

C-IMMSIM simulation results

July 18, 2025

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)

Technical problems: Ilaria Gonnella (ilaria dot gonnella at cnr dot it)

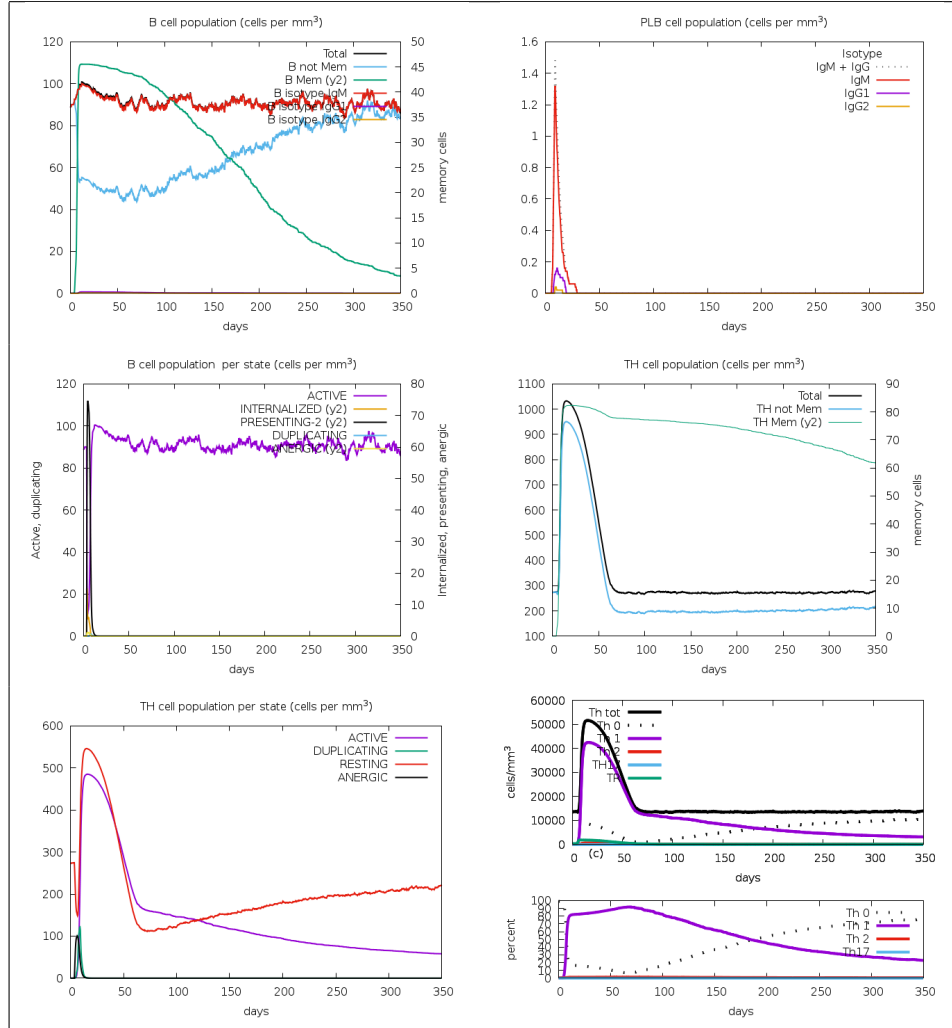


Figure 1: Cell counts shown. Legend: Act=active, Intern=internalized the Ag, Pres II = presenting on MHC II, Dup = in the mitotic cycle, Anergic = anergic, Resting = not active.

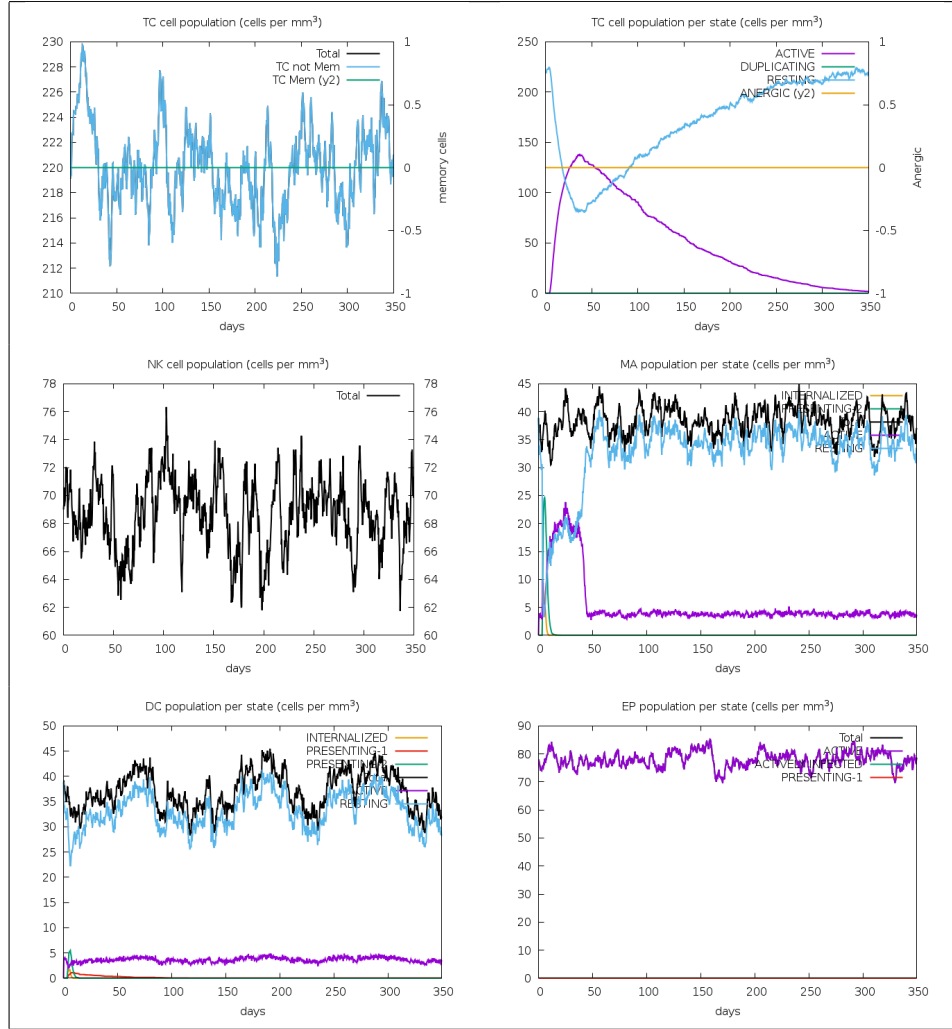


Figure 2: Legend: symbols as figure above.

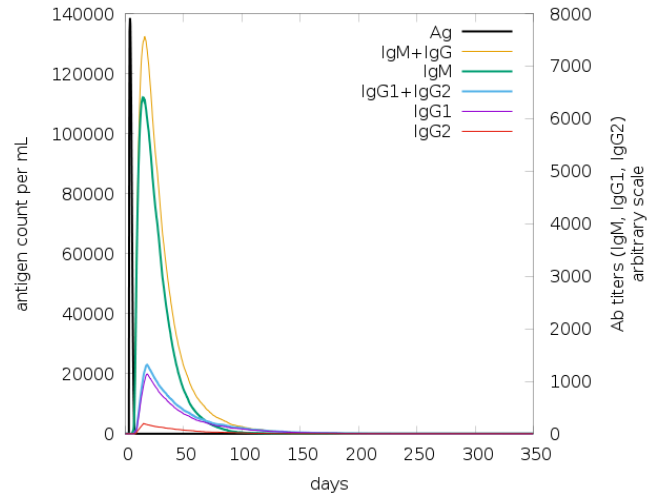


Figure 3: The virus, the immunoglobulins and the immunocomplexes.

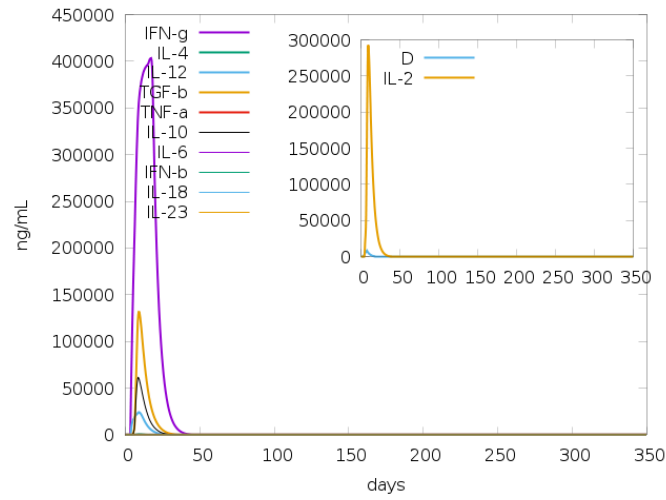


Figure 4: Concentration of cytokines and interleukins. Inset plot shows danger signal together with leukocyte growth factor IL-2.

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/38253_20250718-130113_5_UmQfQ5F1nBD3.FSA_1_001

[illegible]

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

    Read class I peptide list from file? NO
```

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/38253_20250718-130113_5_UmQfQ5F1nBD3.FSA_1_001

```
Epitopes of protein 0 -----
0]      pos=  -1 score=1.000000 unnormalised=104.8410000000      non-binding event
```

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/38253_20250718-130113_5-UmQfQ5F1nBD3.FSA_1_001

GIINTLQKYYCRVGGRCVLSCLPKKEQIGKCSTRGRKCCRRKKEAAAKTPVGRLVTVAAYFLAVGGVLLAAYVLLFLS
VNVAAYFSITPSAPSYTLGPGPGFSITPSAPSKKSITPSAPSYTLKLGEKKVTIMSKDKPTIDVKMKKKMEKLQLKGTTY
GVC

Epitopes of protein 0 -----

0]	pos=	77	score=0.005470	unnormalised=0.5766000000	FLSVNVAAY
1]	pos=	-1	score=0.994530	unnormalised=104.8410000000	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/38253_20250718-130113_5_UmQfQ5F1nBD3.FSA_1_001

GIINTLQKYYCRVGGRCVLSCLPKKEQIGKCSTRGRKCCRRKKEAAAKTPVGRLVTVAAYFLAVGGVLLAAYVLLFLS
VNVAAYFSITPSAPSYTLGPGPGFSITPSAPSKKSITPSAPSYTLKLGEKKVTIMSKDKPTIDVKMKKKMEKLQLKGTTY
GVC

Epitopes of protein 0 -----

0]	pos=	50	score=0.005479	unnormalised=0.6582000000	TPVGRLVTV
1]	pos=	89	score=0.060909	unnormalised=7.3172000000	TPSAPSYTL
2]	pos=	116	score=0.060909	unnormalised=7.3172000000	TPSAPSYTL
3]	pos=	-1	score=0.872703	unnormalised=104.8410000000	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/38253_20250718-130113_5_UmQfQ5F1nBD3.FSA_1_001

GIINTLQKYYCRVGGRCVLSCLPKKEQIGKCSTRGRKCCRRKKEAAAKTPVGRLVTVAAYFLAVGGVLLAAYVLLFLS
VNVAAYFSITPSAPSYTLGPGPGFSITPSAPSKKSITPSAPSYTLKLGEKKVTIMSKDKPTIDVKMKKKMEKLQLKGTTY
GVC

Epitopes of protein 0 -----

0]	pos=	50	score=0.005479	unnormalised=0.6582000000	TPVGRLVTV
1]	pos=	89	score=0.060909	unnormalised=7.3172000000	TPSAPSYTL
2]	pos=	116	score=0.060909	unnormalised=7.3172000000	TPSAPSYTL
3]	pos=	-1	score=0.872703	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_0401
Pseudo sequence: KFAAHVEQRKAQTRV
Threshold: 2.842330
Max score: 29.818000

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/38253_20250718-130113_5_UmQfQ5F1nBD3.FSA_1_001

GIINTLQKYYCRVRGGRCVLSCLPKKEQIGKCSTRGRKCCRRKKEAAAKTPVGRGLVTVAAYFLAVGGVLLAAYVLLFLS
VNVAAYFSITPSAPSYTLGPGPGFSITPSAPSKKSITPSAPSYTLKLGEKKVTIMSKDKPTIDVKMKKKMEKLQLKGT
GVC

Epitopes of protein 0 -----

0]	pos=	52	score=0.034569	unnormalised=4.1646700000	VGRLVTVAA
1]	pos=	69	score=0.005019	unnormalised=0.6046700000	LLAAYVLLF
2]	pos=	73	score=0.028609	unnormalised=3.4466700000	YVLLFLSVN
3]	pos=	75	score=0.031805	unnormalised=3.8316700000	LLFLSVNVA
4]	pos=	76	score=0.045285	unnormalised=5.4556700000	LFLSVNVAA
5]	pos=	77	score=0.011410	unnormalised=1.3746700000	FLSVNVAA
6]	pos=	85	score=0.049468	unnormalised=5.9596700000	YFSITPSAP
7]	pos=	86	score=0.122305	unnormalised=14.7346700000	FSITPSAPS
8]	pos=	103	score=0.122305	unnormalised=14.7346700000	FSITPSAPS
9]	pos=	-1	score=0.549226	unnormalised=66.1680000000	non-binding event

=====

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

Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/38253_20250718-130113_5_UmQfQ5F1nBD3.FSA_1_001

GIINTLQKYYCRVRGGRCVLSCLPKKEQIGKCSTRGRKCCRRKKEAAAKTPVGRGLVTVAAYFLAVGGVLLAAYVLLFLS
VNVAAYFSITPSAPSYTLGPGPGFSITPSAPSKKSITPSAPSYTLKLGEKKVTIMSKDKPTIDVKMKKKMEKLQLKGT
GVC

Epitopes of protein 0 -----

0]	pos=	9	score=0.024348	unnormalised=3.2015600000	YCRVRGGRC
1]	pos=	52	score=0.005062	unnormalised=0.6655600000	VGRLVTVAA
2]	pos=	55	score=0.065650	unnormalised=8.6325600000	LVTVAAYFL
3]	pos=	61	score=0.014530	unnormalised=1.9105600000	YFLAVGGVL
4]	pos=	62	score=0.092047	unnormalised=12.1035600000	FLAVGGVLL
5]	pos=	74	score=0.000179	unnormalised=0.0235600000	VLLFLSVNV
6]	pos=	76	score=0.013047	unnormalised=1.7155600000	LFLSVNVAA
7]	pos=	85	score=0.038318	unnormalised=5.0385600000	YFSITPSAP
8]	pos=	86	score=0.079788	unnormalised=10.4915600000	FSITPSAPS
9]	pos=	88	score=0.036721	unnormalised=4.8285600000	ITPSAPSYT
10]	pos=	95	score=0.010598	unnormalised=1.3935600000	YTLGPGPGF
11]	pos=	103	score=0.079788	unnormalised=10.4915600000	FSITPSAPS
12]	pos=	115	score=0.036721	unnormalised=4.8285600000	ITPSAPSYT
13]	pos=	-1	score=0.503204	unnormalised=66.1680000000	non-binding event