

SUPPEMENTARY MATERIAL

| Peptide epitope | Sequence | Amino acids | mw (g/mol) | Predicted aqueous solubility | Net charge at pH 7.0 | Isoelectric point | Type | SVM Score | Prediction |
|-----------------|---------------|-------------|------------|------------------------------|----------------------|-------------------|------|-----------|------------|
| pPGT122 | DIIGDIRQAH | 10 | 1137.26 | Soluble | -0.9 | 5.1 | acid | -0.62 | Non-toxic |
| pVRC03 | DGGANNTSNETFR | 13 | 1382.37 | Soluble | -1 | 4.07 | acid | -1.05 | Non-toxic |

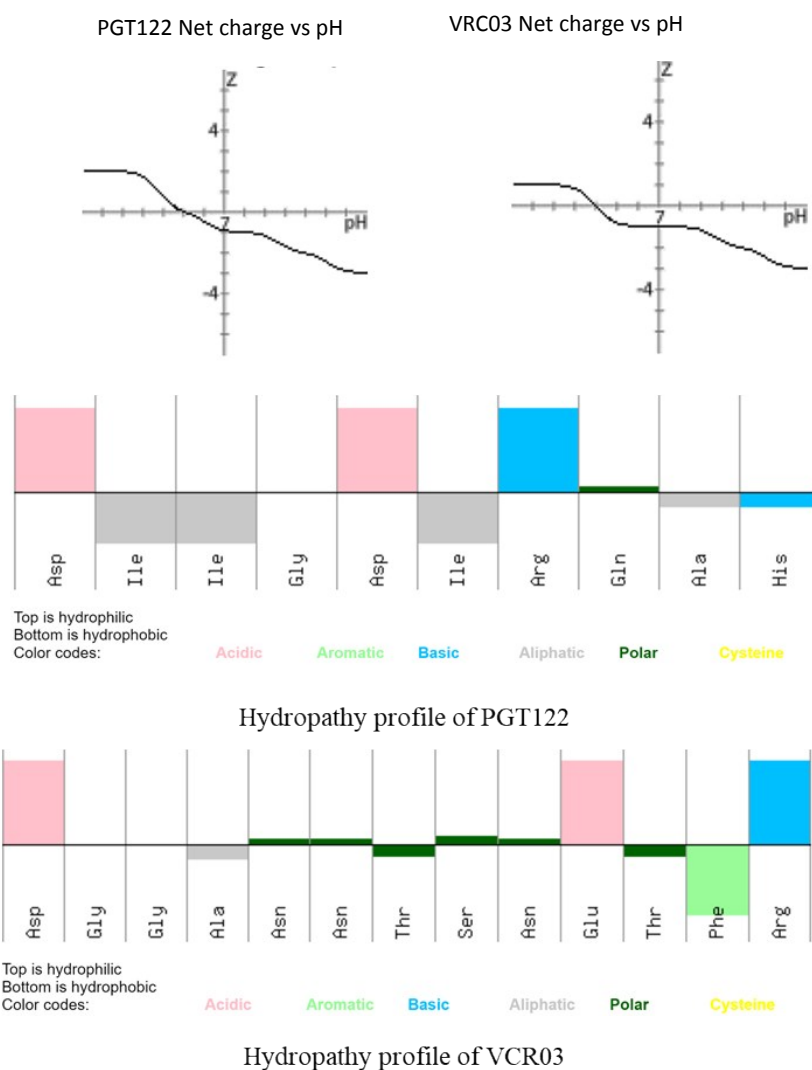


Figure 1S Physicochemical properties and toxicity of pPGT122 and pVRC03.

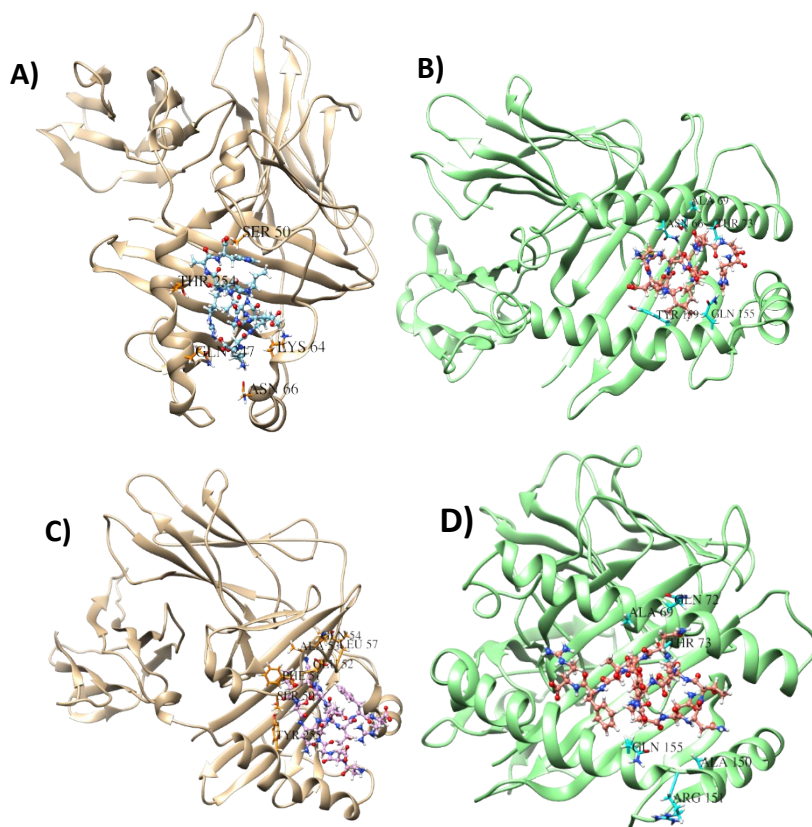


Figure 2S.- Docking studies of peptides on MHC I/II **A)** PGT122-MHC-II complex, **B)** pVRC03-MHC-II complex, **C)** pPGT122-MHC-I complex, and **D)** pVRC03-MHC-I complex at the end of the MD simulations.