

# C-IMMSIM simulation results

April 20, 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](http://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)

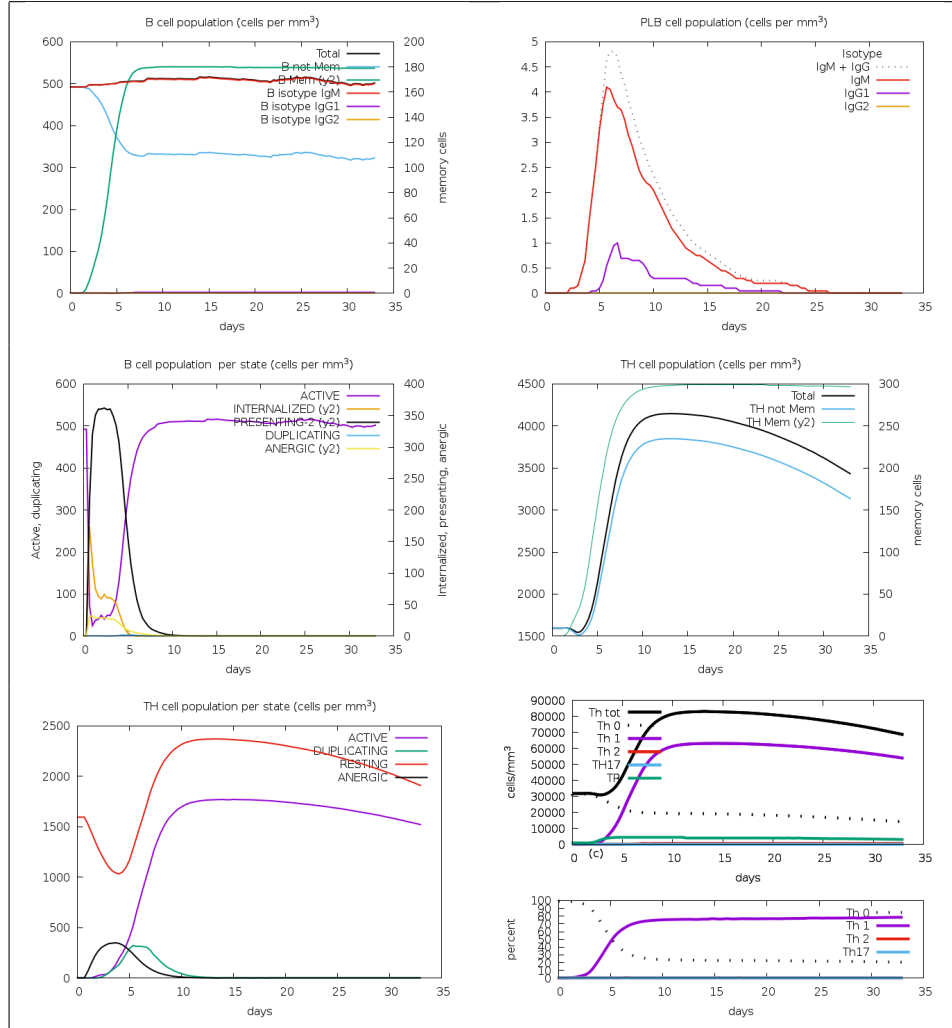


Figure 1: Cell counts shown. Legend: Act=active, Intern=internalized the Ag, Pres II = presenting on MHC II, Dup = in the mitotic cycle, Anergic = anergic, Resting = not active.

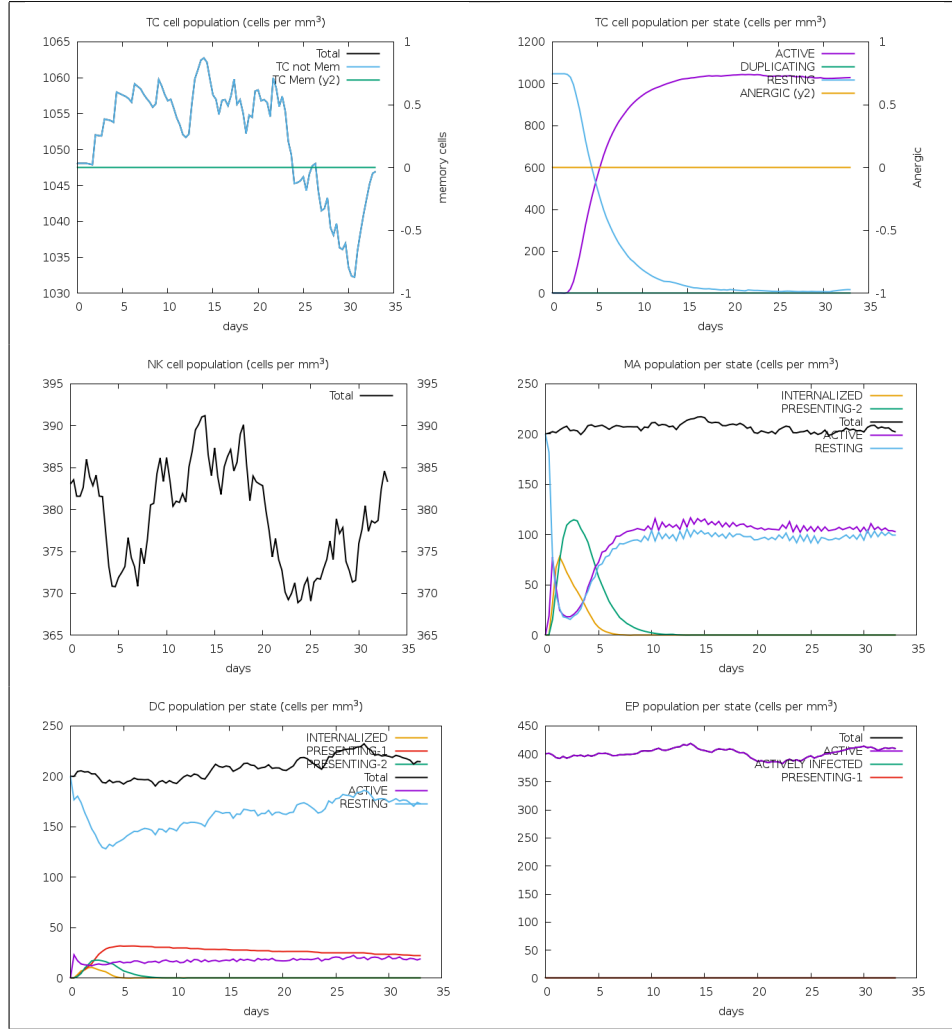


Figure 2: Legend: symbols as figure above.

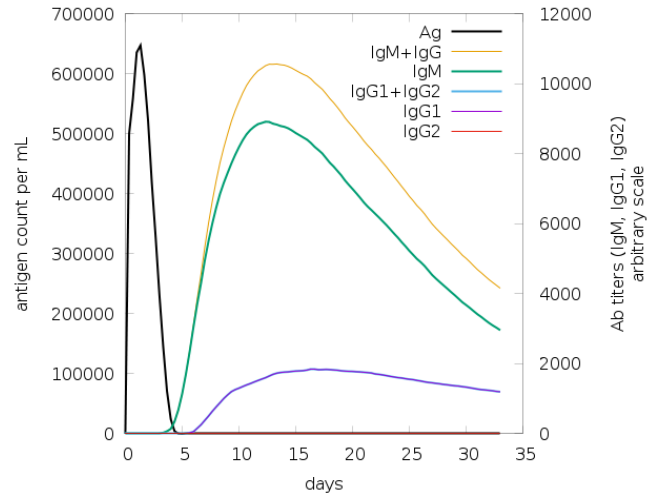


Figure 3: The virus, the immunoglobulins and the immunocomplexes.

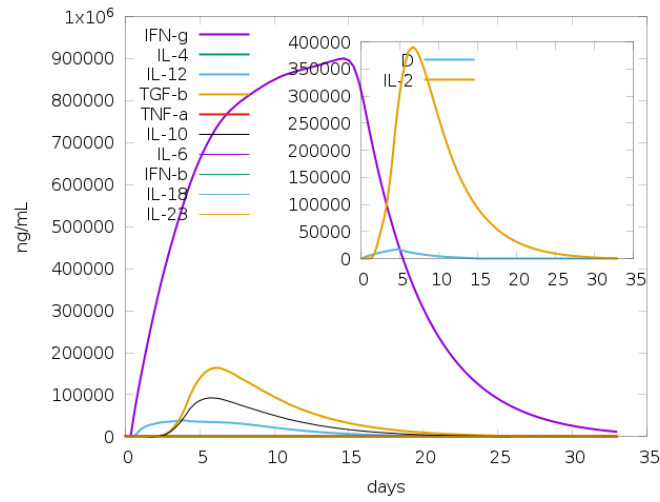


Figure 4: Concentration of cytokines and interleukins. Inset plot shows danger signal together with leukocyte growth factor IL-2.

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/12364\_20230420-135143\_5\_3WBpIhMm0EHq.FSA\_1\_001

[illegible]

```

1]      pos=83 len=6      TNKKKV
2]      pos=100 len=12     DNKTVESKSGPG
3]      pos=146 len=5      DTKGP
4]      pos=162 len=10     NSQPDPKPGPG
5]      pos=187 len=6      NKGPGP
6]      pos=271 len=4      GPGK
7]      pos=310 len=27     KDINSHQTDKRKKKNQIDKNNSTDNNH

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

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Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/12364\_20230420-135143\_5\_3WBpIhMm0EHq.FSA\_1\_001

Epitopes of protein 0 -----

5

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Allele: A0202  
Pseudo sequence: KAAHVEQRKKAQTRV  
Threshold: 9.589400  
Max score: 27.292000

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Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/12364\_20230420-135143\_5\_3WbPihMmOEhQ.FSA\_1\_001

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ILIFALILVAAYLYFDLIYSIAAYNYDNVRVEFAAYMMPAPGDKFAAYDVFGANYYYAAYKYRSITVRVGP GPKNLLSF  
DVQTNKKKVGPGPGYLLIYNDNKTVESKSGPGPGTVQVTIDNRQSLGFTGPGPGQFLYFDLIYSIKDTKGPGGVFHNIN  
YANSQDPKPGPGPFVYPYKFLNIYGNKGP GQSLGFTITTNKNMVTGPGPGSEINIKAEKFLQHDGPGGNMRYLY  
DDKHVSEINGPGPGSAINVKSIDQFLYFDGPGPGDKYVDVFGANYYYQGP GGGFTITTNKNMVTIQEKDINSHQTDK  
RKKKNQIDKNNSTDNHHHHHH

Epitopes of protein 0 -----

0]	pos=	4	score=0.011639	unnormalised=1.2346000000	ALILVAAYL
1]	pos=	-1	score=0.988361	unnormalised=104.8410000000	non-binding event

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

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Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/12364\_20230420-135143\_5\_3WbPihMmOEhQ.FSA\_1\_001

-----

ILIFALILVAAYLYFDLIYSIAAYNYDNVRVEFAAYMMPAPGDKFAAYDVFGANYYYAAYKYRSITVRVGP GPKNLLSF  
DVQTNKKKVGPGPGYLLIYNDNKTVESKSGPGPGTVQVTIDNRQSLGFTGPGPGQFLYFDLIYSIKDTKGPGGVFHNIN  
YANSQDPKPGPGPFVYPYKFLNIYGNKGP GQSLGFTITTNKNMVTGPGPGSEINIKAEKFLQHDGPGGNMRYLY  
DDKHVSEINGPGPGSAINVKSIDQFLYFDGPGPGDKYVDVFGANYYYQGP GGGFTITTNKNMVTIQEKDINSHQTDK  
RKKKNQIDKNNSTDNHHHHHH

Epitopes of protein 0 -----

0]	pos=	37	score=0.002446	unnormalised=0.2572000000	MPAPGDKFA
1]	pos=	109	score=0.000677	unnormalised=0.0712000000	GPGPGTVQV
2]	pos=	-1	score=0.996877	unnormalised=104.8410000000	non-binding event

=====

Allele: B5801  
Pseudo sequence: KAAREEQRNKAQTRE  
Threshold: -11.757400  
Max score: 26.104000

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Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/12364\_20230420-135143\_5\_3WbPihMmOEhQ.FSA\_1\_001

-----

ILIFALILVAAYLYFDLIYSIAAYNYDNVRVEFAAYMMPAPGDKFAAYDVFGANYYYAAYKYRSITVRVGP GPKNLLSF  
DVQTNKKKVGPGPGYLLIYNDNKTVESKSGPGPGTVQVTIDNRQSLGFTGPGPGQFLYFDLIYSIKDTKGPGGVFHNIN  
YANSQDPKPGPGPFVYPYKFLNIYGNKGP GQSLGFTITTNKNMVTGPGPGSEINIKAEKFLQHDGPGGNMRYLY  
DDKHVSEINGPGPGSAINVKSIDQFLYFDGPGPGDKYVDVFGANYYYQGP GGGFTITTNKNMVTIQEKDINSHQTDK  
RKKKNQIDKNNSTDNHHHHHH

Epitopes of protein 0 -----

0]	pos=	0	score=0.005490	unnormalised=7.1904000000	ILIFALILV
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1]	pos=	1	score=0.006094	unnormalised=7.9814000000	LIFALILVA
2]	pos=	2	score=0.001577	unnormalised=2.0654000000	IFALILVAA
3]	pos=	3	score=0.012658	unnormalised=16.5774000000	FALILVAAAY
4]	pos=	4	score=0.008968	unnormalised=11.7454000000	ALILVAAAYL
5]	pos=	5	score=0.012562	unnormalised=16.4524000000	LILVAAAYLY
6]	pos=	6	score=0.017025	unnormalised=22.2974000000	ILVAAAYLYF
7]	pos=	7	score=0.006317	unnormalised=8.2734000000	LVAAYLYFD
8]	pos=	8	score=0.011308	unnormalised=14.8094000000	VAAAYLYFDL
9]	pos=	9	score=0.010525	unnormalised=13.7844000000	AAYLYFDLI
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11]	pos=	11	score=0.003006	unnormalised=3.9364000000	YLYFDLIYS
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18]	pos=	20	score=0.007284	unnormalised=9.5394000000	IAAYNYDNV
19]	pos=	21	score=0.005241	unnormalised=6.8644000000	AAYNYDNVR
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21]	pos=	27	score=0.007922	unnormalised=10.3754000000	NVRVEFAAY
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23]	pos=	29	score=0.009135	unnormalised=11.9644000000	RVEFAAYMM
24]	pos=	30	score=0.001501	unnormalised=1.9664000000	VEFAAYMMP
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26]	pos=	33	score=0.007199	unnormalised=9.4284000000	AAYMMPAPG
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131]	pos= 207	score=0.006902	unnormalised=9.0394000000	VTGPGPGSE
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169]	pos= 289	score=0.007156	unnormalised=9.3724000000	GP GPGGFTI
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177]	pos= 303	score=0.001028	unnormalised=1.3464000000	MVTIQEKKD
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182]	pos= 313	score=0.001163	unnormalised=1.5234000000	NSHQTDKRR
183]	pos= 328	score=0.005418	unnormalised=7.0954000000	KNNSTDNHH
184]	pos= 329	score=0.000816	unnormalised=1.0684000000	NNSTDNHHH
185]	pos= 330	score=0.005581	unnormalised=7.3094000000	NSTDNHHHH
186]	pos= 331	score=0.005506	unnormalised=7.2104000000	STDNHHHHH
187]	pos= -1	score=0.080052	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

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Allele: DRB1\_0101  
Pseudo sequence: KAFHVEQRKAQTRV  
Threshold: 2.392440  
Max score: 26.461000

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Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/12364\_20230420-135143\_5\_3WBpIhMmOEhQ.FSA\_1\_001

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ILIFALILVAAYLYFDLIYSIAAYNYDNVRVEFAAYMMPAPGDKFAAYDVFGANYYYAAYKYRSITVRVGP GPKNLLSF  
DVQTNKKKVGPGPGYLLIYNDNKTVESKSGPGPGTVQVTIDNRQSLGFTGPGPGQFLYFDLIYSIKDTKGPGGVFHNIN  
YANSQDPKGP GPGPFVYPYKFLNIYDNGKPGPGQSLGFTITTNKNMVTGPGPGSEINIKAEKFLQHDGPGPGNMRYLY  
DDKHVSEINGPGPGSAINVKSIDQFLYFDGPGPGKDKYVDVFGANYYYQGP GPGGFTITTNKNMVTIQEKDINSHQTDK  
RKKKNQIDKNNSTDNNHHHHH

Epitopes of protein 0 -----

0]	pos=	5	score=0.024928	unnormalised=2.5395600000	LILVAAYLY
1]	pos=	14	score=0.066271	unnormalised=6.7515600000	FDLIYSIAA
2]	pos=	17	score=0.021914	unnormalised=2.2325600000	IYSIAAYNY
3]	pos=	50	score=0.000329	unnormalised=0.0335600000	FGANYYYAA
4]	pos=	55	score=0.016172	unnormalised=1.6475600000	YYAAYKYRS
5]	pos=	88	score=0.004256	unnormalised=0.4335600000	VGP GPGYLL
6]	pos=	155	score=0.012157	unnormalised=1.2385600000	FHNINYANS
7]	pos=	198	score=0.018204	unnormalised=1.8545600000	FTITTNKNM
8]	pos=	200	score=0.014484	unnormalised=1.4755600000	ITTNKNMVT
9]	pos=	206	score=0.028736	unnormalised=2.9275600000	MVTGPGPGS
10]	pos=	285	score=0.049820	unnormalised=5.0755600000	YYYQGPGPG
11]	pos=	286	score=0.060558	unnormalised=6.1695600000	YYQGP GPG
12]	pos=	295	score=0.018204	unnormalised=1.8545600000	FTITTNKNM
13]	pos=	297	score=0.014484	unnormalised=1.4755600000	ITTNKNMVT
14]	pos=	-1	score=0.649484	unnormalised=66.1680000000	non-binding event

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

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Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/12364\_20230420-135143\_5\_3WBpIhMmOEhQ.FSA\_1\_001

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ILIFALILVAAYLYFDLIYSIAAYNYDNVRVEFAAYMMPAPGDKFAAYDVFGANYYYAAYKYRSITVRVGP GPKNLLSF  
DVQTNKKKVGPGPGYLLIYNDNKTVESKSGPGPGTVQVTIDNRQSLGFTGPGPGQFLYFDLIYSIKDTKGPGGVFHNIN  
YANSQDPKGP GPGPFVYPYKFLNIYDNGKPGPGQSLGFTITTNKNMVTGPGPGSEINIKAEKFLQHDGPGPGNMRYLY  
DDKHVSEINGPGPGSAINVKSIDQFLYFDGPGPGKDKYVDVFGANYYYQGP GPGGFTITTNKNMVTIQEKDINSHQTDK  
RKKKNQIDKNNSTDNNHHHHH

Epitopes of protein 0 -----

0]	pos=	0	score=0.069176	unnormalised=6.7358200000	ILIFALILV
1]	pos=	5	score=0.022489	unnormalised=2.1898200000	LILVAAYLY
2]	pos=	14	score=0.063938	unnormalised=6.2258200000	FDLIYSIAA
3]	pos=	17	score=0.029996	unnormalised=2.9208200000	IYSIAAYNY
4]	pos=	58	score=0.077607	unnormalised=7.5568200000	AYKYRSITV
5]	pos=	200	score=0.028630	unnormalised=2.7878200000	ITTNKNMVT
6]	pos=	297	score=0.028630	unnormalised=2.7878200000	ITTNKNMVT

7] pos= -1 score=0.679533 unnormalised=66.1680000000 non-binding event

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