

C-IMMSIM simulation results

February 7, 2023

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://kraken.iac.rm.cnr.it/C-IMMSIM>

CITATIONS: For publication of results, please cite:

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.

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

GETTING HELP: Scientific problems: Filippo Castiglione (f dot castiglione at iac dot cnr dot it) Technical problems: Ilaria Gonnella (ilaria dot gonnella at cnr dot it)

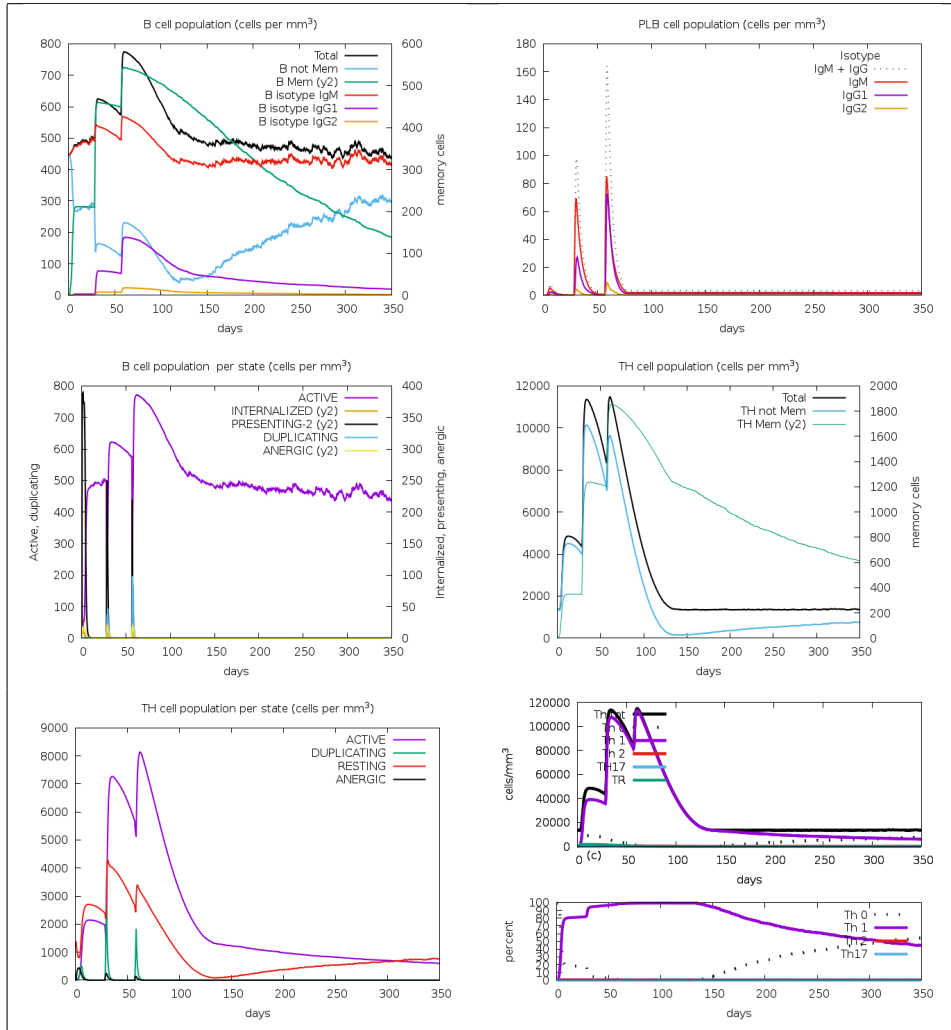


Figure 1: Cell counts shown. Legend: Act=active, Intern=internalized the Ag, Pres II = presenting on MHC II, Dup = in the mitotic cycle, Anergic = anergic, Resting = not active.

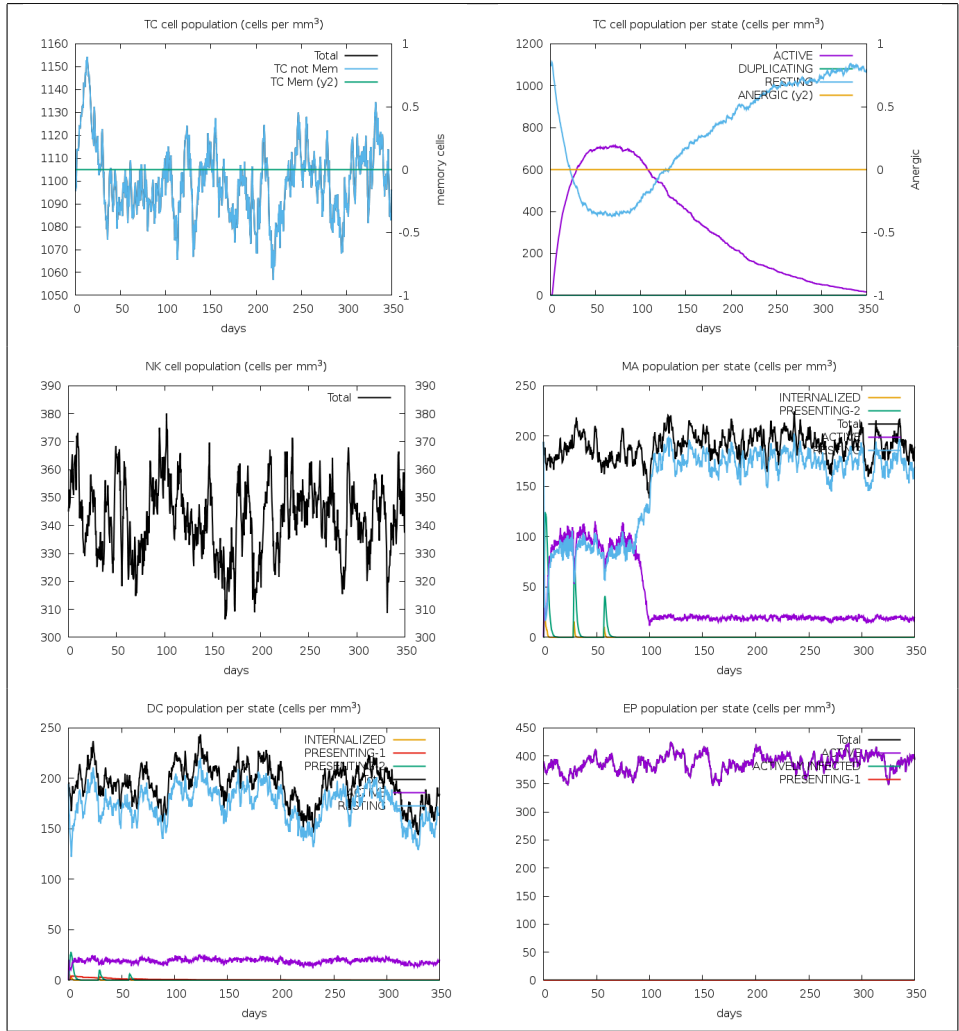


Figure 2: Legend: symbols as figure above.

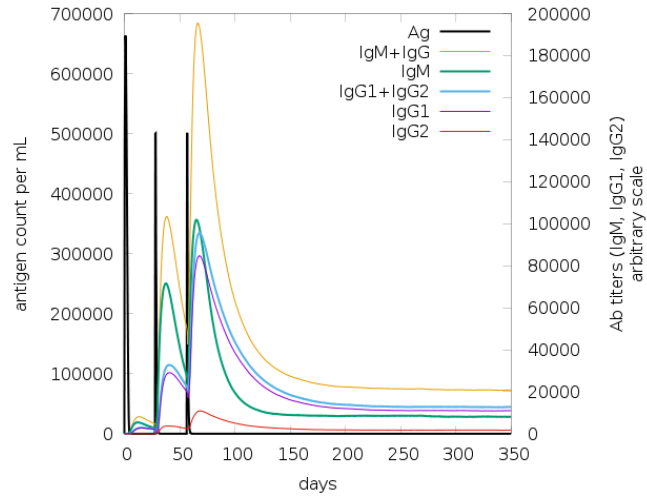


Figure 3: The virus, the immunoglobulins and the immunocomplexes.

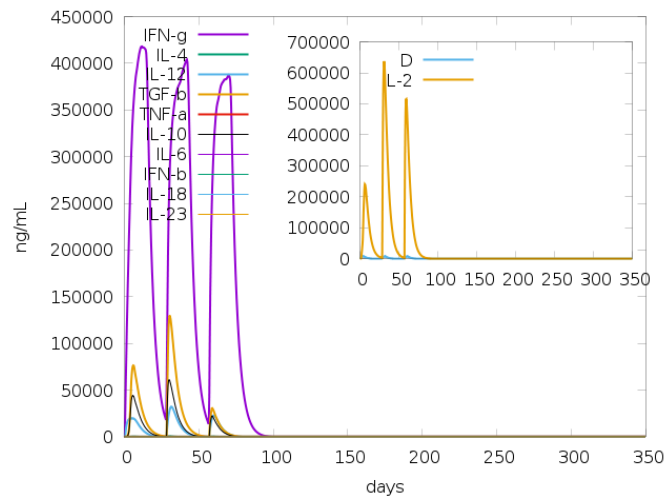


Figure 4: Concentration of cytokines and interleukins. Inset plot shows danger signal together with leukocyte growth factor IL-2.

RAGPGGAQGGYGAMALAAAFHGGPGMSDPAYNINISLPSYYPDGGPGGALSAGVAVAMSLTVGAGPGPGRRRSLRWSW
LLSVLAAGPGGAEELTAAQVRVAAAAAYETAGPGPGYGYAAASAVAARLNPLGPGGTVGGAAPGGGAAAAVAHGPGPGV
APSVMPAAAAGSSATGPGPGTGAVLGGGGIAMAAGPGGLLLVLAFAGGYAVAACAAAYGS AVVGLSMAAYNAAGGHNAVA
AYTAAQAAVVRAAYAMSGDIVGAAAYRTADGINYRAAYAAIGGGVAVAAAYATATATATLAAYFLNLDVPLFVAAYQAETA
VNTLAAAYAVNGEPAPLAAYGLSNATPREVAAYQVTRNRIKKAAYNLPPPLAPDFKAKFLEGFVRTSNIKFQDAYNKKAP
DDPICTGGGNIMAHVS YVKKAGLSASSGLAHADSLASSASKKIGQAAEAMGNSRMFYNQYRSKKALGQTVQASDSLGTGAE
ETLNKKVNTLFEKLEPMASILDGASKKAVGERVLATQGRGAWPVCGRKKAYHAMSSTHEANTMAMMARDEAAAKAPPHA
LSHHHHHH

Epitopes of protein 0 -----

0] pos= 453 score=0.000978 unnormalised=0.102600000 TATATLAAY
1] pos= -1 score=0.999022 unnormalised=104.841000000 non-binding event

Allele: A0201

Pseudo sequence: KAAHVEQRKAQTRTV

Threshold: 9.523800

Max score: 27.437000

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/9107_20230207-091852_5_5fvJbmMTm4C6.FSA_1_001

IALTALPVAAMADVTLTYGTIKAGVETSRVAVHNGAQAASVETGTGIVDLGSKIGFKGQEDLGNGLKAIWQVEQEA
AGLFQRHGEGTKATVGEVPGPGPTGS AVVGLSMAASSALTLGPGGAAIGLSMAGSSAMILAAGPGPGTNI
RAGPGGAQGGYGAMALAAAFHGGPGMSDPAYNINISLPSYYPDGGPGGALSAGVAVAMSLTVGAGPGPGR
RRSLRWSW LLSVLAAGPGGAEELTAAQVRVAAAAAYETAGPGPGYGYAAASAVAARLNPLGPGGTVGGA
APGGGAAAAVAHGPGPGV APSVMPAAAAGSSATGPGPGTGAVLGGGGIAMAAGPGGLLLVLAFAGGYAV
AACAAAYGS AVVGLSMAAYNAAGGHNAVA
AYTAAQAAVVRAAYAMSGDIVGAAAYRTADGINYRAAYAAIGGGVAVAAAYATATATATLAAYFLNLDV
PLFVAAYQAETA VNTLAAAYAVNGEPAPLAAYGLSNATPREVAAYQVTRNRIKKAAYNLPPPLAPDFK
AKFLEGFVRTSNIKFQDAYNKKAP
DDPICTGGGNIMAHVS YVKKAGLSASSGLAHADSLASSASKKIGQAAEAMGNSRMFYNQYRSKKALGQ
TVQASDSLGTGAE ETLNKKVNTLFEKLEPMASILDGASKKAVGERVLATQGRGAWPVCGRKKAYHAMS
STHEANTMAMMARDEAAAKAPPHA
LSHHHHHH

Epitopes of protein 0 -----

0] pos= 132 score=0.006134 unnormalised=0.686200000 SMAGSSAMI
1] pos= 185 score=0.005848 unnormalised=0.654200000 GMSDPAYNI
2] pos= 209 score=0.008833 unnormalised=0.988200000 ALSAGVGAV
3] pos= 457 score=0.019507 unnormalised=2.182200000 TLAAAYFLNL
4] pos= 569 score=0.019605 unnormalised=2.193200000 NIMAHVS YV
5] pos= 648 score=0.002907 unnormalised=0.325200000 TLFEKLEPM
6] pos= -1 score=0.937166 unnormalised=104.841000000 non-binding event

Allele: B0702

Pseudo sequence: KAAREEQIKAQTRE

Threshold: 8.702800

Max score: 28.406000

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/9107_20230207-091852_5_5fvJbmMTm4C6.FSA_1_001

IALTALPVAAMADVTLTYGTIKAGVETSRVAVHNGAQAASVETGTGIVDLGSKIGFKGQEDLGNGLKAIWQVEQEA
AGLFQRHGEGTKATVGEVPGPGPTGS AVVGLSMAASSALTLGPGGAAIGLSMAGSSAMILAAGPGPGTNI
RAGPGGAQGGYGAMALAAAFHGGPGMSDPAYNINISLPSYYPDGGPGGALSAGVAVAMSLTVGAGPGPGR
RRSLRWSW LLSVLAAGPGGAEELTAAQVRVAAAAAYETAGPGPGYGYAAASAVAARLNPLGPGGTVGGA
APGGGAAAAVAHGPGPGV APSVMPAAAAGSSATGPGPGTGAVLGGGGIAMAAGPGGLLLVLAFAGGYAV
AACAAAYGS AVVGLSMAAYNAAGGHNAVA
AYTAAQAAVVRAAYAMSGDIVGAAAYRTADGINYRAAYAAIGGGVAVAAAYATATATATLAAYFLNLDV
PLFVAAYQAETA VNTLAAAYAVNGEPAPLAAYGLSNATPREVAAYQVTRNRIKKAAYNLPPPLAPDFK
AKFLEGFVRTSNIKFQDAYNKKAP
DDPICTGGGNIMAHVS YVKKAGLSASSGLAHADSLASSASKKIGQAAEAMGNSRMFYNQYRSKKALGQ
TVQASDSLGTGAE ETLNKKVNTLFEKLEPMASILDGASKKAVGERVLATQGRGAWPVCGRKKAYHAMS
STHEANTMAMMARDEAAAKAPPHA
LSHHHHHH

ETLNKKVNTLFEKLEPMASILDPGASKKAVGERVLATQGRGAWPVCGRKKAYHAMSSTHEANTMAMMARDEAAAKAPPHA
LSHHHHHH

Epitopes of protein 0 -----

0]	pos= 7	score=0.004079	unnormalised=0.5162000000	LPVAAMADV
1]	pos= 99	score=0.012274	unnormalised=1.5532000000	GPGPGTGSA
2]	pos= 101	score=0.001977	unnormalised=0.2502000000	GPGTGSAVV
3]	pos= 113	score=0.010915	unnormalised=1.3812000000	MAASSALTL
4]	pos= 204	score=0.005549	unnormalised=0.7022000000	GPGPGALSA
5]	pos= 282	score=0.002040	unnormalised=0.2582000000	AVAARLNPL
6]	pos= 302	score=0.026720	unnormalised=3.3812000000	APGGGAAAA
7]	pos= 316	score=0.006252	unnormalised=0.7912000000	GPGVAPSVM
8]	pos= 320	score=0.031019	unnormalised=3.9252000000	APSVMPAAA
9]	pos= 324	score=0.031264	unnormalised=3.9562000000	MPAAAAGSS
10]	pos= 335	score=0.027984	unnormalised=3.5412000000	GPGPGTGAV
11]	pos= 525	score=0.000081	unnormalised=0.0102000000	LPPPLAPDF
12]	pos= 712	score=0.011334	unnormalised=1.4342000000	AAKAPPHAL
13]	pos= -1	score=0.828510	unnormalised=104.8410000000	non-binding event

=====

Allele: B0801
Pseudo sequence: KAAREEQIKAQTRE
Threshold: 8.405400
Max score: 30.890000

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/9107_20230207-091852_5_5fvJbmMTm4C6.FSA_1_001

IALTALPVAAMADVTLTYGTIKAGVETSRVSAHNGAQAASVETGTGIVDLGSKIGFKGQEDLGNLKAIWQVEQEAAAK
AGLFQRHGEGETKATVGEVPGPGTGSVAVGLSMAASSALTLGPGGAAIGLSMAGSSAMILAAGPGPTNIRQAGVQYS
RAGPGPGAQGGYGAMALAAAFHGPMSDPAYNINISLPSYYPDGPAGALSAGVAVAMSLTVGAGPGPGRRLRWSW
LLSVLAAGPGGAELTAAQVRVAAAAAYETAGPGPGYGYAAASAVAARLNPLGPGTGVGAAPGGGAAAAVAHGPGPGV
APSVMPAAAAGSSATGPGPGTGAVLGGGGIAMAAGPGPGLLLVLAFAAGGYAVAACAAYGSVAVGLSMAAYNAAGGHNAVA
AYTAAQAQAVVRAAYAMSGDIVGAAAYRTADGINYRAAYAAIGGGVAVAAATATATATLAAYFLNLDVPLFVAAYQAETA
VNTLAAAYAVNGEPAPLAAYGLSNATPREVAAYQVTRNRIKKAAYNLPPPLAPDFKAKFLEGFVRTSNIKFKQDAYNKKAP
DDP ICTGGG NIMAHVSYVKKAGLSASSGLAHADSLASSASKKIGQAAEAMGNSRMFYNQYRSKKALGQTVQASDSL TGAE
ETLNKKVNTLFEKLEPMASILDPGASKKAVGERVLATQGRGAWPVCGRKKAYHAMSSTHEANTMAMMARDEAAAKAPPHA
LSHHHHHH

Epitopes of protein 0 -----

0]	pos= 282	score=0.003797	unnormalised=0.4096000000	AVAARLNPL
1]	pos= 641	score=0.020703	unnormalised=2.2336000000	TLNKKVNTL
2]	pos= 712	score=0.003732	unnormalised=0.4026000000	AAKAPPHAL
3]	pos= -1	score=0.971769	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: KFAHVEQRKAQTRV
Threshold: 2.392440
Max score: 26.461000

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/9107_20230207-091852_5_5fvJbmMTm4C6.FSA_1_001

IALTLAALPVAAMADVTLTYGTIKAGVETSRVAVHNGAQAASVETGTGIVDLGSKIGFKGQEDLGNGLKAIWQVEQEAAAK
AGLFQRHGEKTKATVGEVPGPGPTGSVAVGLSMAASSALTLGPGGAAIGLSMAGSSAMILAAGPGPGTNRQAGVQYS
RAGPGPGAQGGYGAMALAAFHGPGPGMSDPAYNINISLPSYYPDGPGLSAGVAVAMSLTVGAGPGPGRRRSLRWSW
LLSVLAAGPGPGAELTAAQVRVAAAAYETAGPGPGYGYAAASAVAARLNPLGPGGTVGGAAPGGGAAAAVAHGPVGPV
APSVMPAAAAGSSATGPGGTGAVLGGGGIAMAAGPGPGLLLVLAFAAGGYAVAACAAVGSVAVGLSMAAYNAAGGHNAVA
AYTAAQAAVVRAAYAMSGDIVGAAAYRTADGINYRAAYAAIGGGVAVAAATATATATLAAYFLNLDVPLFVAAYQAETA
VNTLAAAYAVNGEPAPLAAAYGLSNATPREVAAYQVTRNRIKKAAYNLPPPLAPDFKAKFLEGFVRTSNIKFDAYNKKAP
DDPICTGGGNIMAHVSVYKKAGLSASSGLAHADSLASSAKKIGQAAEAMGNSRMFYNQYRSKKALGQTVQASDSLGTAE
ETLNKKVNTLFEKLEPMASILDPGASKKAVGERVLATQGRGAWPVCGRKKAYHAMSSTHEANTMAMMARDEAAAKAPPHA
LSHHHHHH

Epitopes of protein 0 -----

0]	pos=	1	score=0.000194	unnormalised=0.0685600000	ALTLAALPV
1]	pos=	4	score=0.014020	unnormalised=4.9635600000	LAALPVAAM
2]	pos=	9	score=0.005857	unnormalised=2.0735600000	VAAMADVTL
3]	pos=	31	score=0.012947	unnormalised=4.5835600000	VAHNGAQAA
4]	pos=	72	score=0.010433	unnormalised=3.6935600000	VEQEAAAKA
5]	pos=	108	score=0.007058	unnormalised=2.4985600000	VVGLSMAAS
6]	pos=	110	score=0.004304	unnormalised=1.5235600000	GLSMAASSA
7]	pos=	111	score=0.031963	unnormalised=11.3155600000	LSMAASSAL
8]	pos=	113	score=0.016613	unnormalised=5.8815600000	MAASSALTL
9]	pos=	119	score=0.006625	unnormalised=2.3455600000	LTLGPGPGA
10]	pos=	121	score=0.001609	unnormalised=0.5695600000	LGPGGAAI
11]	pos=	130	score=0.001516	unnormalised=0.5365600000	GLSMAGSSA
12]	pos=	131	score=0.026878	unnormalised=9.5155600000	LSMAGSSAM
13]	pos=	133	score=0.014170	unnormalised=5.0165600000	MAGSSAMIL
14]	pos=	140	score=0.003450	unnormalised=1.2215600000	ILAAGPGPG
15]	pos=	141	score=0.009555	unnormalised=3.3825600000	LAAGPGPGT
16]	pos=	156	score=0.002838	unnormalised=1.0045600000	VQYSRAGPG
17]	pos=	158	score=0.015950	unnormalised=5.6465600000	YSRAGPGPG
18]	pos=	171	score=0.004476	unnormalised=1.5845600000	YGAMALAAF
19]	pos=	179	score=0.011941	unnormalised=4.2275600000	FHGPVPGMS
20]	pos=	191	score=0.018582	unnormalised=6.5785600000	YNINISLPS
21]	pos=	237	score=0.039120	unnormalised=13.8495600000	WSWLLSVLA
22]	pos=	241	score=0.007086	unnormalised=2.5085600000	LSVLAAGPG
23]	pos=	244	score=0.009134	unnormalised=3.2335600000	LAAGPGPGA
24]	pos=	266	score=0.008930	unnormalised=3.1615600000	YETAGPGPG
25]	pos=	275	score=0.030316	unnormalised=10.7325600000	YGYAAASAV
26]	pos=	277	score=0.035061	unnormalised=12.4125600000	YAAASAVAA
27]	pos=	287	score=0.007552	unnormalised=2.6735600000	LNPLGPGPG
28]	pos=	311	score=0.007860	unnormalised=2.7825600000	VAHGPVGPV
29]	pos=	323	score=0.009628	unnormalised=3.4085600000	VMPAAAAGS
30]	pos=	351	score=0.010580	unnormalised=3.7455600000	MAAGPGPGL
31]	pos=	359	score=0.009139	unnormalised=3.2355600000	LLLVLAFAF
32]	pos=	363	score=0.014619	unnormalised=5.1755600000	LAFAGGYAV
33]	pos=	365	score=0.017562	unnormalised=6.2175600000	FAGGYAVAA
34]	pos=	371	score=0.002936	unnormalised=1.0395600000	VAACAAVGS
35]	pos=	384	score=0.005933	unnormalised=2.1005600000	LSMAAYNAA
36]	pos=	389	score=0.025203	unnormalised=8.9225600000	YNAAGGHNA
37]	pos=	401	score=0.026867	unnormalised=9.5115600000	YTAAQAAVV
38]	pos=	409	score=0.011650	unnormalised=4.1245600000	VRAAYAMSG
39]	pos=	419	score=0.026822	unnormalised=9.4955600000	IVGAAAYRT
40]	pos=	431	score=0.011215	unnormalised=3.9705600000	INYRAAYAA
41]	pos=	433	score=0.022373	unnormalised=7.9205600000	YRAAYAAIG
42]	pos=	437	score=0.016082	unnormalised=5.6935600000	YAAIGGGVA
43]	pos=	449	score=0.027282	unnormalised=9.6585600000	YATATATAT
44]	pos=	461	score=0.002818	unnormalised=0.9975600000	YFLNLDVPL
45]	pos=	470	score=0.003572	unnormalised=1.2645600000	FVAAYQAET
46]	pos=	474	score=0.023669	unnormalised=8.3795600000	YQAETAVNT

47]	pos= 480	score=0.032914	unnormalised=11.6525600000	VNTLAAYAV
48]	pos= 488	score=0.017385	unnormalised=6.1545600000	VNGEPAPLA
49]	pos= 498	score=0.000233	unnormalised=0.0825600000	YGLSNATPR
50]	pos= 500	score=0.008334	unnormalised=2.9505600000	LSNATPREV
51]	pos= 522	score=0.002182	unnormalised=0.7725600000	AYNLPPPLA
52]	pos= 523	score=0.007651	unnormalised=2.7085600000	YNLPPPLAP
53]	pos= 542	score=0.008800	unnormalised=3.1155600000	FVRTSNIKF
54]	pos= 550	score=0.000137	unnormalised=0.0485600000	FQDAYNKKA
55]	pos= 563	score=0.000674	unnormalised=0.2385600000	ICTGGGNIM
56]	pos= 576	score=0.012190	unnormalised=4.3155600000	YVKKAGLSA
57]	pos= 588	score=0.011769	unnormalised=4.1665600000	LAHADSLAS
58]	pos= 594	score=0.010521	unnormalised=3.7245600000	LASSASKKI
59]	pos= 606	score=0.000527	unnormalised=0.1865600000	AEAMGNSRM
60]	pos= 616	score=0.014097	unnormalised=4.9905600000	YNQYRSKKA
61]	pos= 650	score=0.029994	unnormalised=10.6185600000	FEKLEPMAS
62]	pos= 653	score=0.001259	unnormalised=0.4455600000	LEPMASILD
63]	pos= 673	score=0.001459	unnormalised=0.5165600000	VLATQGRGA
64]	pos= 691	score=0.018983	unnormalised=6.7205600000	YHAMSSTHE
65]	pos= -1	score=0.186902	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/9107_20230207-091852_5_5fvJbmMtM4C6.FSA_1_001

IALLTLAALPVAAMADVTLTYGTIKAGVETSRVAHNGAQAASVETGTGIVDLGSKIGFKGQEDLGNLKAIWQVEQEA
AGLFQRHGEGTKATVGPVPGPGTGSVAVGLSMAASSALTLGPGGAAIGLSMAGSSAMILAAGPGPGTNRQAGVQYS
RAGPGPGAQGGYGAMALAAFHGPGGMSDPAYNINISLPSYYPDGGPGGALSAGVAVAMSLTVGAGPGPGRRLRWSW
LLSVLAAGPGPGAELTAAQVRVAAAAYETAGPGPGYGYAAASVAARLNPLGPGGTVGGAAPGGAAAAVAHGP
APSVMPAAAAGSSATGPGGTGAVLGGGGIAMAAGPGPGLLLVLAFAAGYAVAACAAYGSVAVGLSMAAYNAAGGHNAVA
AYTAAQAQAVVRAAYAMSGDIVGAAAYRTADGINYRAAYAAIGGGVAVAAAYATATATLAAYFLNLDVPLFVAAYQAETA
VNTLAAYAVNGEPAPLAAYGLSNATPREVAAYQVTRNRIKKAAYNLPPPLAPDFKKAKFLEGFVRTSNIKFQDAYNKKAP
DDPICTGGGNIMAHVSYVKKAGLSASSGLAHADSLASSASKKIGQAAEAMGNSRMFYNQYRSKKALGQTVQASD
ETLNKRVNTLFEKLEPMASILDPGASKKAVGERVLATQGRGAWPVCGRKKAYHAMSSTHEANTMAMMARDEAAAKAPPHA
LSHHHHHH

Epitopes of protein 0 -----

0]	pos= 9	score=0.015642	unnormalised=2.2588200000	VAAMADVTL
1]	pos= 15	score=0.030772	unnormalised=4.4438200000	VTLTYTIKA
2]	pos= 25	score=0.036035	unnormalised=5.2038200000	VETSRVAH
3]	pos= 108	score=0.028023	unnormalised=4.0468200000	VVGLSMAAS
4]	pos= 113	score=0.032420	unnormalised=4.6818200000	MAASSALTL
5]	pos= 119	score=0.001799	unnormalised=0.2598200000	LTLP GPGGA
6]	pos= 133	score=0.011570	unnormalised=1.6708200000	MAGSSAMIL
7]	pos= 141	score=0.001065	unnormalised=0.1538200000	LAAGPGPGT
8]	pos= 156	score=0.019436	unnormalised=2.8068200000	VQYSRAGPG
9]	pos= 237	score=0.048658	unnormalised=7.0268200000	WSWLLSVLA
10]	pos= 311	score=0.004174	unnormalised=0.6028200000	VAHGP GPGV
11]	pos= 359	score=0.000580	unnormalised=0.0838200000	LLLVLAFAG
12]	pos= 362	score=0.011591	unnormalised=1.6738200000	VLAFA GGYA
13]	pos= 374	score=0.012512	unnormalised=1.8068200000	CAAYGS AVV
14]	pos= 419	score=0.004465	unnormalised=0.6448200000	IVGAA YRT
15]	pos= 431	score=0.002409	unnormalised=0.3478200000	INYRA AYAA
16]	pos= 446	score=0.014125	unnormalised=2.0398200000	VAAYAT ATA
17]	pos= 471	score=0.014201	unnormalised=2.0508200000	VAAYQ AETA
18]	pos= 480	score=0.047350	unnormalised=6.8378200000	VNTLA AYAV
19]	pos= 495	score=0.010220	unnormalised=1.4758200000	LAAYG LSNA
20]	pos= 570	score=0.057467	unnormalised=8.2988200000	IMAHV SYVK

21]	pos= 582	score=0.027787	unnormalised=4.0128200000	LSASSGLAH
22]	pos= 591	score=0.012747	unnormalised=1.8408200000	ADSLASSAS
23]	pos= 606	score=0.017400	unnormalised=2.5128200000	AEAMGNSRM
24]	pos= 612	score=0.037904	unnormalised=5.4738200000	SRMFYNQYR
25]	pos= 616	score=0.023764	unnormalised=3.4318200000	YNQYRSKKA
26]	pos= 653	score=0.017691	unnormalised=2.5548200000	LEPMASILD
27]	pos= -1	score=0.458192	unnormalised=66.1680000000	non-binding event
