Supplementary Information

Vaccine formulation and optimization for Human Herpes virus-5 through immunoinformatics framework

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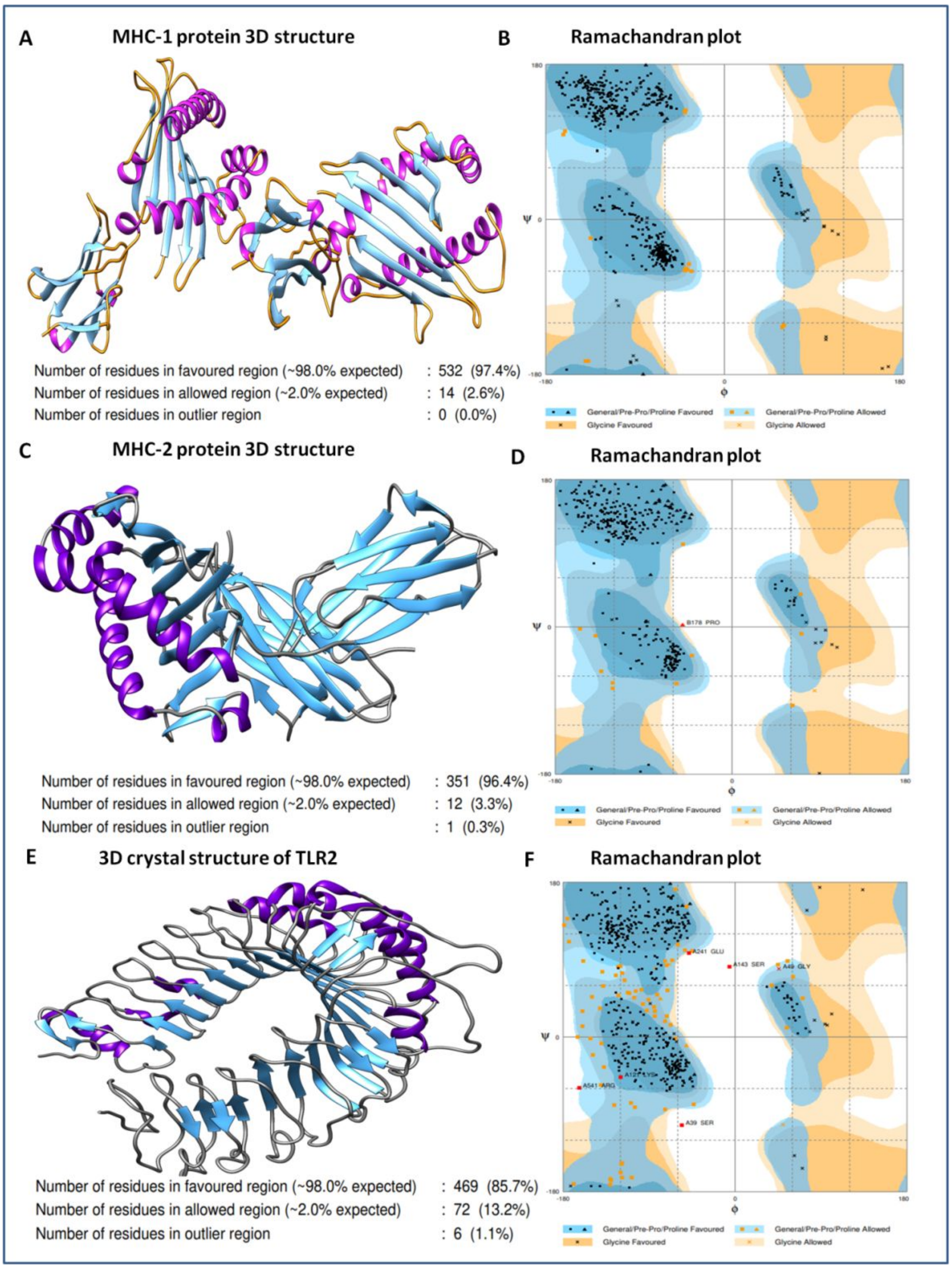
Protein sequence of multi epitope vaccine construct

EAAAKMTPQNITDLCAEYHNTQIYTLNDKIFSYTESLAGKREMAIITFKNGAIFQVEV
PGSQHIDSQKKAIERMKDTLRIAYLTEAKVEKLCVWNNKTPHAIAAISMANGTEAAA
KAAYNDIISDISGFNSSVITYPDAQLVPGINGKAIHLVNNEAAYIEYNDMFNNFTVSF
WLRVPKVSASHLEQYGTAAYLRVGYNAPGIPLYKKMEAVKLRDLKGPGPGSTVDS
MIALGPGPGKRNIVAHTFGPGPGNPSAILSAIGPGPGAAYNLFPYLVSAAAYYIYSTY
LLGAAYYEYVDYLFKAAYKKVGVAIGAVGGAVKKRKGPGPPSSDASKKKRSTNNT
TTLSLKKRVYQKVLTFHEYGAEALERAGKVVDPLPPYHEYGAEALERAGRLRHRKN
GYHEYGAEALERAG.

Relevant Linkers used for constriction of vaccine construct

CTL epitopes - AAY linker, HTLs, TTFrC - GPGPG linker, B-cell epitopes -KK linker, and CTB adjuvant -EAAAK linkers”.

Three- dimensional structure assessment of MHC-1, MHC-2 and TLR2



Number of residues in favoured region (~98.0% expected) : 532 (97.4%)
Number of residues in allowed region (~2.0% expected) : 14 (2.6%)
Number of residues in outlier region : 0 (0.0%)

Number of residues in favoured region (~98.0% expected) : 351 (96.4%)
Number of residues in allowed region (~2.0% expected) : 12 (3.3%)
Number of residues in outlier region : 1 (0.3%)

Number of residues in favoured region (~98.0% expected) : 469 (85.7%)
Number of residues in allowed region (~2.0% expected) : 72 (13.2%)
Number of residues in outlier region : 6 (1.1%)

Figure S1: **(A)** The 3D structure of MHC-1 **(B)** The Ramachandran plot of MHC-1 **(C)** The 3D structure of MHC-2 **(D)** The Ramachandran plot of MHC-2 **(E)** The 3D structure of TLR-2 receptor **(F)** The Ramachandran plot of TLR-2.

Molecular dynamics simulation analyses results for Secondary structure element analysis

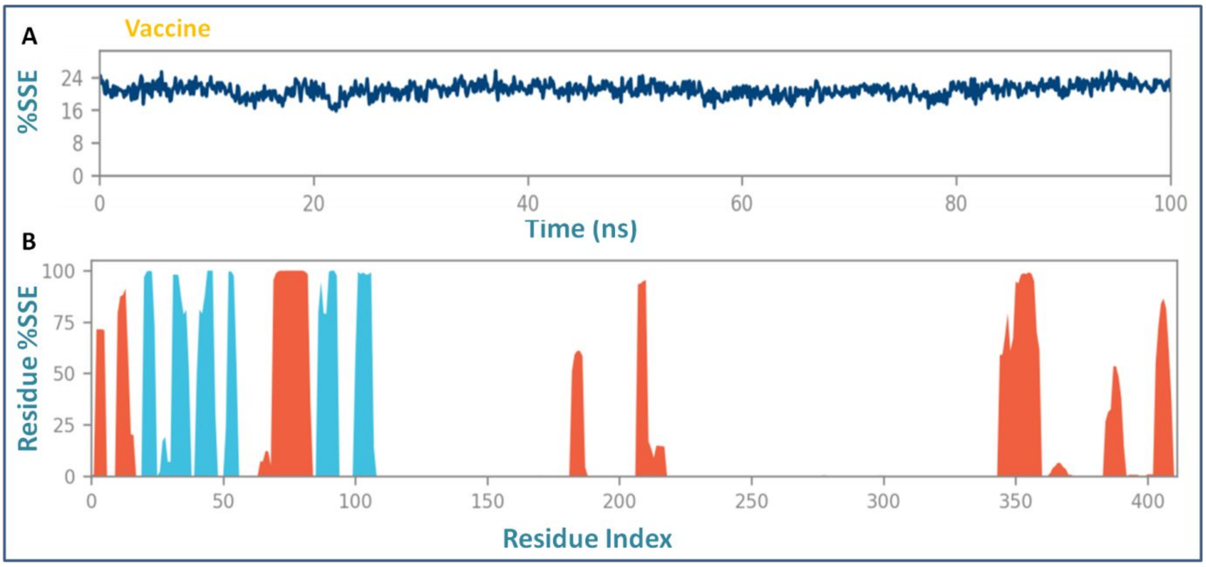


Figure S2: (A) Secondary structure element analysis of vaccine in singlet state **(B)** Residue content fluctuation plot of secondary structural elements of Vaccine.

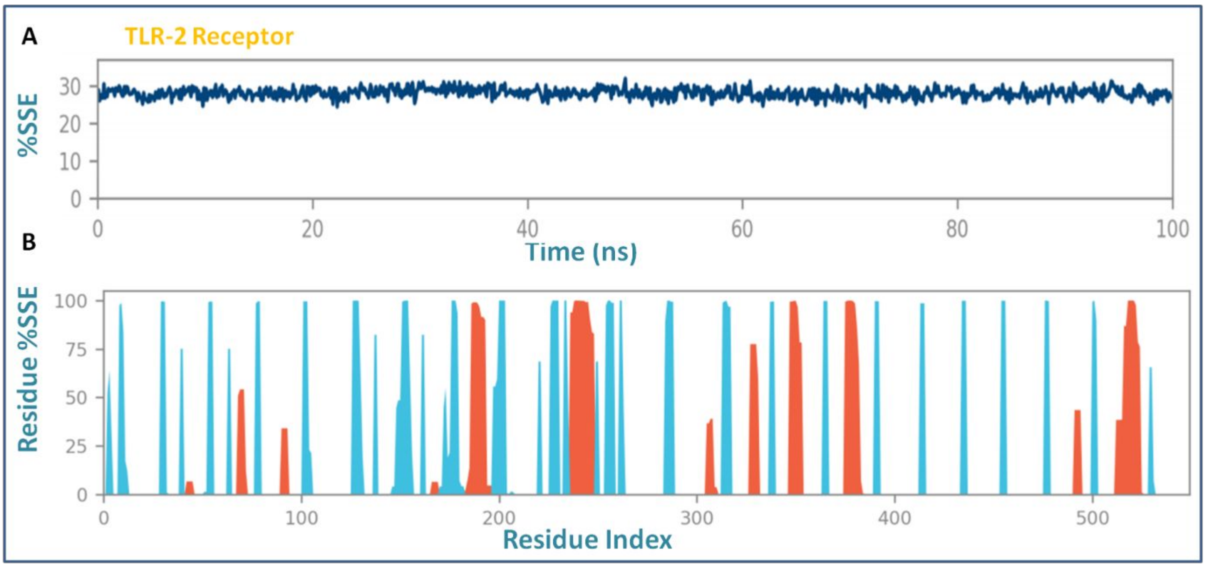


Figure S3: (A) Secondary structure element analysis of TLR2 receptor **(B)** Residue content fluctuation plot of secondary structural elements of TLR2 receptor.

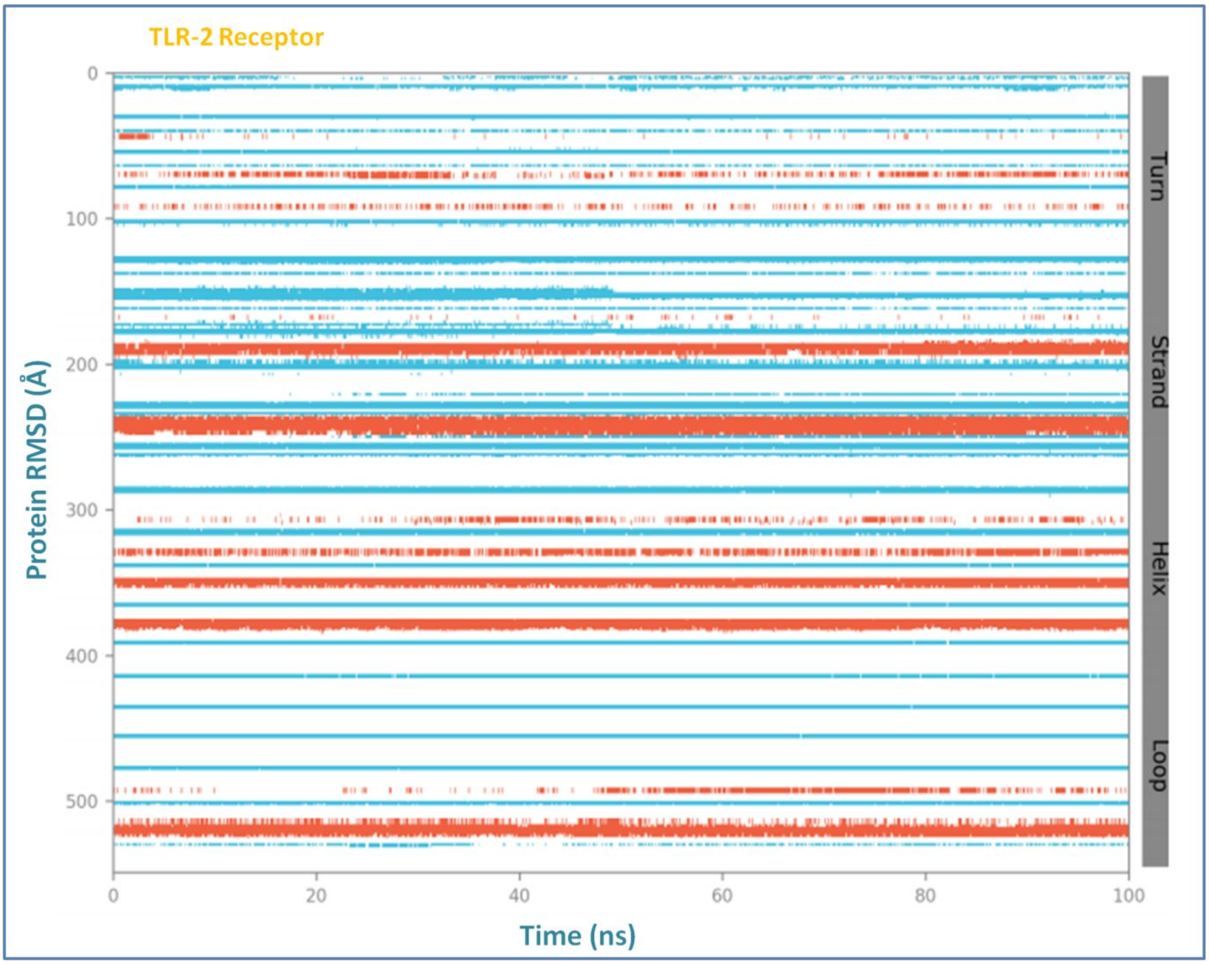


Figure S4: Residue content fluctuation of Secondary structure element analysis of TLR2 receptor for 100 ns molecular dynamics simulation run.

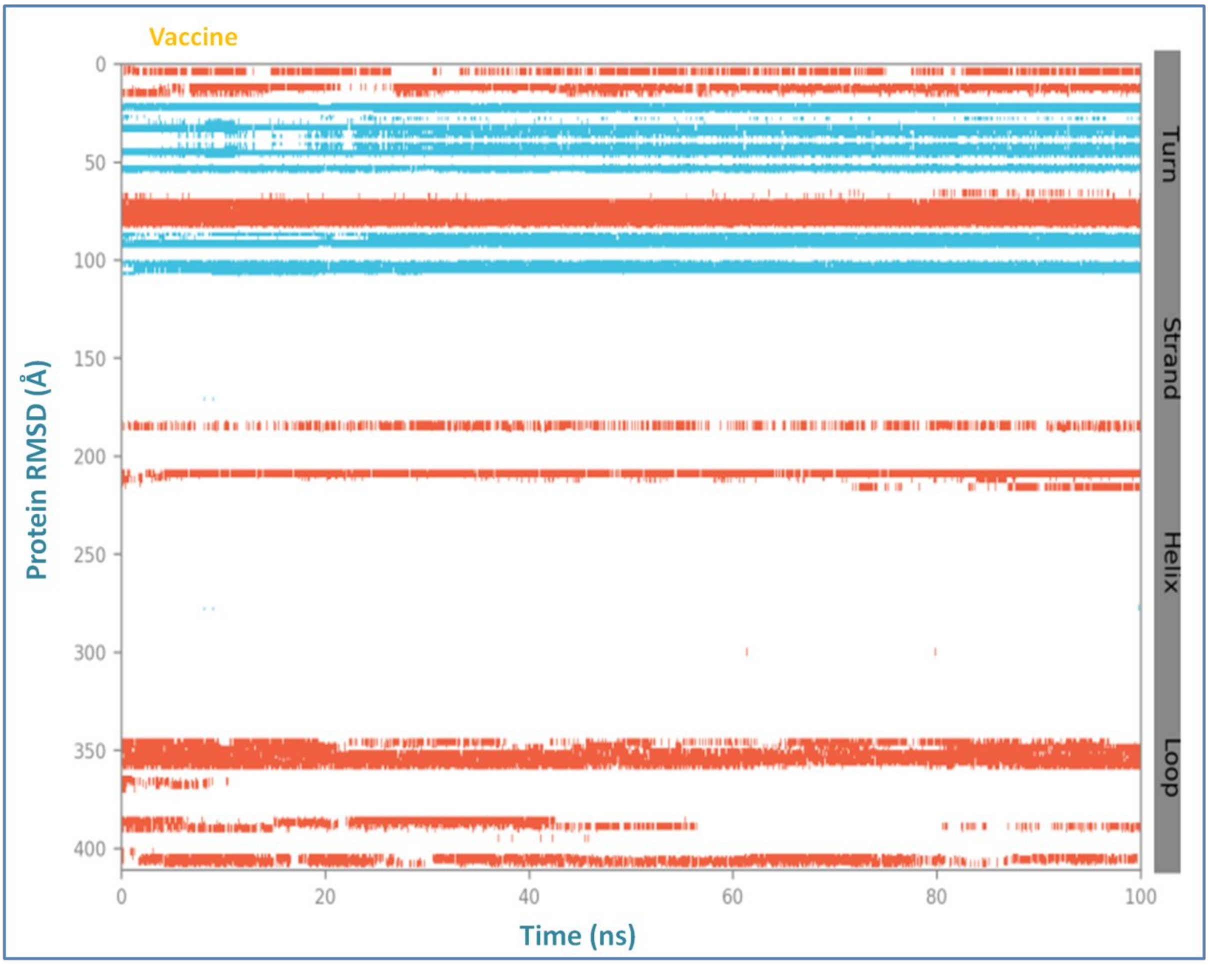


Figure S5: Residue content fluctuation of Secondary structure element analysis of vaccine construct for 100 ns molecular dynamics simulation run.

In silico immune response results for vaccine

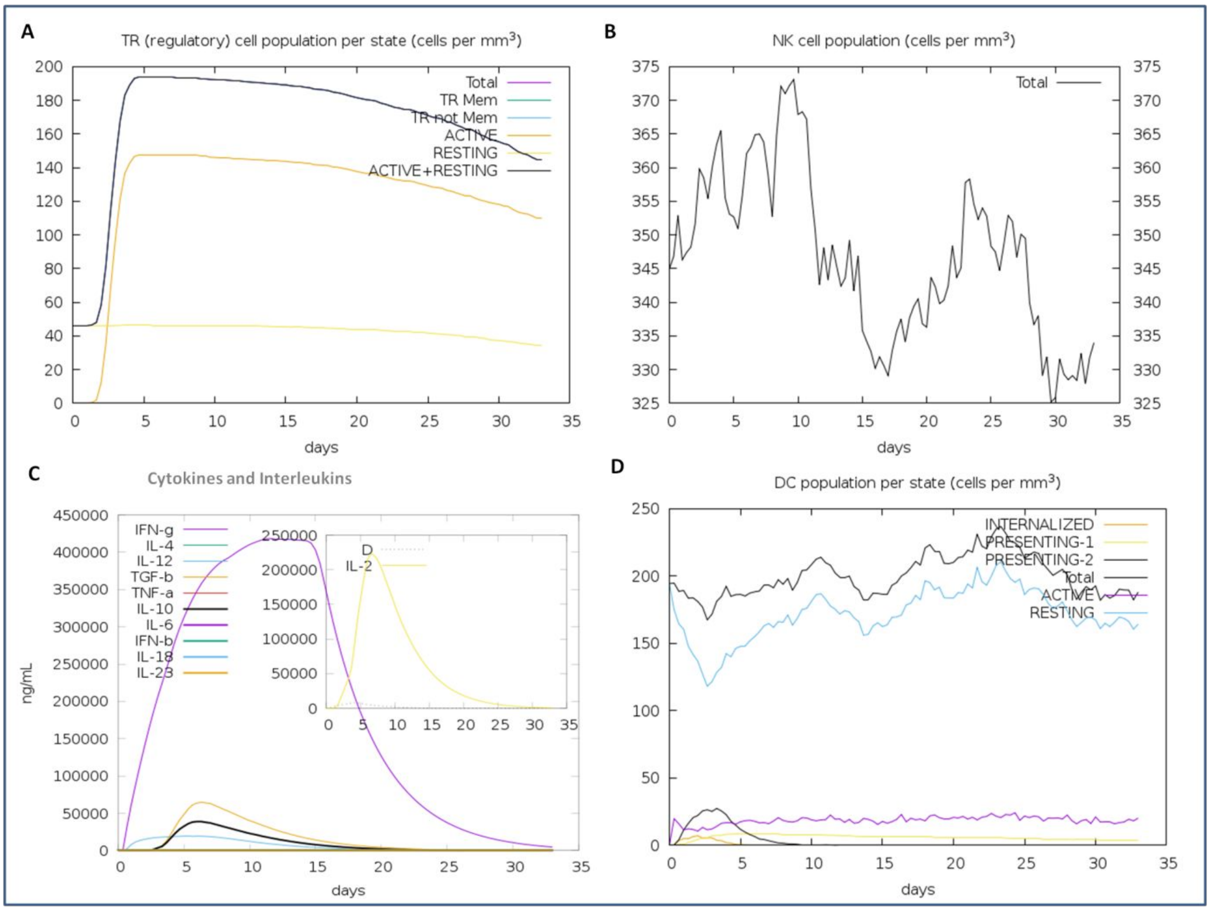


Figure S6: Predicted immune response **(A)** Elevation of regulatory T-cell populations at different concentration of antigen, resting and active state **(B)** Natural Killer cell count **(C)** Cytokines and dendritic cells populations **(D)** Dendritic cell population in response to vaccine.