C-IMMSIM simulation results

May 23, 2026

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://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)

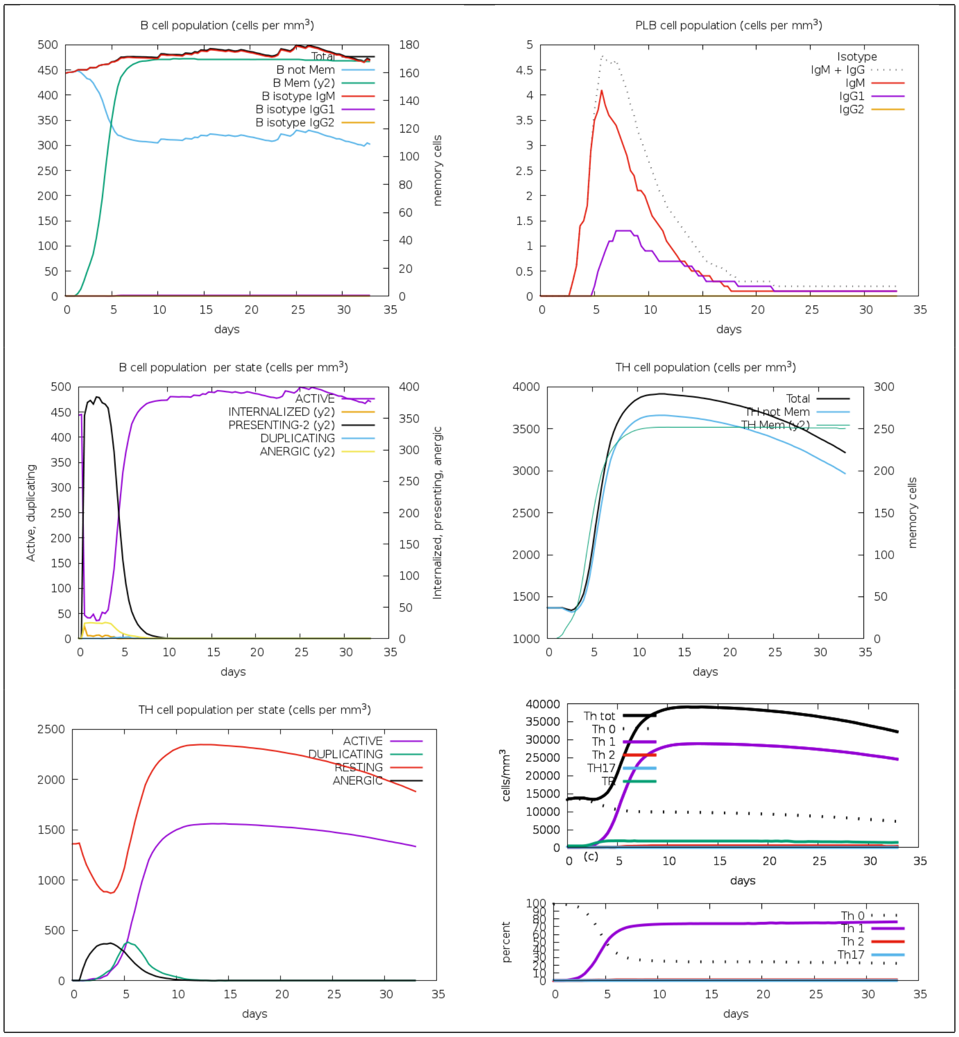

Figure 1: Cell counts shown. Legend: Act=active, Intern=internalized the Ag, Pres II = presenting on MHC II, Dup = in the mitotic cycle, Anergic = anergic, Resting = not active.

Figure 2: Legend: symbols as figure above.

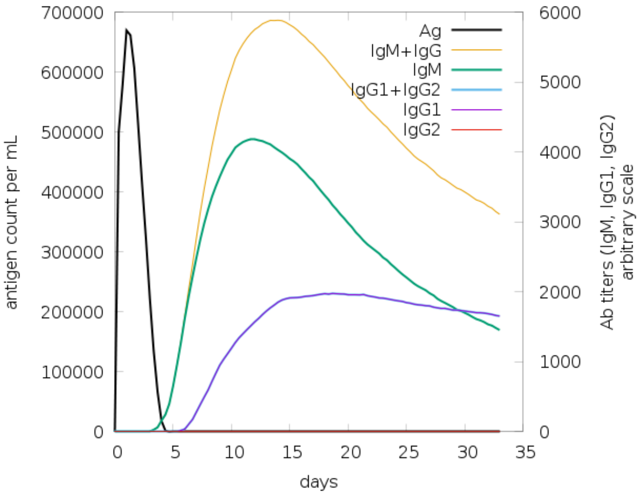

Figure 3: The virus, the immunoglobulins and the immunocomplexes.

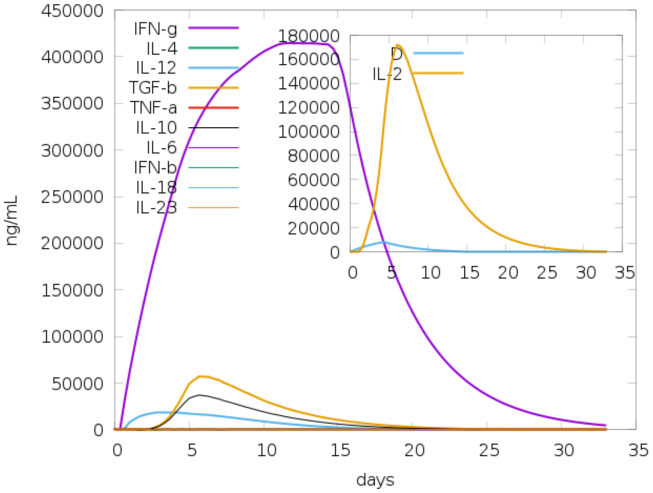

Figure 4: Concentration of cytokines and interleukins. Inset plot shows danger signal together with leukocyte growth factor IL-2.

```
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/50712_20260523-104210_5_km0OQLjwdbkx.FSA_1_001
----------------------------------


MARGKKIGYSGLKSRQTKDKAAEAAAPAAPAPAPEVTPAAAPVVAPAPAPAEAKKSEESDDMGFGLFDVAKNVAAESAAE
AAAPAEEAAAAPAPAPVVKEAKKDLHSLLELGTKPTAPHVRNKKVILFDTNHQVSICNQIIDAINSGIDLGDLLEGGLLT
LCVEHYYNSDKDSIISNSVGQTRFSGLLIVKTVLEFILQKTDSGVTLHPLVRTSKVKNEVASFKQALSNLARHGEYAPFA
NLSGINNLEHGLYPQLSAIALGVATAHGSTLAGVNVGEQYQQLREAAHDAEVKLQRRHEHQEIQAIATVQARPMNRPTAL
PPPVDDKIEHESTEDSSSSSSFVDLNDPFALLNEDEDTLDDSVMIPGTTSREFQGPQRVVTKKGRTFLYPNDLLQTNPPE
SLITALVEEYQNPVSAKELQADWPDMSFDERRHVAMCPGPGGLYPQLSAILIHQGVNLVLTLCVEHYYQLSAIALGVQTL
AVLSQKRPMNRPTALTEITHSQTLTVQARPMNRYPQLSAIALAAYVIFGILRSSFILKFVPLILALKTLESTESQKILEQ
FHLQKTEITHTVLEFILQKTDSGVTRGRIGLFLSFCSLFLIALGVATAHGSTLAGATRFLDVIPNEPHYSEHGLYPQLSA
IALGVPQLSAIALGVATAHGSQTLAVLSQKREKLAHHHHHH

00000000000010011111110000000000000000000000000000001111111110000000000001001110
00000000000000000000110000000000001000000000000000010000000000000000000000000000
00000011111000000011000000000000000000001110000000000011100000000000000000000000
00000000000000000000000000100000000001100000001100000000011000000000000000000000
00010001111111111110000000000000001111110000000011110000000000100000000000000100
00000000011000100000000000010100000000000000000000000000000000000000000000000000
00000010000000000000000000000000000000000000000000000000000000000000011111000000
00000000000000000001111110000000000000000000000001000000000000000001110000000000
00000000000000000011000000000110000000000
Epitopes of protein 0 ------------
1]        pos=15 len=7        QTKDKAA
2]        pos=52 len=9        AKKSEESDD
3]        pos=166 len=5        YNSDK
4]        pos=327 len=12        IEHESTEDSSSS
5]        pos=354 len=6        DEDTLD
6]        pos=368 len=4        TSRE
7]        pos=549 len=5        ESTES
8]        pos=579 len=6        TDSGVT
```

```
DoPeptideList_I:
        Given the antigen injected creates the list of peptides for all the
        NumAgProts proteins and for all i.e., 4 MHCI molecules

        Read class I peptide list from file? NO

=========================================================================

Allele: A0101
Pseudo sequence: KAVHAEQRNKAQTRA
Threshold: 9.456400
Max score: 29.236000


----------------------------------
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/50712_20260523-104210_5_km0OQLjwdbkx.FSA_1_001
----------------------------------

MARGKKIGYSGLKSRQTKDKAAEAAAPAAPAPAPEVTPAAAPVVAPAPAPAEAKKSEESDDMGFGLFDVAKNVAAESAAE
```

```
AAAPAEEAAAAPAPAPVVKEAKKDLHSLLELGTKPTAPHVRNKKVILFDTNHQVSICNQIIDAINSGIDLGDLLEGGLLT
LCVEHYYNSDKDSIISNSVGQTRFSGLLIVKTVLEFILQKTDSGVTLHPLVRTSKVKNEVASFKQALSNLARHGEYAPFA
NLSGINNLEHGLYPQLSAIALGVATAHGSTLAGVNVGEQYQQLREAAHDAEVKLQRRHEHQEIQAIATVQARPMNRPTAL
PPPVDDKIEHESTEDSSSSSSFVDLNDPFALLNEDEDTLDDSVMIPGTTSREFQGPQRVVTKKGRTFLYPNDLLQTNPPE
SLITALVEEYQNPVSAKELQADWPDMSFDERRHVAMCPGPGGLYPQLSAILIHQGVNLVLTLCVEHYYQLSAIALGVQTL
AVLSQKRPMNRPTALTEITHSQTLTVQARPMNRYPQLSAIALAAYVIFGILRSSFILKFVPLILALKTLESTESQKILEQ
FHLQKTEITHTVLEFILQKTDSGVTRGRIGLFLSFCSLFLIALGVATAHGSTLAGATRFLDVIPNEPHYSEHGLYPQLSA
IALGVPQLSAIALGVATAHGSQTLAVLSQKREKLAHHHHHH

Epitopes of protein 0 ------------
0]        pos= 158 score=0.001019 unnormalised=0.1106000000        LTLCVEHYY
1]        pos= 199 score=0.008216 unnormalised=0.8916000000        KTDSGVTLH
2]        pos= 459 score=0.001019 unnormalised=0.1106000000        LTLCVEHYY
3]        pos= 516 score=0.023615 unnormalised=2.5626000000        LSAIALAAY
4]        pos=  -1 score=0.966130 unnormalised=104.8410000000        non-binding event

=========================================================================

Allele: A0101
Pseudo sequence: KAVHAEQRNKAQTRA
Threshold: 9.456400
Max score: 29.236000


----------------------------------
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/50712_20260523-104210_5_km0OQLjwdbkx.FSA_1_001
----------------------------------

MARGKKIGYSGLKSRQTKDKAAEAAAPAAPAPAPEVTPAAAPVVAPAPAPAEAKKSEESDDMGFGLFDVAKNVAAESAAE
AAAPAEEAAAAPAPAPVVKEAKKDLHSLLELGTKPTAPHVRNKKVILFDTNHQVSICNQIIDAINSGIDLGDLLEGGLLT
LCVEHYYNSDKDSIISNSVGQTRFSGLLIVKTVLEFILQKTDSGVTLHPLVRTSKVKNEVASFKQALSNLARHGEYAPFA
NLSGINNLEHGLYPQLSAIALGVATAHGSTLAGVNVGEQYQQLREAAHDAEVKLQRRHEHQEIQAIATVQARPMNRPTAL
PPPVDDKIEHESTEDSSSSSSFVDLNDPFALLNEDEDTLDDSVMIPGTTSREFQGPQRVVTKKGRTFLYPNDLLQTNPPE
SLITALVEEYQNPVSAKELQADWPDMSFDERRHVAMCPGPGGLYPQLSAILIHQGVNLVLTLCVEHYYQLSAIALGVQTL
AVLSQKRPMNRPTALTEITHSQTLTVQARPMNRYPQLSAIALAAYVIFGILRSSFILKFVPLILALKTLESTESQKILEQ
FHLQKTEITHTVLEFILQKTDSGVTRGRIGLFLSFCSLFLIALGVATAHGSTLAGATRFLDVIPNEPHYSEHGLYPQLSA
IALGVPQLSAIALGVATAHGSQTLAVLSQKREKLAHHHHHH

Epitopes of protein 0 ------------
0]        pos= 158 score=0.001019 unnormalised=0.1106000000        LTLCVEHYY
1]        pos= 199 score=0.008216 unnormalised=0.8916000000        KTDSGVTLH
2]        pos= 459 score=0.001019 unnormalised=0.1106000000        LTLCVEHYY
3]        pos= 516 score=0.023615 unnormalised=2.5626000000        LSAIALAAY
4]        pos=  -1 score=0.966130 unnormalised=104.8410000000        non-binding event

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


----------------------------------
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/50712_20260523-104210_5_km0OQLjwdbkx.FSA_1_001
----------------------------------

MARGKKIGYSGLKSRQTKDKAAEAAAPAAPAPAPEVTPAAAPVVAPAPAPAEAKKSEESDDMGFGLFDVAKNVAAESAAE
AAAPAEEAAAAPAPAPVVKEAKKDLHSLLELGTKPTAPHVRNKKVILFDTNHQVSICNQIIDAINSGIDLGDLLEGGLLT
LCVEHYYNSDKDSIISNSVGQTRFSGLLIVKTVLEFILQKTDSGVTLHPLVRTSKVKNEVASFKQALSNLARHGEYAPFA
NLSGINNLEHGLYPQLSAIALGVATAHGSTLAGVNVGEQYQQLREAAHDAEVKLQRRHEHQEIQAIATVQARPMNRPTAL
PPPVDDKIEHESTEDSSSSSSFVDLNDPFALLNEDEDTLDDSVMIPGTTSREFQGPQRVVTKKGRTFLYPNDLLQTNPPE
SLITALVEEYQNPVSAKELQADWPDMSFDERRHVAMCPGPGGLYPQLSAILIHQGVNLVLTLCVEHYYQLSAIALGVQTL
AVLSQKRPMNRPTALTEITHSQTLTVQARPMNRYPQLSAIALAAYVIFGILRSSFILKFVPLILALKTLESTESQKILEQ
FHLQKTEITHTVLEFILQKTDSGVTRGRIGLFLSFCSLFLIALGVATAHGSTLAGATRFLDVIPNEPHYSEHGLYPQLSA
```

```
IALGVPQLSAIALGVATAHGSQTLAVLSQKREKLAHHHHHH

Epitopes of protein 0 ------------
0]        pos=  25 score=0.014627 unnormalised=3.0192000000        APAAPAPAP
1]        pos=  28 score=0.010882 unnormalised=2.2462000000        APAPAPEVT
2]        pos=  30 score=0.020314 unnormalised=4.1932000000        APAPEVTPA
3]        pos=  32 score=0.011425 unnormalised=2.3582000000        APEVTPAAA
4]        pos=  36 score=0.014850 unnormalised=3.0652000000        TPAAAPVVA
5]        pos=  40 score=0.022601 unnormalised=4.6652000000        APVVAPAPA
6]        pos=  44 score=0.027848 unnormalised=5.7482000000        APAPAPAEA
7]        pos=  82 score=0.020048 unnormalised=4.1382000000        APAEEAAAA
8]        pos=  88 score=0.006594 unnormalised=1.3612000000        AAAPAPAPV
9]        pos=  92 score=0.006822 unnormalised=1.4082000000        APAPVVKEA
10]        pos= 116 score=0.000960 unnormalised=0.1982000000        APHVRNKKV
11]        pos= 207 score=0.008775 unnormalised=1.8112000000        HPLVRTSKV
12]        pos= 236 score=0.012960 unnormalised=2.6752000000        APFANLSGI
13]        pos= 252 score=0.031815 unnormalised=6.5672000000        YPQLSAIAL
14]        pos= 311 score=0.055297 unnormalised=11.4142000000        RPMNRPTAL
15]        pos= 315 score=0.035095 unnormalised=7.2442000000        RPTALPPPV
16]        pos= 364 score=0.007592 unnormalised=1.5672000000        IPGTTSREF
17]        pos= 486 score=0.055297 unnormalised=11.4142000000        RPMNRPTAL
18]        pos= 490 score=0.000645 unnormalised=0.1332000000        RPTALTEIT
19]        pos= 508 score=0.030241 unnormalised=6.2422000000        RPMNRYPQL
20]        pos= 513 score=0.031815 unnormalised=6.5672000000        YPQLSAIAL
21]        pos= 625 score=0.007297 unnormalised=1.5062000000        EPHYSEHGL
22]        pos= 634 score=0.031815 unnormalised=6.5672000000        YPQLSAIAL
23]        pos= 644 score=0.026472 unnormalised=5.4642000000        VPQLSAIAL
24]        pos=  -1 score=0.507912 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/50712_20260523-104210_5_km0OQLjwdbkx.FSA_1_001
----------------------------------

MARGKKIGYSGLKSRQTKDKAAEAAAPAAPAPAPEVTPAAAPVVAPAPAPAEAKKSEESDDMGFGLFDVAKNVAAESAAE
AAAPAEEAAAAPAPAPVVKEAKKDLHSLLELGTKPTAPHVRNKKVILFDTNHQVSICNQIIDAINSGIDLGDLLEGGLLT
LCVEHYYNSDKDSIISNSVGQTRFSGLLIVKTVLEFILQKTDSGVTLHPLVRTSKVKNEVASFKQALSNLARHGEYAPFA
NLSGINNLEHGLYPQLSAIALGVATAHGSTLAGVNVGEQYQQLREAAHDAEVKLQRRHEHQEIQAIATVQARPMNRPTAL
PPPVDDKIEHESTEDSSSSSSFVDLNDPFALLNEDEDTLDDSVMIPGTTSREFQGPQRVVTKKGRTFLYPNDLLQTNPPE
SLITALVEEYQNPVSAKELQADWPDMSFDERRHVAMCPGPGGLYPQLSAILIHQGVNLVLTLCVEHYYQLSAIALGVQTL
AVLSQKRPMNRPTALTEITHSQTLTVQARPMNRYPQLSAIALAAYVIFGILRSSFILKFVPLILALKTLESTESQKILEQ
FHLQKTEITHTVLEFILQKTDSGVTRGRIGLFLSFCSLFLIALGVATAHGSTLAGATRFLDVIPNEPHYSEHGLYPQLSA
IALGVPQLSAIALGVATAHGSQTLAVLSQKREKLAHHHHHH

Epitopes of protein 0 ------------
0]        pos=  25 score=0.014627 unnormalised=3.0192000000        APAAPAPAP
1]        pos=  28 score=0.010882 unnormalised=2.2462000000        APAPAPEVT
2]        pos=  30 score=0.020314 unnormalised=4.1932000000        APAPEVTPA
3]        pos=  32 score=0.011425 unnormalised=2.3582000000        APEVTPAAA
4]        pos=  36 score=0.014850 unnormalised=3.0652000000        TPAAAPVVA
5]        pos=  40 score=0.022601 unnormalised=4.6652000000        APVVAPAPA
6]        pos=  44 score=0.027848 unnormalised=5.7482000000        APAPAPAEA
7]        pos=  82 score=0.020048 unnormalised=4.1382000000        APAEEAAAA
8]        pos=  88 score=0.006594 unnormalised=1.3612000000        AAAPAPAPV
9]        pos=  92 score=0.006822 unnormalised=1.4082000000        APAPVVKEA
10]        pos= 116 score=0.000960 unnormalised=0.1982000000        APHVRNKKV
11]        pos= 207 score=0.008775 unnormalised=1.8112000000        HPLVRTSKV
12]        pos= 236 score=0.012960 unnormalised=2.6752000000        APFANLSGI
```

```
13]        pos= 252 score=0.031815 unnormalised=6.5672000000        YPQLSAIAL
14]        pos= 311 score=0.055297 unnormalised=11.4142000000        RPMNRPTAL
15]        pos= 315 score=0.035095 unnormalised=7.2442000000        RPTALPPPV
16]        pos= 364 score=0.007592 unnormalised=1.5672000000        IPGTTSREF
17]        pos= 486 score=0.055297 unnormalised=11.4142000000        RPMNRPTAL
18]        pos= 490 score=0.000645 unnormalised=0.1332000000        RPTALTEIT
19]        pos= 508 score=0.030241 unnormalised=6.2422000000        RPMNRYPQL
20]        pos= 513 score=0.031815 unnormalised=6.5672000000        YPQLSAIAL
21]        pos= 625 score=0.007297 unnormalised=1.5062000000        EPHYSEHGL
22]        pos= 634 score=0.031815 unnormalised=6.5672000000        YPQLSAIAL
23]        pos= 644 score=0.026472 unnormalised=5.4642000000        VPQLSAIAL
24]        pos=  -1 score=0.507912 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_0101
Pseudo sequence: KAFAHVEQRKAQTRV
Threshold: 2.392440
Max score: 26.461000


----------------------------------
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/50712_20260523-104210_5_km0OQLjwdbkx.FSA_1_001
----------------------------------

MARGKKIGYSGLKSRQTKDKAAEAAAPAAPAPAPEVTPAAAPVVAPAPAPAEAKKSEESDDMGFGLFDVAKNVAAESAAE
AAAPAEEAAAAPAPAPVVKEAKKDLHSLLELGTKPTAPHVRNKKVILFDTNHQVSICNQIIDAINSGIDLGDLLEGGLLT
LCVEHYYNSDKDSIISNSVGQTRFSGLLIVKTVLEFILQKTDSGVTLHPLVRTSKVKNEVASFKQALSNLARHGEYAPFA
NLSGINNLEHGLYPQLSAIALGVATAHGSTLAGVNVGEQYQQLREAAHDAEVKLQRRHEHQEIQAIATVQARPMNRPTAL
PPPVDDKIEHESTEDSSSSSSFVDLNDPFALLNEDEDTLDDSVMIPGTTSREFQGPQRVVTKKGRTFLYPNDLLQTNPPE
SLITALVEEYQNPVSAKELQADWPDMSFDERRHVAMCPGPGGLYPQLSAILIHQGVNLVLTLCVEHYYQLSAIALGVQTL
AVLSQKRPMNRPTALTEITHSQTLTVQARPMNRYPQLSAIALAAYVIFGILRSSFILKFVPLILALKTLESTESQKILEQ
FHLQKTEITHTVLEFILQKTDSGVTRGRIGLFLSFCSLFLIALGVATAHGSTLAGATRFLDVIPNEPHYSEHGLYPQLSA
IALGVPQLSAIALGVATAHGSQTLAVLSQKREKLAHHHHHH

Epitopes of protein 0 ------------
0]        pos=   8 score=0.043680 unnormalised=11.8545600000        YSGLKSRQT
1]        pos=  35 score=0.011841 unnormalised=3.2135600000        VTPAAAPVV
2]        pos=  42 score=0.015382 unnormalised=4.1745600000        VVAPAPAPA
3]        pos=  66 score=0.011262 unnormalised=3.0565600000        FDVAKNVAA
4]        pos=  72 score=0.006122 unnormalised=1.6615600000        VAAESAAEA
5]        pos= 104 score=0.002419 unnormalised=0.6565600000        LHSLLELGT
6]        pos= 183 score=0.014317 unnormalised=3.8855600000        FSGLLIVKT
7]        pos= 222 score=0.055058 unnormalised=14.9425600000        FKQALSNLA
8]        pos= 235 score=0.009011 unnormalised=2.4455600000        YAPFANLSG
9]        pos= 238 score=0.021222 unnormalised=5.7595600000        FANLSGINN
10]        pos= 251 score=0.017714 unnormalised=4.8075600000        LYPQLSAIA
11]        pos= 252 score=0.033882 unnormalised=9.1955600000        YPQLSAIAL
12]        pos= 262 score=0.005308 unnormalised=1.4405600000        VATAHGSTL
13]        pos= 279 score=0.012423 unnormalised=3.3715600000        YQQLREAAH
14]        pos= 302 score=0.025153 unnormalised=6.8265600000        IQAIATVQA
15]        pos= 305 score=0.020227 unnormalised=5.4895600000        IATVQARPM
16]        pos= 392 score=0.008609 unnormalised=2.3365600000        LLQTNPPES
17]        pos= 393 score=0.032243 unnormalised=8.7505600000        LQTNPPESL
```

```
18]        pos= 442 score=0.020172 unnormalised=5.4745600000        LYPQLSAIL
19]        pos= 443 score=0.033355 unnormalised=9.0525600000        YPQLSAILI
20]        pos= 450 score=0.003753 unnormalised=1.0185600000        LIHQGVNLV
21]        pos= 451 score=0.001472 unnormalised=0.3995600000        IHQGVNLVL
22]        pos= 455 score=0.000945 unnormalised=0.2565600000        VNLVLTLCV
23]        pos= 466 score=0.059752 unnormalised=16.2165600000        YYQLSAIAL
24]        pos= 467 score=0.010621 unnormalised=2.8825600000        YQLSAIALG
25]        pos= 497 score=0.005835 unnormalised=1.5835600000        ITHSQTLTV
26]        pos= 513 score=0.033882 unnormalised=9.1955600000        YPQLSAIAL
27]        pos= 527 score=0.037290 unnormalised=10.1205600000        FGILRSSFI
28]        pos= 542 score=0.010894 unnormalised=2.9565600000        ILALKTLES
29]        pos= 545 score=0.020573 unnormalised=5.5835600000        LKTLESTES
30]        pos= 548 score=0.007427 unnormalised=2.0155600000        LESTESQKI
31]        pos= 560 score=0.021413 unnormalised=5.8115600000        FHLQKTEIT
32]        pos= 591 score=0.015673 unnormalised=4.2535600000        FLSFCSLFL
33]        pos= 594 score=0.012261 unnormalised=3.3275600000        FCSLFLIAL
34]        pos= 598 score=0.034534 unnormalised=9.3725600000        FLIALGVAT
35]        pos= 604 score=0.005308 unnormalised=1.4405600000        VATAHGSTL
36]        pos= 633 score=0.017714 unnormalised=4.8075600000        LYPQLSAIA
37]        pos= 634 score=0.033882 unnormalised=9.1955600000        YPQLSAIAL
38]        pos= 640 score=0.005544 unnormalised=1.5045600000        IALGVPQLS
39]        pos= 644 score=0.012268 unnormalised=3.3295600000        VPQLSAIAL
40]        pos= 654 score=0.005754 unnormalised=1.5615600000        VATAHGSQT
41]        pos=  -1 score=0.243804 unnormalised=66.1680000000        non-binding event

=========================================================================

Allele: DRB1_0101
Pseudo sequence: KAFAHVEQRKAQTRV
Threshold: 2.392440
Max score: 26.461000


----------------------------------
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/50712_20260523-104210_5_km0OQLjwdbkx.FSA_1_001
----------------------------------

MARGKKIGYSGLKSRQTKDKAAEAAAPAAPAPAPEVTPAAAPVVAPAPAPAEAKKSEESDDMGFGLFDVAKNVAAESAAE
AAAPAEEAAAAPAPAPVVKEAKKDLHSLLELGTKPTAPHVRNKKVILFDTNHQVSICNQIIDAINSGIDLGDLLEGGLLT
LCVEHYYNSDKDSIISNSVGQTRFSGLLIVKTVLEFILQKTDSGVTLHPLVRTSKVKNEVASFKQALSNLARHGEYAPFA
NLSGINNLEHGLYPQLSAIALGVATAHGSTLAGVNVGEQYQQLREAAHDAEVKLQRRHEHQEIQAIATVQARPMNRPTAL
PPPVDDKIEHESTEDSSSSSSFVDLNDPFALLNEDEDTLDDSVMIPGTTSREFQGPQRVVTKKGRTFLYPNDLLQTNPPE
SLITALVEEYQNPVSAKELQADWPDMSFDERRHVAMCPGPGGLYPQLSAILIHQGVNLVLTLCVEHYYQLSAIALGVQTL
AVLSQKRPMNRPTALTEITHSQTLTVQARPMNRYPQLSAIALAAYVIFGILRSSFILKFVPLILALKTLESTESQKILEQ
FHLQKTEITHTVLEFILQKTDSGVTRGRIGLFLSFCSLFLIALGVATAHGSTLAGATRFLDVIPNEPHYSEHGLYPQLSA
IALGVPQLSAIALGVATAHGSQTLAVLSQKREKLAHHHHHH

Epitopes of protein 0 ------------
0]        pos=   8 score=0.043680 unnormalised=11.8545600000        YSGLKSRQT
1]        pos=  35 score=0.011841 unnormalised=3.2135600000        VTPAAAPVV
2]        pos=  42 score=0.015382 unnormalised=4.1745600000        VVAPAPAPA
3]        pos=  66 score=0.011262 unnormalised=3.0565600000        FDVAKNVAA
4]        pos=  72 score=0.006122 unnormalised=1.6615600000        VAAESAAEA
5]        pos= 104 score=0.002419 unnormalised=0.6565600000        LHSLLELGT
6]        pos= 183 score=0.014317 unnormalised=3.8855600000        FSGLLIVKT
7]        pos= 222 score=0.055058 unnormalised=14.9425600000        FKQALSNLA
8]        pos= 235 score=0.009011 unnormalised=2.4455600000        YAPFANLSG
9]        pos= 238 score=0.021222 unnormalised=5.7595600000        FANLSGINN
10]        pos= 251 score=0.017714 unnormalised=4.8075600000        LYPQLSAIA
11]        pos= 252 score=0.033882 unnormalised=9.1955600000        YPQLSAIAL
12]        pos= 262 score=0.005308 unnormalised=1.4405600000        VATAHGSTL
13]        pos= 279 score=0.012423 unnormalised=3.3715600000        YQQLREAAH
14]        pos= 302 score=0.025153 unnormalised=6.8265600000        IQAIATVQA
15]        pos= 305 score=0.020227 unnormalised=5.4895600000        IATVQARPM
16]        pos= 392 score=0.008609 unnormalised=2.3365600000        LLQTNPPES
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17]        pos= 393 score=0.032243 unnormalised=8.7505600000        LQTNPPESL
18]        pos= 442 score=0.020172 unnormalised=5.4745600000        LYPQLSAIL
19]        pos= 443 score=0.033355 unnormalised=9.0525600000        YPQLSAILI
20]        pos= 450 score=0.003753 unnormalised=1.0185600000        LIHQGVNLV
21]        pos= 451 score=0.001472 unnormalised=0.3995600000        IHQGVNLVL
22]        pos= 455 score=0.000945 unnormalised=0.2565600000        VNLVLTLCV
23]        pos= 466 score=0.059752 unnormalised=16.2165600000        YYQLSAIAL
24]        pos= 467 score=0.010621 unnormalised=2.8825600000        YQLSAIALG
25]        pos= 497 score=0.005835 unnormalised=1.5835600000        ITHSQTLTV
26]        pos= 513 score=0.033882 unnormalised=9.1955600000        YPQLSAIAL
27]        pos= 527 score=0.037290 unnormalised=10.1205600000        FGILRSSFI
28]        pos= 542 score=0.010894 unnormalised=2.9565600000        ILALKTLES
29]        pos= 545 score=0.020573 unnormalised=5.5835600000        LKTLESTES
30]        pos= 548 score=0.007427 unnormalised=2.0155600000        LESTESQKI
31]        pos= 560 score=0.021413 unnormalised=5.8115600000        FHLQKTEIT
32]        pos= 591 score=0.015673 unnormalised=4.2535600000        FLSFCSLFL
33]        pos= 594 score=0.012261 unnormalised=3.3275600000        FCSLFLIAL
34]        pos= 598 score=0.034534 unnormalised=9.3725600000        FLIALGVAT
35]        pos= 604 score=0.005308 unnormalised=1.4405600000        VATAHGSTL
36]        pos= 633 score=0.017714 unnormalised=4.8075600000        LYPQLSAIA
37]        pos= 634 score=0.033882 unnormalised=9.1955600000        YPQLSAIAL
38]        pos= 640 score=0.005544 unnormalised=1.5045600000        IALGVPQLS
39]        pos= 644 score=0.012268 unnormalised=3.3295600000        VPQLSAIAL
40]        pos= 654 score=0.005754 unnormalised=1.5615600000        VATAHGSQT
41]        pos=  -1 score=0.243804 unnormalised=66.1680000000        non-binding event
```