

C-IMMSIM simulation results

November 20, 2022

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)

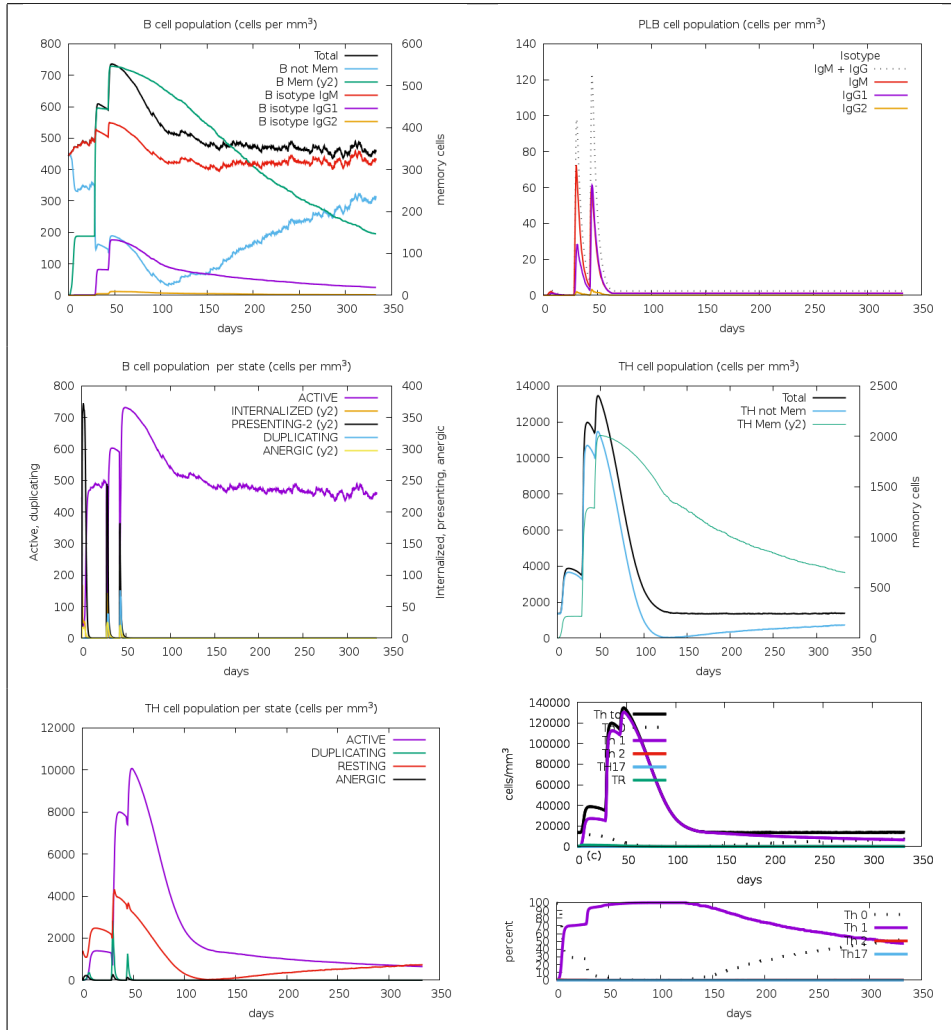


Figure 1: Cell counts shown. Legend: Act=active, Intern=internalized the Ag, Pres II = presenting on MHC II, Dup = in the mitotic cycle, Anergic = anergic, Resting = not active.

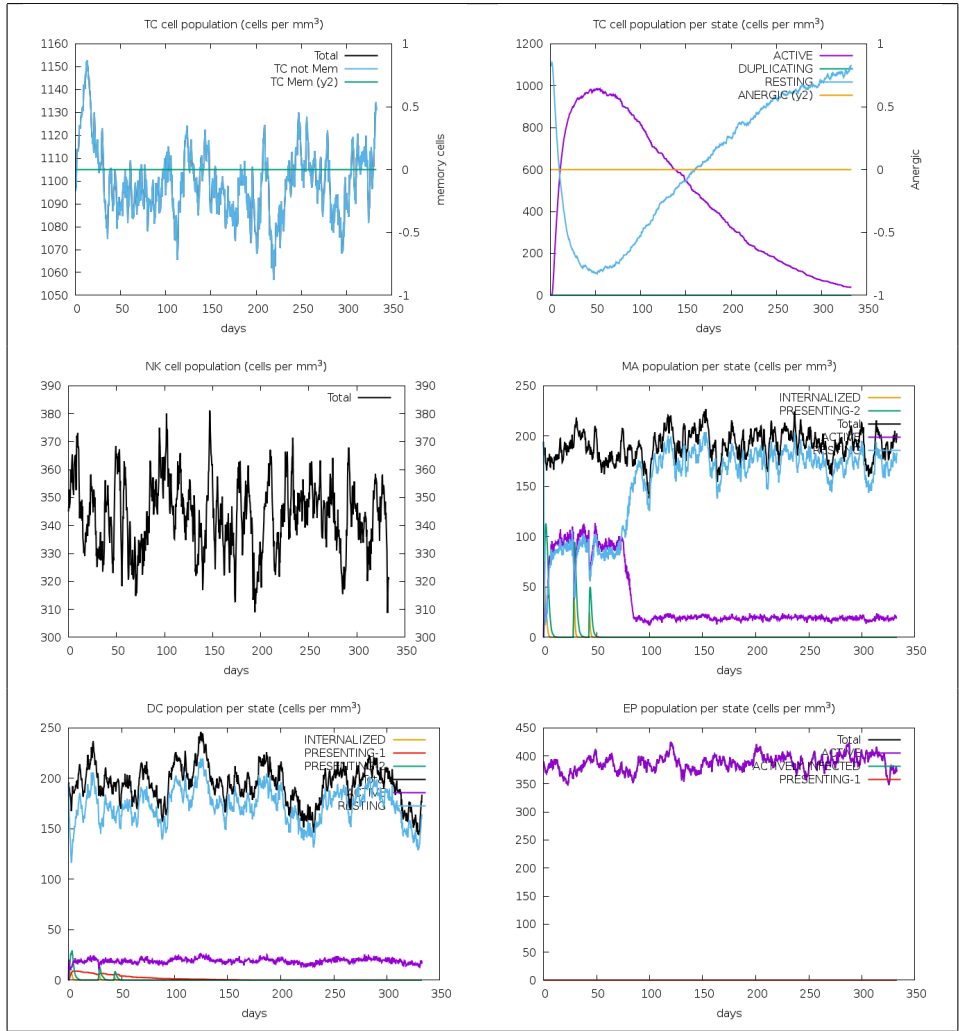


Figure 2: Legend: symbols as figure above.

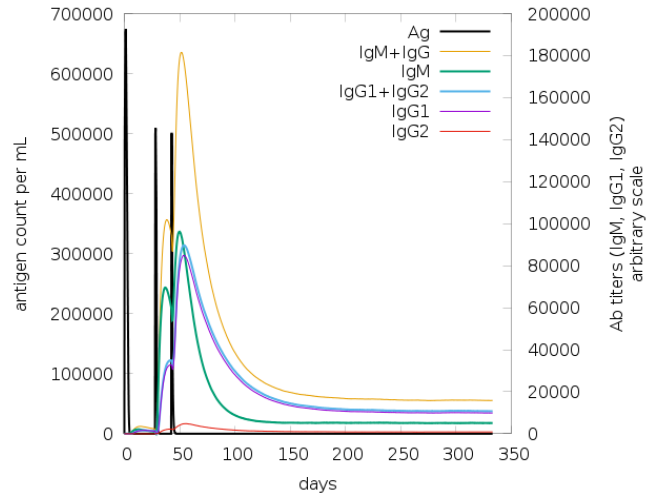


Figure 3: The virus, the immunoglobulins and the immunocomplexes.

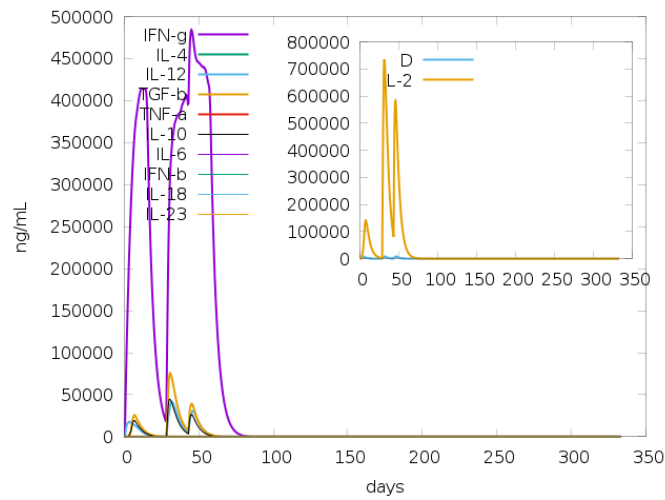


Figure 4: Concentration of cytokines and interleukins. Inset plot shows danger signal together with leukocyte growth factor IL-2.

Threshold: 9.523800
Max score: 27.437000

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/6827_20221120-033933_5_F2TRTG0UfqFj.FSA_1_001

APPHALSEAAKAGLFQRHGEGTKATVGEVVAAYFPRGQGVPIAAYLSYFIASFRAAYRLFRKSNLKAAYGELFWTVVPY
AAYAGLRPTFDTRAAYLTDRDIVIKGPGGGTWTLYTGAIKLDKGGPGGITRFQTLALHRSYLGPGGSLLENKSLT
ILDDNGPGPKDCDPVFAEYFVSVLKKTRRIRGGDGKMKDLSPKKYACWHHSIGFDYVYNPKKTSNCTRITTSVAVGDVHPG
EPVKKYSDICSKHMDARYCSEFIRIKKSFKFRPGSLIYYQNEVTPEYEAANKFNFTVSFVLRVVKVSASHLEHHHHHH

Epitopes of protein 0 -----
0] pos= 4 score=0.005518 unnormalised=0.5982000000 ALSEAAKA
1] pos= 274 score=0.027479 unnormalised=2.9792000000 SLIYYQNEV
2] pos= -1 score=0.967004 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/6827_20221120-033933_5_F2TRTG0UfqFj.FSA_1_001

APPHALSEAAKAGLFQRHGEGTKATVGEVVAAYFPRGQGVPIAAYLSYFIASFRAAYRLFRKSNLKAAYGELFWTVVPY
AAYAGLRPTFDTRAAYLTDRDIVIKGPGGGTWTLYTGAIKLDKGGPGGITRFQTLALHRSYLGPGGSLLENKSLT
ILDDNGPGPKDCDPVFAEYFVSVLKKTRRIRGGDGKMKDLSPKKYACWHHSIGFDYVYNPKKTSNCTRITTSVAVGDVHPG
EPVKKYSDICSKHMDARYCSEFIRIKKSFKFRPGSLIYYQNEVTPEYEAANKFNFTVSFVLRVVKVSASHLEHHHHHH

Epitopes of protein 0 -----
0] pos= 0 score=0.016572 unnormalised=2.1552000000 APPHALSEA
1] pos= 34 score=0.064939 unnormalised=8.4452000000 FPRGQGVPI
2] pos= 77 score=0.022570 unnormalised=2.9352000000 VPYAAAYAGL
3] pos= 86 score=0.050660 unnormalised=6.5882000000 RPTFDTRAA
4] pos= 105 score=0.009314 unnormalised=1.2112000000 GPGPGGTWL
5] pos= 145 score=0.008037 unnormalised=1.0452000000 GPGPGSLLL
6] pos= 303 score=0.021732 unnormalised=2.8262000000 VPKVSASHL
7] pos= -1 score=0.806175 unnormalised=104.8410000000 non-binding event

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

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/6827_20221120-033933_5_F2TRTG0UfqFj.FSA_1_001

APPHALSEAAKAGLFQRHGEGTKATVGEVVAAYFPRGQGVPIAAYLSYFIASFRAAYRLFRKSNLKAAYGELFWTVVPY
AAYAGLRPTFDTRAAYLTDRDIVIKGPGGGTWTLYTGAIKLDKGGPGGITRFQTLALHRSYLGPGGSLLENKSLT
ILDDNGPGPKDCDPVFAEYFVSVLKKTRRIRGGDGKMKDLSPKKYACWHHSIGFDYVYNPKKTSNCTRITTSVAVGDVHPG
EPVKKYSDICSKHMDARYCSEFIRIKKSFKFRPGSLIYYQNEVTPEYEAANKFNFTVSFVLRVVKVSASHLEHHHHHH

Epitopes of protein 0 -----
0] pos= 57 score=0.006614 unnormalised=0.7446000000 YRLFRKSNL
1] pos= 136 score=0.021120 unnormalised=2.3776000000 LLALHRSYL

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2]      pos= 176 score=0.001746 unnormalised=0.1966000000      FRAEYFSVL
3]      pos= 267 score=0.039206 unnormalised=4.4136000000      SFKFRPGSL
4]      pos=  -1 score=0.931312 unnormalised=104.8410000000      non-binding event

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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: KFAHVEQRKAQTRV
Threshold: 2.392440
Max score: 26.461000

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Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/6827_20221120-033933_5_F2TRTGOUfqFj.FSA_1_001

```

APPHALSEAAAKAGLFQRHGEGTKATVGEVVAAYFPRGQGVPIAAYLSYFIASFRAAYRFRKSNLKAAYGELFWTVVVPY
AAYAGLRPTFDTRAAYLTDRDIVIKGPGGWTWLTGTGAIKLDKGGPGGITRFQTLALHRSYLGPGPGSLLLENKSLT
ILDDNGPGPKDCDPVFAEYFVSVLKKTRRIRGGDGKMKDLSPKKYACWHHSIGFDYVYNPKKTSNCTRRTTSAVGDVHPG
EPVKKYSDICSKHMDARYCSEFIRIKKSFKFRPGSLIYYQNEVTPEYEAANKFNFTVSFVLRVVKVSASHLEHHHHHH

```

Epitopes of protein 0 -----

```

0]      pos= 34 score=0.003560 unnormalised=0.4135600000      FPRGQGVPI
1]      pos= 42 score=0.010172 unnormalised=1.1815600000      IAAYLSYFI
2]      pos= 65 score=0.011695 unnormalised=1.3585600000      LKAAYGELF
3]      pos= 73 score=0.066576 unnormalised=7.7335600000      FWTVVVPYAA
4]      pos= 82 score=0.022353 unnormalised=2.5965600000      YAGLRPTFD
5]      pos= 89 score=0.042497 unnormalised=4.9365600000      FDTRAAYLT
6]      pos= 113 score=0.022448 unnormalised=2.6075600000      LTYTGAIKL
7]      pos= 130 score=0.001692 unnormalised=0.1965600000      ITRFQTLA
8]      pos= 133 score=0.071810 unnormalised=8.3415600000      FQTLALHR
9]      pos= 137 score=0.038219 unnormalised=4.4395600000      LALHRSYLG
10]     pos= 143 score=0.037556 unnormalised=4.3625600000      YLPGPGSL
11]     pos= 144 score=0.020778 unnormalised=2.4135600000      LGPGPGSLL
12]     pos= 152 score=0.001537 unnormalised=0.1785600000      LLENKSLTI
13]     pos= 268 score=0.062754 unnormalised=7.2895600000      FKFRPGSLI
14]     pos= 300 score=0.016732 unnormalised=1.9435600000      WLRVVKVSA
15]     pos=  -1 score=0.569621 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/6827_20221120-033933_5_F2TRTGOUfqFj.FSA_1_001

```

APPHALSEAAAKAGLFQRHGEGTKATVGEVVAAYFPRGQGVPIAAYLSYFIASFRAAYRFRKSNLKAAYGELFWTVVVPY
AAYAGLRPTFDTRAAYLTDRDIVIKGPGGWTWLTGTGAIKLDKGGPGGITRFQTLALHRSYLGPGPGSLLLENKSLT
ILDDNGPGPKDCDPVFAEYFVSVLKKTRRIRGGDGKMKDLSPKKYACWHHSIGFDYVYNPKKTSNCTRRTTSAVGDVHPG

```

EPVKKYSDICSKHMDARYCSEFIRIKKSFKFRPGSLIYYQNEVTPEYEAANKFNFTVSWFLRVPKVSASHLEHHHHHH

Epitopes of protein 0 -----

0]	pos= 39	score=0.001733	unnormalised=0.2578200000	GVPIAAYLS
1]	pos= 42	score=0.055646	unnormalised=8.2788200000	IAAYLSYFI
2]	pos= 46	score=0.042156	unnormalised=6.2718200000	LSYFIASFR
3]	pos= 47	score=0.018046	unnormalised=2.6848200000	SYFIASFRA
4]	pos= 50	score=0.063806	unnormalised=9.4928200000	IASFRAAYR
5]	pos= 54	score=0.003749	unnormalised=0.5578200000	RAAYRLFRK
6]	pos= 57	score=0.014047	unnormalised=2.0898200000	YRLFRKSNL
7]	pos= 59	score=0.025567	unnormalised=3.8038200000	LFRKSNLKA
8]	pos= 76	score=0.036806	unnormalised=5.4758200000	VVPYAAYAG
9]	pos= 130	score=0.074096	unnormalised=11.0238200000	ITRFQTLA
10]	pos= 133	score=0.037733	unnormalised=5.6138200000	FQTLALHR
11]	pos= 136	score=0.006727	unnormalised=1.0008200000	LLALHRSYL
12]	pos= 137	score=0.051909	unnormalised=7.7228200000	LALHRSYLG
13]	pos= 214	score=0.018853	unnormalised=2.8048200000	FDYVYNPKK
14]	pos= 242	score=0.014349	unnormalised=2.1348200000	VKKYSDICS
15]	pos= 262	score=0.025144	unnormalised=3.7408200000	IRIKKSFKF
16]	pos= 275	score=0.057864	unnormalised=8.6088200000	LIYYQNEVT
17]	pos= 303	score=0.007023	unnormalised=1.0448200000	VPKVSASHL
18]	pos= -1	score=0.444747	unnormalised=66.1680000000	non-binding event
