

C-IMMSIM simulation results

May 22, 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
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](mailto:filippo.castiglione@iac.cnr.it))

Technical problems: Ilaria Gonnella ([ilaria dot gonnella at cnr dot it](mailto:ilaria.gonnella@iac.cnr.it))

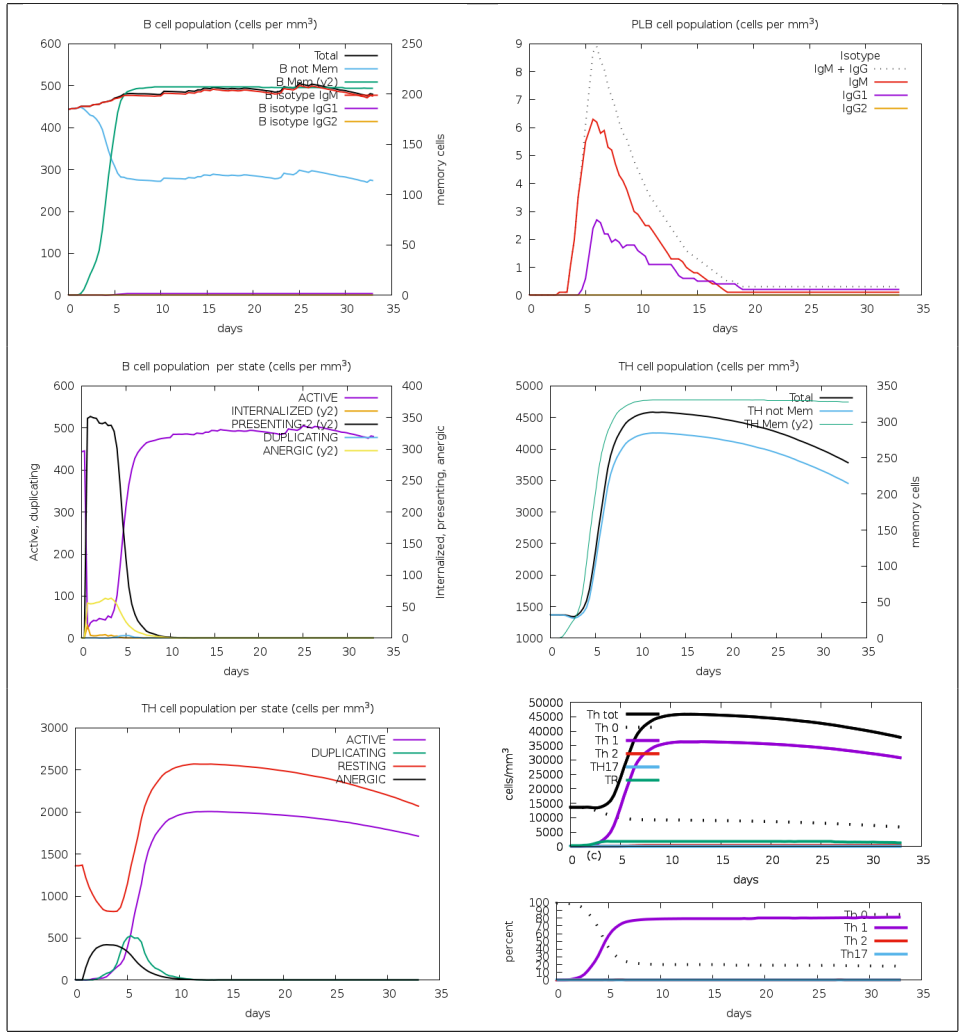


Figure 1: Cell counts shown. Legend: Act=active, Intern=internalized the Ag, Pres II = presenting on MHC II, Dup = in the mitotic cycle, Anergic = anergic, Resting = not active.

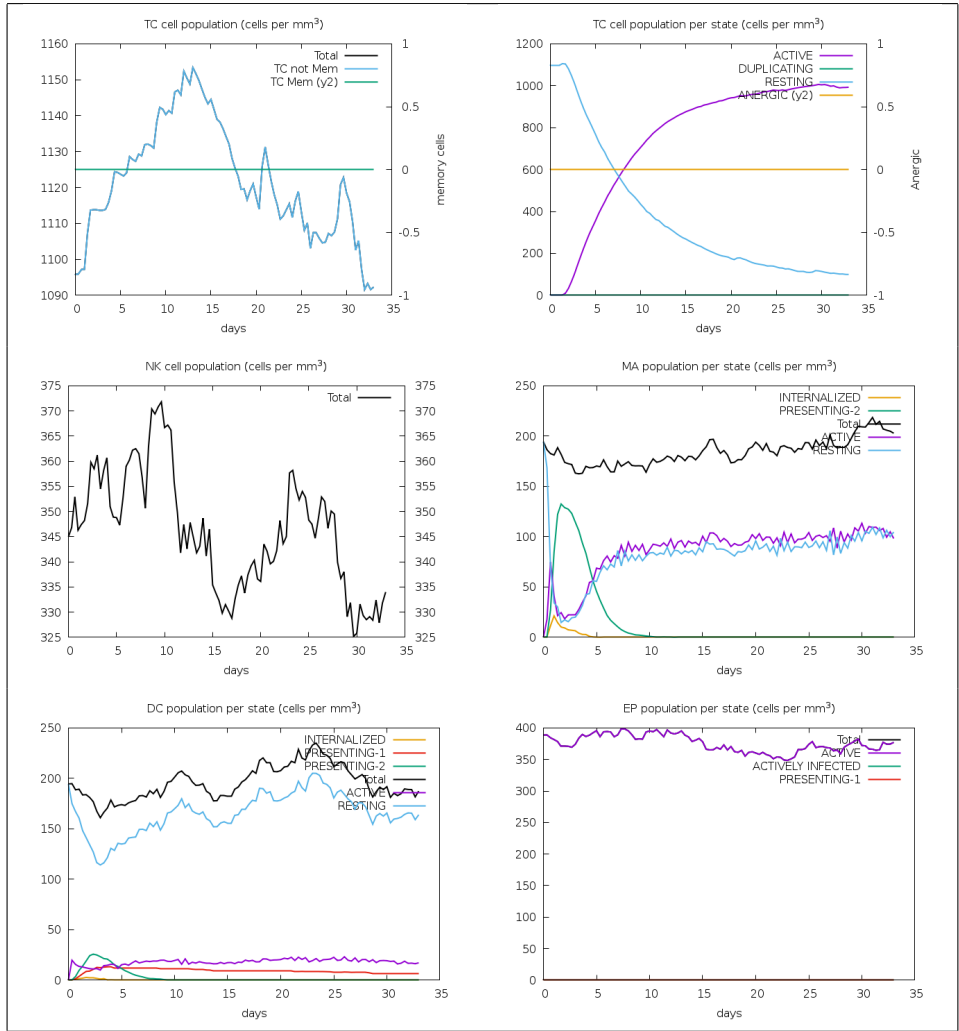


Figure 2: Legend: symbols as figure above.

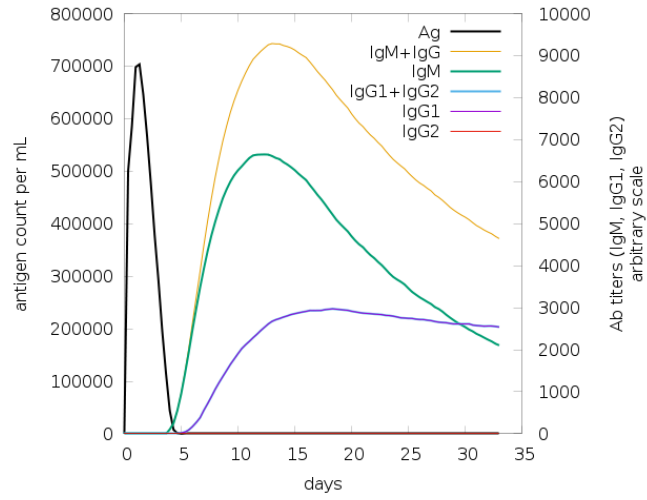


Figure 3: The virus, the immunoglobulins and the immunocomplexes.

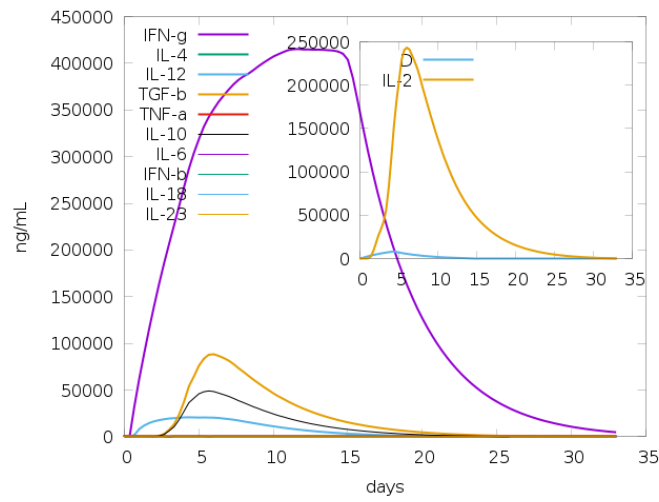


Figure 4: Concentration of cytokines and interleukins. Inset plot shows danger signal together with leukocyte growth factor IL-2.

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

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/50712_20260522-092940_5_XkLfjnfTr3nx.FSA_1_001

MARGKKIGYSGLSRQTKDKAAEAAAAPAPAPAEVTPAAAPVVAPAPAPAEAKKSEESDDMGFLFDVAKNVAESAAE
AAAPAEAAAAPAPAPVVKEAKKEAAKMDSRPQKIWMAPSLTESMDYHKILTAGLSVQQGIVRQVIVPYQVNNLEEI
CQLIIQAFEAGVDFQEFLLIHQGMHVMAGHDANDAVISNSVAQARFSGLLIVKTVLDHILKQTERGVRLHPLARTAKVKN
EVNSFLSSLAKHGEYAPFARLLNLSGVNLEHGLFPQLSAIALGVATAHGSTLAGVNVGEQYQQLREAAATLQQYAESRE
LDHLGLDDQEKKILMNFHQKNEISFQQTAMVTLRKRERLAKLTEAITAASLPKTSGHDDDDIPFPGPINDDDNPGHQD
DDPTDSQDTTIPDVVVDVDDGSYGEYQSYSENGMNPDDLVLFDLDEEDTKPVPNRSTKGGQKNSQKQGHIEGRQTQSR
PIQNVPGPHRTIHHASAPLTDNDRRNEPSGSTSPRLTPIINEEADPLDDADDETSLLPPLSDDEEQDRDGTNRTPTVAP
PAPVYRDHSEKKELPQDEQQDQDHEKEAMNEENRFVTLDGQFYWPVMNHKNKFMAILQHHCPPGQLSAIALGVYQVNVN
NLEEIRLEELLPAVFPQLSAIALFLSFASLFLQTNAMVTLRAAYISFQQTAMVTLRKEVQGGIVRQVIVPYQFARLLN
LSGVNLEHLSAIALGVATAHGSTRLEELLPAVSSGKNIDANDAVISNSVAQARHHHHHH

Epitopes of protein 0 -----
0] pos= 306 score=0.000960 unnormalised=0.1086000000 EAATQLQQY
1] pos= 402 score=0.003946 unnormalised=0.4466000000 PTDSQDTTI
2] pos= 414 score=0.010759 unnormalised=1.2176000000 VVDPDDGSY
3] pos= 420 score=0.005298 unnormalised=0.5996000000 GSYGEYQSY
4] pos= 596 score=0.027229 unnormalised=3.0816000000 VTLDGQQFY
5] pos= 597 score=0.018145 unnormalised=2.0536000000 TLDGQQFYW
6] pos= 628 score=0.007295 unnormalised=0.8256000000 LSAIALGVY
7] pos= -1 score=0.926368 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_20260522-092940_5_XkLfjnfTr3nx.FSA_1_001

MARGKKIGYSGLSRQTKDKAAEAAAAPAPAPAEVTPAAAPVVAPAPAPAEAKKSEESDDMGFLFDVAKNVAESAAE
AAAPAEAAAAPAPAPVVKEAKKEAAKMDSRPQKIWMAPSLTESMDYHKILTAGLSVQQGIVRQVIVPYQVNNLEEI
CQLIIQAFEAGVDFQEFLLIHQGMHVMAGHDANDAVISNSVAQARFSGLLIVKTVLDHILKQTERGVRLHPLARTAKVKN
EVNSFLSSLAKHGEYAPFARLLNLSGVNLEHGLFPQLSAIALGVATAHGSTLAGVNVGEQYQQLREAAATLQQYAESRE
LDHLGLDDQEKKILMNFHQKNEISFQQTAMVTLRKRERLAKLTEAITAASLPKTSGHDDDDIPFPGPINDDDNPGHQD
DDPTDSQDTTIPDVVVDVDDGSYGEYQSYSENGMNPDDLVLFDLDEEDTKPVPNRSTKGGQKNSQKQGHIEGRQTQSR
PIQNVPGPHRTIHHASAPLTDNDRRNEPSGSTSPRLTPIINEEADPLDDADDETSLLPPLSDDEEQDRDGTNRTPTVAP
PAPVYRDHSEKKELPQDEQQDQDHEKEAMNEENRFVTLDGQFYWPVMNHKNKFMAILQHHCPPGQLSAIALGVYQVNVN
NLEEIRLEELLPAVFPQLSAIALFLSFASLFLQTNAMVTLRAAYISFQQTAMVTLRKEVQGGIVRQVIVPYQFARLLN
LSGVNLEHLSAIALGVATAHGSTRLEELLPAVSSGKNIDANDAVISNSVAQARHHHHHH

Epitopes of protein 0 -----
0] pos= 306 score=0.000960 unnormalised=0.1086000000 EAATQLQQY
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3] pos= 420 score=0.005298 unnormalised=0.5996000000 GSYGEYQSY
4] pos= 596 score=0.027229 unnormalised=3.0816000000 VTLDGQQFY
5] pos= 597 score=0.018145 unnormalised=2.0536000000 TLDGQQFYW
6] pos= 628 score=0.007295 unnormalised=0.8256000000 LSAIALGVY
7] pos= -1 score=0.926368 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_20260522-092940_5_XkLfjnfTr3nx.FSA_1_001

MARGKKIGYSGLSRQTKDKAAEAAAAPAPAPEVTPAAAPVVAPAPAPAEAKKSEESDDMGFLFDVAKNVAESAEE
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NLEEIRLEELLPAVFPQLSAIALFLSFASLFLQTNAMVTLRAAYISFQQTAMVTLRKEVQQGIVRQVIVPYQFARLLN
LSGVNNLEHLSAIALGVATAHGSTRLEELLPAVSSGKNIDANDAVISNSVAQARHHHHHH

Epitopes of protein 0 -----

0]	pos=	25	score=0.018842	unnormalised=3.0192000000	APAAPAPAP
1]	pos=	28	score=0.014018	unnormalised=2.2462000000	APAPAPEVT
2]	pos=	30	score=0.026169	unnormalised=4.1932000000	APAPEVTPA
3]	pos=	32	score=0.014717	unnormalised=2.3582000000	APEVTPAAA
4]	pos=	36	score=0.019129	unnormalised=3.0652000000	TPAAAPVVA
5]	pos=	40	score=0.029114	unnormalised=4.6652000000	APVVAPAPA
6]	pos=	44	score=0.035873	unnormalised=5.7482000000	APAPAPAEA
7]	pos=	82	score=0.025826	unnormalised=4.1382000000	APAEAAAA
8]	pos=	88	score=0.008495	unnormalised=1.3612000000	AAAPAPAPV
9]	pos=	92	score=0.008788	unnormalised=1.4082000000	APAPVVKEA
10]	pos=	118	score=0.009637	unnormalised=1.5442000000	APSLTESDM
11]	pos=	148	score=0.003615	unnormalised=0.5792000000	IPVYQVNNL
12]	pos=	229	score=0.020702	unnormalised=3.3172000000	HPLARTAKV
13]	pos=	255	score=0.026231	unnormalised=4.2032000000	APFARLLNL
14]	pos=	274	score=0.035823	unnormalised=5.7402000000	FPQLSAIAL
15]	pos=	654	score=0.035823	unnormalised=5.7402000000	FPQLSAIAL
16]	pos=	709	score=0.012907	unnormalised=2.0682000000	IPVYQFARL
17]	pos=	-1	score=0.654290	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_20260522-092940_5_XkLfjnfTr3nx.FSA_1_001

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NLEEIRLEELLPAVFPQLSAIALFLSFASLFLQTNAMVTLRAAYISFQQTAMVTLRKEVQQGIVRQVIVPYQFARLLN
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```

Epitopes of protein 0 -----
0] pos= 25 score=0.018842 unnormalised=3.0192000000 APAAPAPAP
1] pos= 28 score=0.014018 unnormalised=2.2462000000 APAPAPEVT
2] pos= 30 score=0.026169 unnormalised=4.1932000000 APAPEVTPA
3] pos= 32 score=0.014717 unnormalised=2.3582000000 APEVTPAAA
4] pos= 36 score=0.019129 unnormalised=3.0652000000 TPAAAPVVA
5] pos= 40 score=0.029114 unnormalised=4.6652000000 APVVAPAPA
6] pos= 44 score=0.035873 unnormalised=5.7482000000 APAPAPAEA
7] pos= 82 score=0.025826 unnormalised=4.1382000000 APAEAAAAA
8] pos= 88 score=0.008495 unnormalised=1.3612000000 AAAPAPAPV
9] pos= 92 score=0.008788 unnormalised=1.4082000000 APAPVVKEA
10] pos= 118 score=0.009637 unnormalised=1.5442000000 APSLTESDM
11] pos= 148 score=0.003615 unnormalised=0.5792000000 IPVYQVNNL
12] pos= 229 score=0.020702 unnormalised=3.3172000000 HPLARTAKV
13] pos= 255 score=0.026231 unnormalised=4.2032000000 APFARLLNL
14] pos= 274 score=0.035823 unnormalised=5.7402000000 FPQLSAIAL
15] pos= 654 score=0.035823 unnormalised=5.7402000000 FPQLSAIAL
16] pos= 709 score=0.012907 unnormalised=2.0682000000 IPVYQFARL
17] pos= -1 score=0.654290 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_20260522-092940_5_XkLfjnfTr3nx.FSA_1_001

```

MARGKKIGYSGLSRQTKDKAAEAAAAPAPAPAPEVTPAAAPVVAPAPAPAEAKKSEESDDMGFGLFDVAKNVAESAEE
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LDHLGLDDQEKKILMNFHQKNEISFQQTNAMVTLRKRERLAKLTEAITAASLPKTSGHDDDDIPFPGPINDDDNPGHQD
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```

```

Epitopes of protein 0 -----
0] pos= 8 score=0.042755 unnormalised=11.8545600000 YSGLKSRQT
1] pos= 35 score=0.011590 unnormalised=3.2135600000 VTPAAAPVV
2] pos= 42 score=0.015056 unnormalised=4.1745600000 VVAPAPAPA
3] pos= 66 score=0.011024 unnormalised=3.0565600000 FDVAKNVAA
4] pos= 72 score=0.005993 unnormalised=1.6615600000 VAAESAEEA
5] pos= 114 score=0.001077 unnormalised=0.2985600000 KIWMAPSLT
6] pos= 128 score=0.025454 unnormalised=7.0575600000 YHKILTAGL
7] pos= 142 score=0.003771 unnormalised=1.0455600000 IVRQVPIPV
8] pos= 178 score=0.007385 unnormalised=2.0475600000 LIHQGMHVM
9] pos= 183 score=0.021249 unnormalised=5.8915600000 MHMVAGHDA

```

10]	pos= 205	score=0.014014	unnormalised=3.8855600000	FSGLLIVKT
11]	pos= 237	score=0.002271	unnormalised=0.6295600000	VKNEVNSFL
12]	pos= 241	score=0.015972	unnormalised=4.4285600000	VNSFLSSLA
13]	pos= 244	score=0.013783	unnormalised=3.8215600000	FLSSLAKHG
14]	pos= 257	score=0.038532	unnormalised=10.6835600000	FARLLNLSG
15]	pos= 260	score=0.011623	unnormalised=3.2225600000	LLNLSGVNN
16]	pos= 273	score=0.013191	unnormalised=3.6575600000	LFPQLSAIA
17]	pos= 274	score=0.034424	unnormalised=9.5445600000	FPQLSAIAL
18]	pos= 284	score=0.005196	unnormalised=1.4405600000	VATAHGSTL
19]	pos= 301	score=0.038229	unnormalised=10.5995600000	YQQLREAAAT
20]	pos= 336	score=0.013332	unnormalised=3.6965600000	FHQKKNEIS
21]	pos= 343	score=0.006743	unnormalised=1.8695600000	ISFQQTNAM
22]	pos= 345	score=0.033273	unnormalised=9.2255600000	FQQTAMVT
23]	pos= 351	score=0.002296	unnormalised=0.6365600000	MVTLRKERL
24]	pos= 481	score=0.007226	unnormalised=2.0035600000	IQNVPGPHR
25]	pos= 491	score=0.038330	unnormalised=10.6275600000	IHHASAPLT
26]	pos= 595	score=0.013938	unnormalised=3.8645600000	FVTLDGQQF
27]	pos= 653	score=0.006209	unnormalised=1.7215600000	VFPQLSAIA
28]	pos= 654	score=0.034424	unnormalised=9.5445600000	FPQLSAIAL
29]	pos= 657	score=0.005571	unnormalised=1.5445600000	LSAIALFLS
30]	pos= 660	score=0.004698	unnormalised=1.3025600000	IALFLSFAS
31]	pos= 663	score=0.030784	unnormalised=8.5355600000	FLSFASLFL
32]	pos= 669	score=0.017263	unnormalised=4.7865600000	LFLQTNAMV
33]	pos= 670	score=0.028671	unnormalised=7.9495600000	FLQTNAMVT
34]	pos= 671	score=0.002794	unnormalised=0.7745600000	LQTNAMVTL
35]	pos= 676	score=0.035682	unnormalised=9.8935600000	MVTLRAAYI
36]	pos= 684	score=0.006743	unnormalised=1.8695600000	ISFQQTNAM
37]	pos= 686	score=0.033273	unnormalised=9.2255600000	FQQTAMVT
38]	pos= 703	score=0.003771	unnormalised=1.0455600000	IVRQRVIPV
39]	pos= 712	score=0.003699	unnormalised=1.0255600000	YQFARLLNL
40]	pos= 714	score=0.038532	unnormalised=10.6835600000	FARLLNLSG
41]	pos= 717	score=0.011623	unnormalised=3.2225600000	LLNLSGVNN
42]	pos= 723	score=0.003800	unnormalised=1.0535600000	VNNLEHLSA
43]	pos= 726	score=0.037799	unnormalised=10.4805600000	LEHLSAIAL
44]	pos= 745	score=0.008301	unnormalised=2.3015600000	LEELLPAVS
45]	pos= -1	score=0.238643	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_20260522-092940_5_XkLfjnfTr3nx.FSA_1_001

MARGKKIGYSGLSRQTKDKAAEAAAPAAPAPEVTPAAAPVVAPAPAPAEAKKSEESDDMGFLFDVAKNVAESAEE
AAAPAEAAAAPAPAPVVKEAKKEAAKMDSRPQKIWMAPSLTESDMYHKILTAGLSVQQGIVRQRVIPVYQVNNLEEI
CQLIIQAFEAGVDFQEFLLIHQGMHMVAGHDANDAVISNSVAQARFSGLLIVKTVLDHILKQTERGVRHLPLARTAKVKN
EVNSFLSSLAKHGEYAPFARLLNLSGVNNLEHGLFQPQLSAIALGVATAHGSTLAGVNVGEQYQQLREAAATLQQAESRE
LDHLGLDDQEKILMNFHQKKNEISFQQTAMVTLRKERLAKL TEA ITAASLPKTS GHDDDDIPFP GPINDDDNPGHQD
DDPDTSDQTTIPDVVVDPDDGSYGEYQSYSENGMNPDDLVLFDLDDDETKPVPNRSTKGGQKNSQKQGHIEGRQTQSR
PIQNVPGPHRTIHHASAPLTDNDRRNEPSPGTSPLTPINEEADPLDADDETSPLPLESDDEEQDRDGTNRTPTVAP
PAPVYRDHSEKKELPQDEQDQDHEKEAMNEENRFVTLDGQQFYWPVMNHKNKFMAILQHHCPCPGQLSAIALGVYQVN
NLEEIRLEELLPAVFPQLSAIALFLSFASLFLQTNAMVTLRAAYISFQQTAMVTLRKEVQGGIVRQRVIPVYQFARLLN
LSGVNNLEHLSAIALGVATAHGSTRLEELLPAVSSGKNIDANDAVISNSVAQARHHHHHH

Epitopes of protein 0 -----
0] pos= 8 score=0.042755 unnormalised=11.8545600000 YSGLKSRQT
1] pos= 35 score=0.011590 unnormalised=3.2135600000 VTPAAAPVV
2] pos= 42 score=0.015056 unnormalised=4.1745600000 VVAPAPAPA
3] pos= 66 score=0.011024 unnormalised=3.0565600000 FDVAKNVAA

4]	pos= 72	score=0.005993	unnormalised=1.6615600000	VAAESAAEA
5]	pos= 114	score=0.001077	unnormalised=0.2985600000	KIWMAPSLT
6]	pos= 128	score=0.025454	unnormalised=7.0575600000	YHKLLTAGL
7]	pos= 142	score=0.003771	unnormalised=1.0455600000	IVRQRVIPV
8]	pos= 178	score=0.007385	unnormalised=2.0475600000	LIHQGMHMV
9]	pos= 183	score=0.021249	unnormalised=5.8915600000	MHMVAGHDA
10]	pos= 205	score=0.014014	unnormalised=3.8855600000	FSGLLIVKT
11]	pos= 237	score=0.002271	unnormalised=0.6295600000	VKNEVNSFL
12]	pos= 241	score=0.015972	unnormalised=4.4285600000	VNSFLSSLA
13]	pos= 244	score=0.013783	unnormalised=3.8215600000	FLSSLAKHG
14]	pos= 257	score=0.038532	unnormalised=10.6835600000	FARLLNLSG
15]	pos= 260	score=0.011623	unnormalised=3.2225600000	LLNLSGVNN
16]	pos= 273	score=0.013191	unnormalised=3.6575600000	LFPQLSAIA
17]	pos= 274	score=0.034424	unnormalised=9.5445600000	FPQLSAIAL
18]	pos= 284	score=0.005196	unnormalised=1.4405600000	VATAHGSTL
19]	pos= 301	score=0.038229	unnormalised=10.5995600000	YQQLREAAAT
20]	pos= 336	score=0.013332	unnormalised=3.6965600000	FHQKKEIS
21]	pos= 343	score=0.006743	unnormalised=1.8695600000	ISFQQTNAM
22]	pos= 345	score=0.033273	unnormalised=9.2255600000	FQQTAMVT
23]	pos= 351	score=0.002296	unnormalised=0.6365600000	MVTLRKERL
24]	pos= 481	score=0.007226	unnormalised=2.0035600000	IQNVPGPHR
25]	pos= 491	score=0.038330	unnormalised=10.6275600000	IHHASAPLT
26]	pos= 595	score=0.013938	unnormalised=3.8645600000	FVTLDGQQF
27]	pos= 653	score=0.006209	unnormalised=1.7215600000	VFPQLSAIA
28]	pos= 654	score=0.034424	unnormalised=9.5445600000	FPQLSAIAL
29]	pos= 657	score=0.005571	unnormalised=1.5445600000	LSAIALFLS
30]	pos= 660	score=0.004698	unnormalised=1.3025600000	IALFLSFAS
31]	pos= 663	score=0.030784	unnormalised=8.5355600000	FLSFASLFL
32]	pos= 669	score=0.017263	unnormalised=4.7865600000	LFLQTNAMV
33]	pos= 670	score=0.028671	unnormalised=7.9495600000	FLQTNAMVT
34]	pos= 671	score=0.002794	unnormalised=0.7745600000	LQTNAMVTL
35]	pos= 676	score=0.035682	unnormalised=9.8935600000	MVTLRAAYI
36]	pos= 684	score=0.006743	unnormalised=1.8695600000	ISFQQTNAM
37]	pos= 686	score=0.033273	unnormalised=9.2255600000	FQQTAMVT
38]	pos= 703	score=0.003771	unnormalised=1.0455600000	IVRQRVIPV
39]	pos= 712	score=0.003699	unnormalised=1.0255600000	YQFARLLNL
40]	pos= 714	score=0.038532	unnormalised=10.6835600000	FARLLNLSG
41]	pos= 717	score=0.011623	unnormalised=3.2225600000	LLNLSGVNN
42]	pos= 723	score=0.003800	unnormalised=1.0535600000	VNNLEHLSA
43]	pos= 726	score=0.037799	unnormalised=10.4805600000	LEHLSAIAL
44]	pos= 745	score=0.008301	unnormalised=2.3015600000	LEELLPAVS
45]	pos= -1	score=0.238643	unnormalised=66.1680000000	non-binding event