

n	Start Position	Sequence	End Position
1	4	PDPSKYAAEVSTLL	17
2	26	PYNKLLP	32
3	39	LITGCVATATAQVLNYFKYPVRG	61
4	63	GSHTVHYPA	71
5	105	EANAVATLMLHCGVAS	120
6	134	YMTDCAAGLRT	144
7	174	KGHPLIYGGVSP	185
8	192	AGHAFVID	199
9	203	KAGLVSV	209
10	217	VDGYKIDL	225
11	240	MVRGVYG	246


Contact **Pedro Reche**
Last Update: 19 August 2022

Figure S1: Antigenic Peptides determinants.

AllergenFP v.1.0

Bioinformatics tool for allergenicity prediction

MISKIL...AVVADQVD...
VMVD...JHRC...
QNTK...EDGL...
MKCPLVKGQYD...
VTVKLIGDNGV...
1000100011011...
0010010001010...
00100110100100...
100100010001100...



Your sequence is:

PROBABLE NON-ALLERGEN

The protein with the highest Tanimoto similarity index 0.8 is:

[UniProtKB accession number O75976](#)

Figure S2. Prediction of Allergenicity.

VaxiJen RESULTS

Model selected: bacteria

Threshold for this model: 0.4

Your Sequence:

```
VIKPDPSKYAAEVSTLLTTTWGQQMPYNKLL  
PKTKKGRLITGCVATATAQVLNYFKYPVRGI  
GSHTVHYPANDPSGTAISADFGNTTYDWANM  
KDNYSGNYTEAEANAVATLMLHCGVASEMQY  
GGPNEGSGAYMTDCAAGLRITYFGFTDAEYIT  
RANYTDEQWMDIVFSELTKGHPLIYGGVSPG  
SMGQDAGHAFVIDGYNKAGLVSVNWGWNGDV  
DGYYKIDLLNPGNMYSFTAQDMVRGVYGKP  
LED
```

Overall Prediction for the Protective Antigen = **0.4690** (Probable **ANTIGEN**).

Figure S3. Antigenicity Prediction.

Cluster	Members	Representative	Weighted Score
0	99	Center	-596.9
		Lowest Energy	-661.2
1	74	Center	-566.8
		Lowest Energy	-645.4
2	57	Center	-580.6
		Lowest Energy	-617.8
3	56	Center	-623.1
		Lowest Energy	-651.1
4	52	Center	-542.0
		Lowest Energy	-639.3
5	46	Center	-632.9
		Lowest Energy	-632.9
6	46	Center	-592.0
		Lowest Energy	-611.0
7	35	Center	-612.6
		Lowest Energy	-612.6
8	32	Center	-542.5
		Lowest Energy	-634.2
9	31	Center	-622.1
		Lowest Energy	-622.1
10	31	Center	-594.8
		Lowest Energy	-594.8

Figure S4: Binding energy of the Predicted vaccine structure with C3.

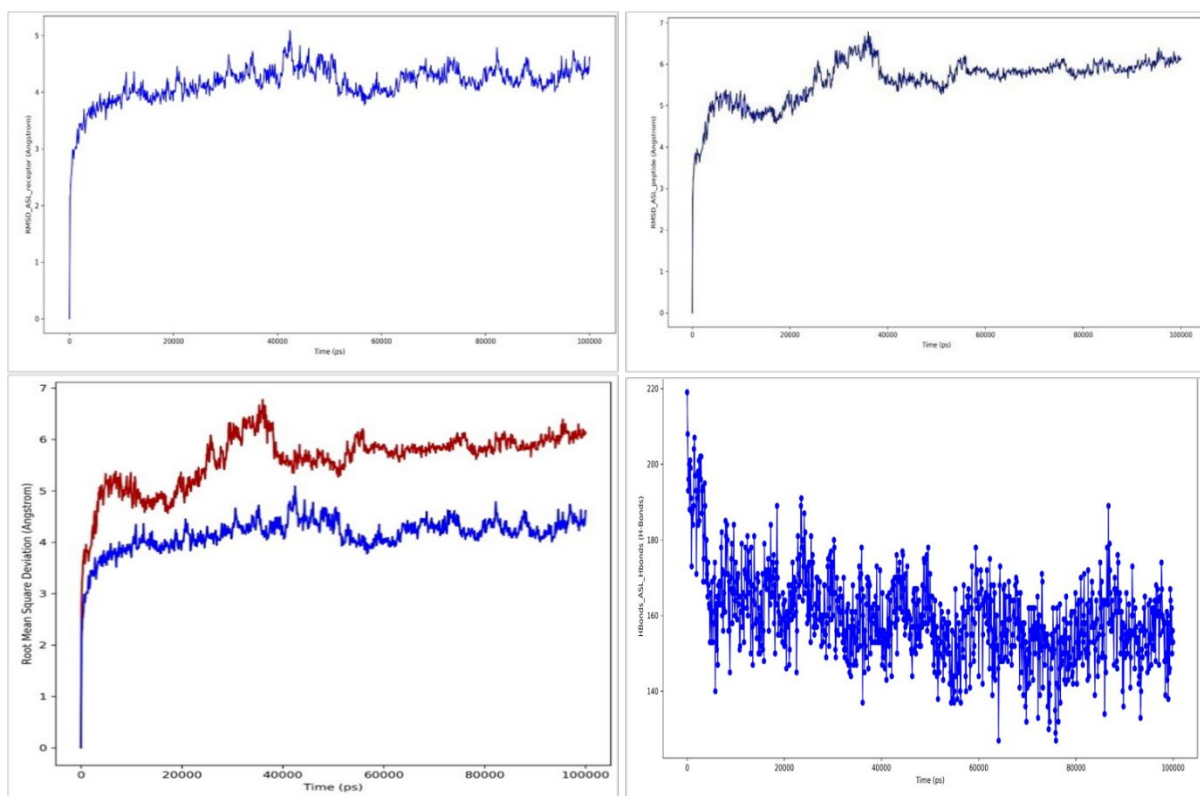


Figure S5: Molecular dynamic simulation analysis.

Table S1: CTL epitopes for N protein (NetCTL1.2).

S. No	Peptide
1.	YAAEVSTLL
2.	TTWGQQMPY
3.	TATAQVLNY
4.	ATAQVLNYF
5.	GIGSHTVHY
6.	SADFGNTTY
7.	MKDNYSGNY
8.	YTEAEANAV
9.	MTDCAAGLR
10.	FTDAEYITR
11.	YTDEQWMDI
12.	WMDIVFSEL
13.	LTKGHPLIY
14.	WNGDVDGYY
15.	EQDMVRGVY