEEYLSKEDRIITILQNIIVNEHDIKYDNKLLNMRDLIVTFRERY

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	YIIITSYL
3]	pos= 47	score=0.045930	unnormalised=5.3858200000	YIIITSYLQ
4]	pos= 75	score=0.043048	unnormalised=5.0478200000	LQRGRPLV
5]	pos= 94	score=0.043048	unnormalised=5.0478200000	LQRGRPLV
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	YRQLTSNVD
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	ITILQNIIV
14]	pos= 221	score=0.011315	unnormalised=1.3268200000	LLNMRDLIV
15]	pos= -1	score=0.564283	unnormalised=66.1680000000	non-binding event
