C-IMMSIM simulation results

May 21, 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
tt 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.2022.998262i`

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)

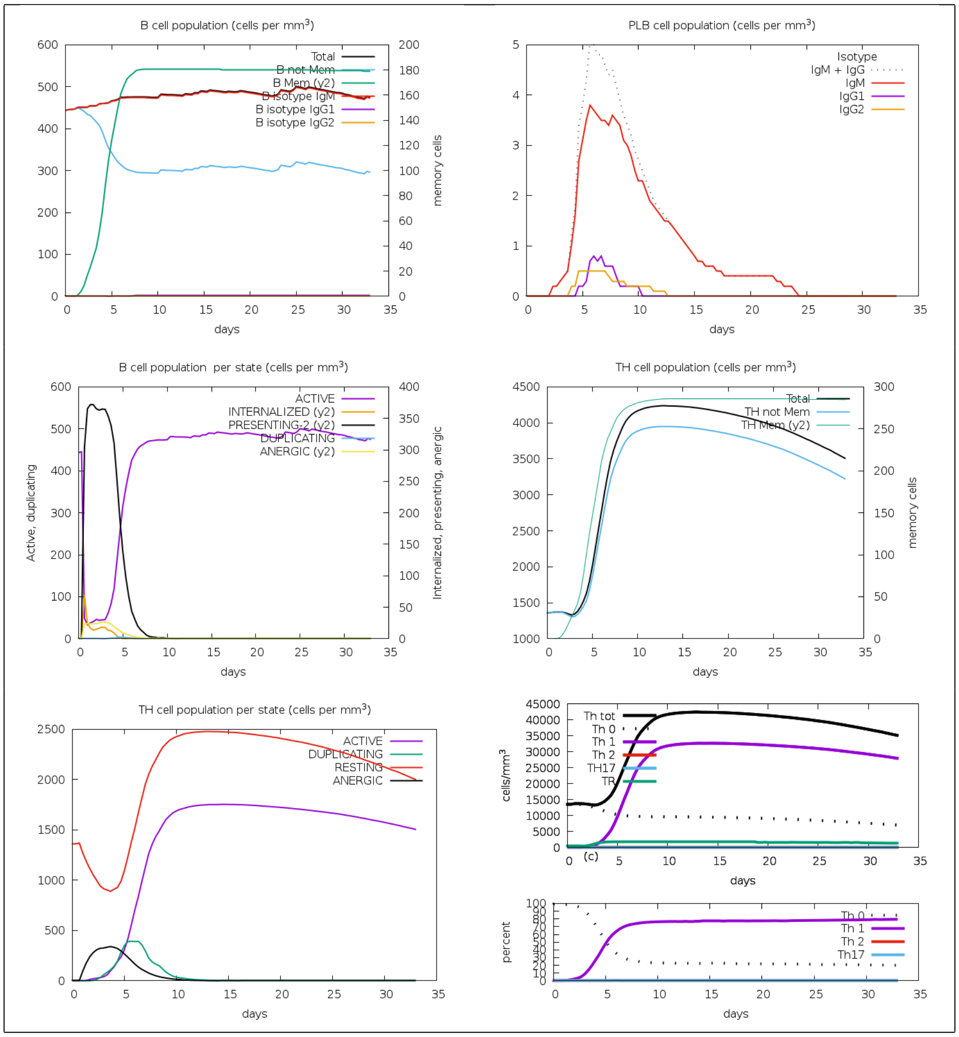

Figure 1: Cell counts shown. Legend: Act=active, Intern=internalized the Ag, Pres II = presenting on MHC II, Dup = in the mitotic cycle, Anergic = anergic, Resting = not active.

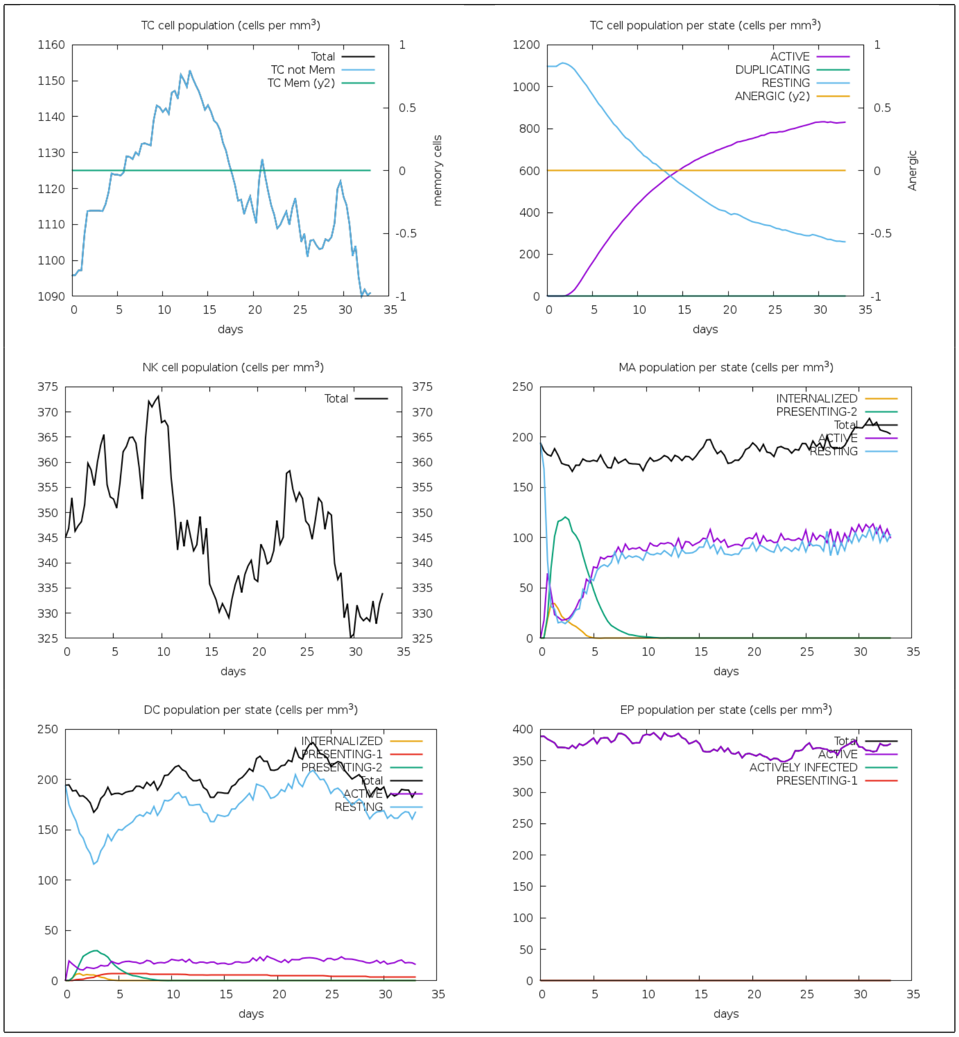

Figure 2: Legend: symbols as figure above.

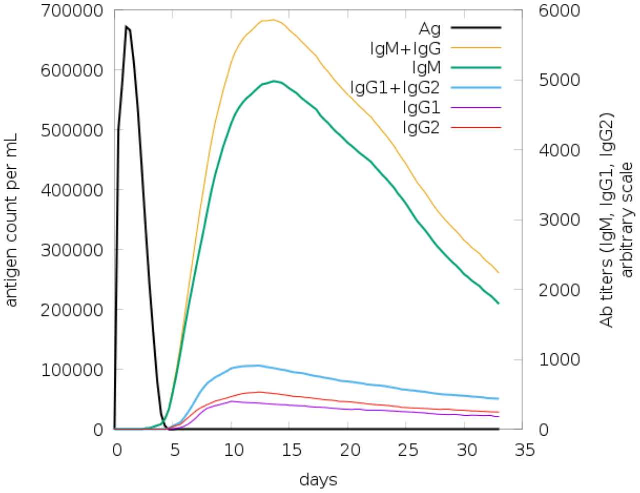

Figure 3: The virus, the immunoglobulins and the immunocomplexes.

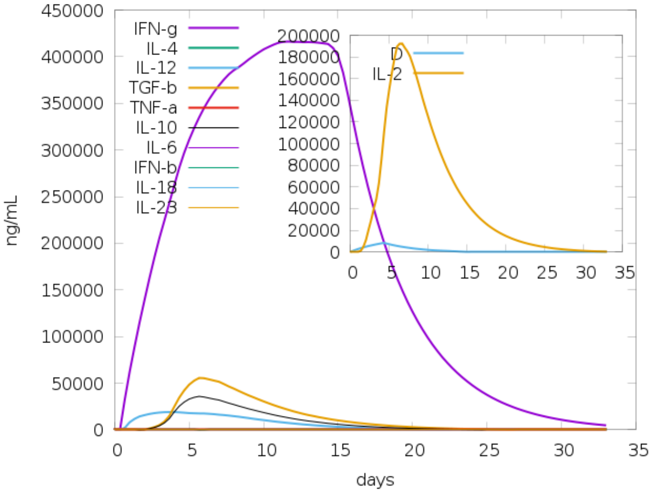

Figure 4: Concentration of cytokines and interleukins. Inset plot shows danger signal together with leukocyte growth factor IL-2.

```
Parker_B_scale_epitope_find
Use Parker’s propensity scale, takes an antigen block as input,
and creates a list of residues that are possible epitopes.


----------------------------------
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/50712_20260521-164125_5_z3nbfLoryBAr.FSA_1_001
----------------------------------


MAKLSTDELLDAFKEMTLLELSDFVKKFEETFEVTAAAPVAVAAAGAAPAAAAPAAEEAAEEAAEEDDIDLMVVGVEVPA
ARAVVNKVDELDGKTAAKIGAILTAAMAKTEAAKPVVEAAGAEEAARKLEDRVNSDILEEAAAKVAAQKLASKPVDPTGL
EPDDHLKEKSALRYGNVLAQSTMKADEITPGRFRMASKSVGTAEEKFHLGDDMDPELRCPGPGKPKHLYVSMRAYFINRQ
KGVIGFGFFVFVIPIVLKAMLFWGKEAVTLQSRRAAVTNRAYFINRGLFPAQIKAAAYRQTVKENKGTRIRFKIPIVLKA
LYMLSTRGKEKSALRYGNVLDVNSFMGTNRAYFINRQKRQTVKENKGTRIRFKDMRNTIMASKSVGTALKRQLADLVAAQ
KLAHHHHHH

00001000000000000000000000000000000000000000000000000000111111111110000000000000
00000000111110100000000000000011000000001111100000001100000000000000000000110000
11011110000000000000001100001000000000111110000000001100000010110000000000000000
00000000000000000000000000000000000000000000000000000000000001111110000000000000
00000011110000000000000000000000000011111111111000000000000000011000000000000000
000000000
Epitopes of protein 0 ------------
1]        pos=57 len=11        EAAEEAAEEDD
2]        pos=88 len=5        DELDG
3]        pos=120 len=5        GAEEA
4]        pos=163 len=4        DHLK
5]        pos=198 len=5        SVGTA
6]        pos=301 len=6        VKENKG
7]        pos=326 len=4        RGKE
8]        pos=356 len=11        QKRQTVKENKG
```

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

        Read class I peptide list from file? NO

=========================================================================

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


----------------------------------
Antigen sequence file: /opt/lampp/htdocs/C-IMMSIM/Jobs/input/50712_20260521-164125_5_z3nbfLoryBAr.FSA_1_001
----------------------------------

MAKLSTDELLDAFKEMTLLELSDFVKKFEETFEVTAAAPVAVAAAGAAPAAAAPAAEEAAEEAAEEDDIDLMVVGVEVPA
ARAVVNKVDELDGKTAAKIGAILTAAMAKTEAAKPVVEAAGAEEAARKLEDRVNSDILEEAAAKVAAQKLASKPVDPTGL
EPDDHLKEKSALRYGNVLAQSTMKADEITPGRFRMASKSVGTAEEKFHLGDDMDPELRCPGPGKPKHLYVSMRAYFINRQ
KGVIGFGFFVFVIPIVLKAMLFWGKEAVTLQSRRAAVTNRAYFINRGLFPAQIKAAAYRQTVKENKGTRIRFKIPIVLKA
LYMLSTRGKEKSALRYGNVLDVNSFMGTNRAYFINRQKRQTVKENKGTRIRFKDMRNTIMASKSVGTALKRQLADLVAAQ
KLAHHHHHH
```

```
Epitopes of protein 0 ------------
0]        pos=   4 score=0.046437 unnormalised=5.1056000000        STDELLDAF
1]        pos=  -1 score=0.953563 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_20260521-164125_5_z3nbfLoryBAr.FSA_1_001
----------------------------------

MAKLSTDELLDAFKEMTLLELSDFVKKFEETFEVTAAAPVAVAAAGAAPAAAAPAAEEAAEEAAEEDDIDLMVVGVEVPA
ARAVVNKVDELDGKTAAKIGAILTAAMAKTEAAKPVVEAAGAEEAARKLEDRVNSDILEEAAAKVAAQKLASKPVDPTGL
EPDDHLKEKSALRYGNVLAQSTMKADEITPGRFRMASKSVGTAEEKFHLGDDMDPELRCPGPGKPKHLYVSMRAYFINRQ
KGVIGFGFFVFVIPIVLKAMLFWGKEAVTLQSRRAAVTNRAYFINRGLFPAQIKAAAYRQTVKENKGTRIRFKIPIVLKA
LYMLSTRGKEKSALRYGNVLDVNSFMGTNRAYFINRQKRQTVKENKGTRIRFKDMRNTIMASKSVGTALKRQLADLVAAQ
KLAHHHHHH

Epitopes of protein 0 ------------
0]        pos=   4 score=0.046437 unnormalised=5.1056000000        STDELLDAF
1]        pos=  -1 score=0.953563 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_20260521-164125_5_z3nbfLoryBAr.FSA_1_001
----------------------------------

MAKLSTDELLDAFKEMTLLELSDFVKKFEETFEVTAAAPVAVAAAGAAPAAAAPAAEEAAEEAAEEDDIDLMVVGVEVPA
ARAVVNKVDELDGKTAAKIGAILTAAMAKTEAAKPVVEAAGAEEAARKLEDRVNSDILEEAAAKVAAQKLASKPVDPTGL
EPDDHLKEKSALRYGNVLAQSTMKADEITPGRFRMASKSVGTAEEKFHLGDDMDPELRCPGPGKPKHLYVSMRAYFINRQ
KGVIGFGFFVFVIPIVLKAMLFWGKEAVTLQSRRAAVTNRAYFINRGLFPAQIKAAAYRQTVKENKGTRIRFKIPIVLKA
LYMLSTRGKEKSALRYGNVLDVNSFMGTNRAYFINRQKRQTVKENKGTRIRFKDMRNTIMASKSVGTALKRQLADLVAAQ
KLAHHHHHH

Epitopes of protein 0 ------------
0]        pos=  47 score=0.063183 unnormalised=7.6042000000        APAAAAPAA
1]        pos= 223 score=0.020591 unnormalised=2.4782000000        KPKHLYVSM
2]        pos= 252 score=0.005510 unnormalised=0.6632000000        IPIVLKAML
3]        pos= 288 score=0.039602 unnormalised=4.7662000000        FPAQIKAAA
4]        pos=  -1 score=0.871114 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_20260521-164125_5_z3nbfLoryBAr.FSA_1_001
----------------------------------
```

```
MAKLSTDELLDAFKEMTLLELSDFVKKFEETFEVTAAAPVAVAAAGAAPAAAAPAAEEAAEEAAEEDDIDLMVVGVEVPA
ARAVVNKVDELDGKTAAKIGAILTAAMAKTEAAKPVVEAAGAEEAARKLEDRVNSDILEEAAAKVAAQKLASKPVDPTGL
EPDDHLKEKSALRYGNVLAQSTMKADEITPGRFRMASKSVGTAEEKFHLGDDMDPELRCPGPGKPKHLYVSMRAYFINRQ
KGVIGFGFFVFVIPIVLKAMLFWGKEAVTLQSRRAAVTNRAYFINRGLFPAQIKAAAYRQTVKENKGTRIRFKIPIVLKA
LYMLSTRGKEKSALRYGNVLDVNSFMGTNRAYFINRQKRQTVKENKGTRIRFKDMRNTIMASKSVGTALKRQLADLVAAQ
KLAHHHHHH

Epitopes of protein 0 ------------
0]        pos=  47 score=0.063183 unnormalised=7.6042000000        APAAAAPAA
1]        pos= 223 score=0.020591 unnormalised=2.4782000000        KPKHLYVSM
2]        pos= 252 score=0.005510 unnormalised=0.6632000000        IPIVLKAML
3]        pos= 288 score=0.039602 unnormalised=4.7662000000        FPAQIKAAA
4]        pos=  -1 score=0.871114 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_20260521-164125_5_z3nbfLoryBAr.FSA_1_001
----------------------------------

MAKLSTDELLDAFKEMTLLELSDFVKKFEETFEVTAAAPVAVAAAGAAPAAAAPAAEEAAEEAAEEDDIDLMVVGVEVPA
ARAVVNKVDELDGKTAAKIGAILTAAMAKTEAAKPVVEAAGAEEAARKLEDRVNSDILEEAAAKVAAQKLASKPVDPTGL
EPDDHLKEKSALRYGNVLAQSTMKADEITPGRFRMASKSVGTAEEKFHLGDDMDPELRCPGPGKPKHLYVSMRAYFINRQ
KGVIGFGFFVFVIPIVLKAMLFWGKEAVTLQSRRAAVTNRAYFINRGLFPAQIKAAAYRQTVKENKGTRIRFKIPIVLKA
LYMLSTRGKEKSALRYGNVLDVNSFMGTNRAYFINRQKRQTVKENKGTRIRFKDMRNTIMASKSVGTALKRQLADLVAAQ
KLAHHHHHH

Epitopes of protein 0 ------------
0]        pos=  12 score=0.005569 unnormalised=0.8815600000        FKEMTLLEL
1]        pos=  31 score=0.050380 unnormalised=7.9755600000        FEVTAAAPV
2]        pos=  33 score=0.049533 unnormalised=7.8415600000        VTAAAPVAV
3]        pos=  39 score=0.001330 unnormalised=0.2105600000        VAVAAAGAA
4]        pos=  41 score=0.031183 unnormalised=4.9365600000        VAAAGAAPA
5]        pos=  75 score=0.001153 unnormalised=0.1825600000        VEVPAARAV
6]        pos=  98 score=0.019251 unnormalised=3.0475600000        IGAILTAAM
7]        pos= 136 score=0.013881 unnormalised=2.1975600000        ILEEAAAKV
8]        pos= 173 score=0.046034 unnormalised=7.2875600000        YGNVLAQST
9]        pos= 176 score=0.017362 unnormalised=2.7485600000        VLAQSTMKA
10]        pos= 228 score=0.107041 unnormalised=16.9455600000        YVSMRAYFI
11]        pos= 236 score=0.021076 unnormalised=3.3365600000        INRQKGVIG
12]        pos= 248 score=0.027121 unnormalised=4.2935600000        FVFVIPIVL
13]        pos= 261 score=0.000698 unnormalised=0.1105600000        FWGKEAVTL
14]        pos= 269 score=0.014936 unnormalised=2.3645600000        LQSRRAAVT
15]        pos= 292 score=0.002574 unnormalised=0.4075600000        IKAAAYRQT
16]        pos= 301 score=0.002972 unnormalised=0.4705600000        VKENKGTRI
17]        pos= 317 score=0.023079 unnormalised=3.6535600000        LKALYMLST
18]        pos= 345 score=0.018297 unnormalised=2.8965600000        MGTNRAYFI
19]        pos= 361 score=0.002972 unnormalised=0.4705600000        VKENKGTRI
```

```
20]        pos= 371 score=0.051068 unnormalised=8.0845600000        FKDMRNTIM
21]        pos= 378 score=0.031676 unnormalised=5.0145600000        IMASKSVGT
22]        pos= 388 score=0.042844 unnormalised=6.7825600000        LKRQLADLV
23]        pos=  -1 score=0.417968 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_20260521-164125_5_z3nbfLoryBAr.FSA_1_001
----------------------------------

MAKLSTDELLDAFKEMTLLELSDFVKKFEETFEVTAAAPVAVAAAGAAPAAAAPAAEEAAEEAAEEDDIDLMVVGVEVPA
ARAVVNKVDELDGKTAAKIGAILTAAMAKTEAAKPVVEAAGAEEAARKLEDRVNSDILEEAAAKVAAQKLASKPVDPTGL
EPDDHLKEKSALRYGNVLAQSTMKADEITPGRFRMASKSVGTAEEKFHLGDDMDPELRCPGPGKPKHLYVSMRAYFINRQ
KGVIGFGFFVFVIPIVLKAMLFWGKEAVTLQSRRAAVTNRAYFINRGLFPAQIKAAAYRQTVKENKGTRIRFKIPIVLKA
LYMLSTRGKEKSALRYGNVLDVNSFMGTNRAYFINRQKRQTVKENKGTRIRFKDMRNTIMASKSVGTALKRQLADLVAAQ
KLAHHHHHH

Epitopes of protein 0 ------------
0]        pos=  12 score=0.005569 unnormalised=0.8815600000        FKEMTLLEL
1]        pos=  31 score=0.050380 unnormalised=7.9755600000        FEVTAAAPV
2]        pos=  33 score=0.049533 unnormalised=7.8415600000        VTAAAPVAV
3]        pos=  39 score=0.001330 unnormalised=0.2105600000        VAVAAAGAA
4]        pos=  41 score=0.031183 unnormalised=4.9365600000        VAAAGAAPA
5]        pos=  75 score=0.001153 unnormalised=0.1825600000        VEVPAARAV
6]        pos=  98 score=0.019251 unnormalised=3.0475600000        IGAILTAAM
7]        pos= 136 score=0.013881 unnormalised=2.1975600000        ILEEAAAKV
8]        pos= 173 score=0.046034 unnormalised=7.2875600000        YGNVLAQST
9]        pos= 176 score=0.017362 unnormalised=2.7485600000        VLAQSTMKA
10]        pos= 228 score=0.107041 unnormalised=16.9455600000        YVSMRAYFI
11]        pos= 236 score=0.021076 unnormalised=3.3365600000        INRQKGVIG
12]        pos= 248 score=0.027121 unnormalised=4.2935600000        FVFVIPIVL
13]        pos= 261 score=0.000698 unnormalised=0.1105600000        FWGKEAVTL
14]        pos= 269 score=0.014936 unnormalised=2.3645600000        LQSRRAAVT
15]        pos= 292 score=0.002574 unnormalised=0.4075600000        IKAAAYRQT
16]        pos= 301 score=0.002972 unnormalised=0.4705600000        VKENKGTRI
17]        pos= 317 score=0.023079 unnormalised=3.6535600000        LKALYMLST
18]        pos= 345 score=0.018297 unnormalised=2.8965600000        MGTNRAYFI
19]        pos= 361 score=0.002972 unnormalised=0.4705600000        VKENKGTRI
20]        pos= 371 score=0.051068 unnormalised=8.0845600000        FKDMRNTIM
21]        pos= 378 score=0.031676 unnormalised=5.0145600000        IMASKSVGT
22]        pos= 388 score=0.042844 unnormalised=6.7825600000        LKRQLADLV
23]        pos=  -1 score=0.417968 unnormalised=66.1680000000        non-binding event
```
