Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Theoretical and experimental analysis in search of new immunogenic peptides from gp120 protein of HIV-1.

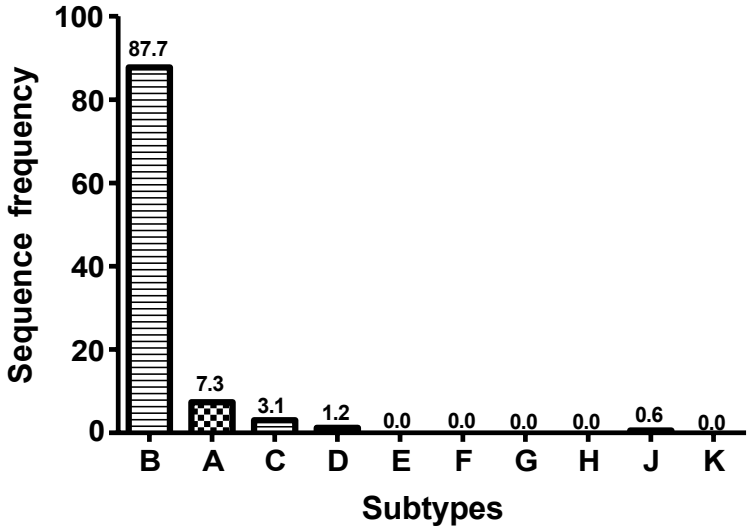

Figure S1. Frequency of sequences obtained by each subtype of HIV-1 found at NCBI in 2015.

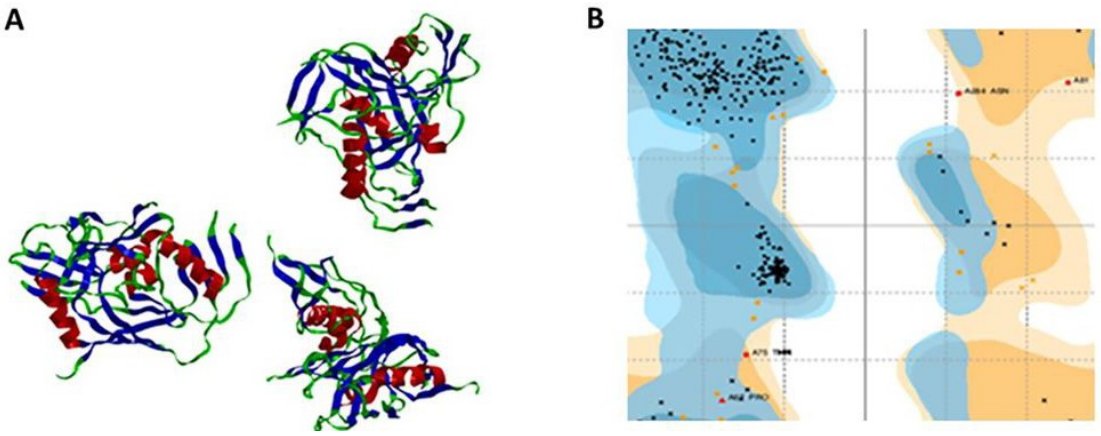

Figure S2. A. 3D structure of the HIV-1 gp120 trimer. **B.** Ramachandran's plot of gp120 protein.

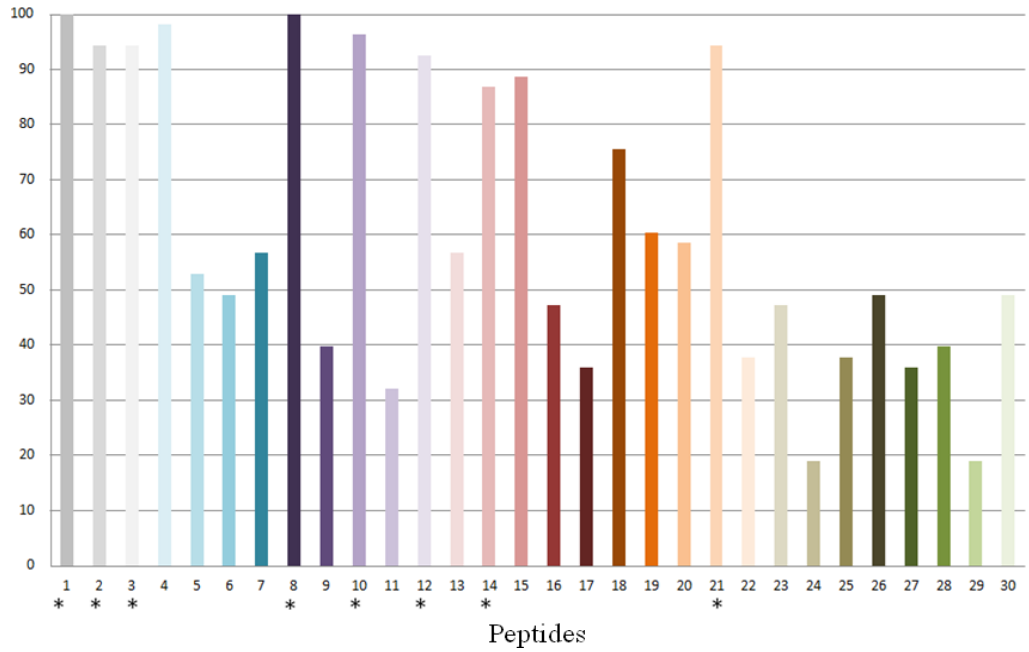

Figure S3. Frequency of the epitopes in the different alleles of the CMH-II predicted by the *ProPred* server. * Asterisks in the graph indicate the peptides that by their structure and the score obtained in the servers are potential candidates for their synthesis.

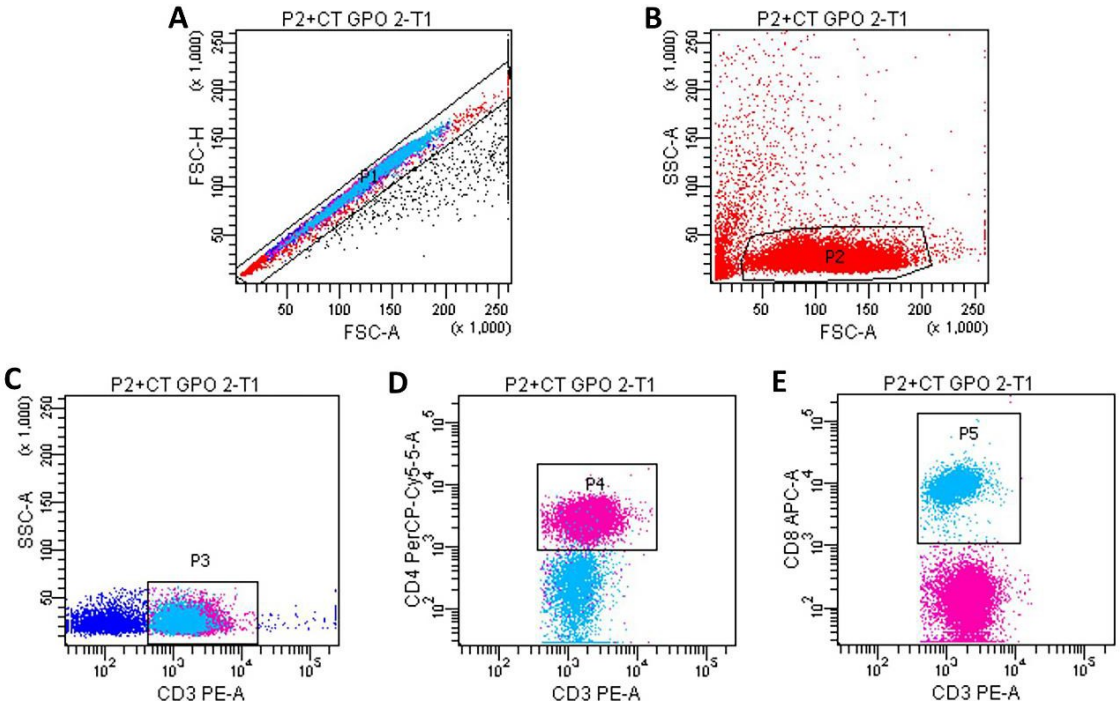

Figure S4. Flow Cytometry Dot-Plots. Representative Dot-Plots for selection criteria of cell populations for the P2+CT from IN group, cells were gated based on size and granularity using FSC-A and SSC-A. Dot-Plots: A: FSC-A and FSC-H; B: FSC-A and SSC-A; C: CD3 and SSCA; D: CD3 and CD4; E: CD3 and CD8. Programs to determinate lymphocyte region; the same procedure was applied to all mice groups.

Table S1. Proteasomal cleavages predicted by the *PaPROC* server

Peptide	**Proteasomal cleavages Type-I**
P31	MTLTVQA|RQLL|SGI|V|QQ|Q|S|NL|L|RAIEA|Q|Q|H|MLQL|T|VWGI|KQL|QA|RVLALERYL|KDQQ
P32	FNVTTNM | RDKV | QG | A | YAL | F | Y | K |LD | VVPI
P37	LTVWGI | KQLQA
Peptide	**Proteasomal cleavages Type-II**
P31	MTLTVQ|A|RQLLSGIVQQ|QSNLL|RAIEAQQH|ML|QL|T|VWGI|KQL|QA|RVLALER|Y|L|KDQQ
P32	FNVTTNM | RDKVQGA | YAL | FY | K |LDVVPI
P37	LTVWGI | KQLQA
P40	MTLTVQ | ARQL
Peptide	**Proteasomal cleavages Type-II**
P31	MTLTVQ|A|RQL|LSGIVQQQSNL|L|RAIEAQQ|H|ML|QL|TV|WGI|KQL|QA|RVLAL|ER|Y|L|KDQQ
P32	FNVTTNM | RDKV | QGA | YAL | FY | K |L | D | VVPI
P37	LTVWGI | KQLQA
P40	MTLTVQ | ARQL

Table S2. Molecular, topological and chemical reactivity parameters calculated by the DFT method with a 6-311G** used to develop the QSAR models.

Peptides		**Descriptors**						
No.	**Secuencias**	***Hy***	***AMR***	***ALOGP***	***ICR***	***Qtot***	***EHOMO***	***I***
P2	FYKLDVVPI	7.776	285.854	3.308	3.968	17.844	-8.37	8.37
P6	IRPVVSTQL	7.576	204.841	-1.86	3.848	13.468	-9.07	9.07
P10	LGFLSAAGS	8.743	267.271	1.108	4.032	18.202	-8.57	8.57
P16	YKLDVVPID	16.755	277.179	-5.496	3.974	19.562	-7.8	7.8
P30	FNSTWTRND	11.574	254.704	-1.643	3.902	16.484	-9.4	9.4

E_{HOMO} = Energy of the HOMO orbital; ***Qtot*** = total absolute charge; ***AlogP*** = Ghose-Crippen octanol-water partition coefficient; ***AMR*** = Molar refractivity; ***ICR*** = radial centric information index; ***Hy*** = hydrophilic factor; ***I*** = Ionization potential.