

Supplementary Materials

Towards an ensemble vaccine against the Pegivirus using computational modelling approaches and its validation through *In silico* cloning and immune simulation

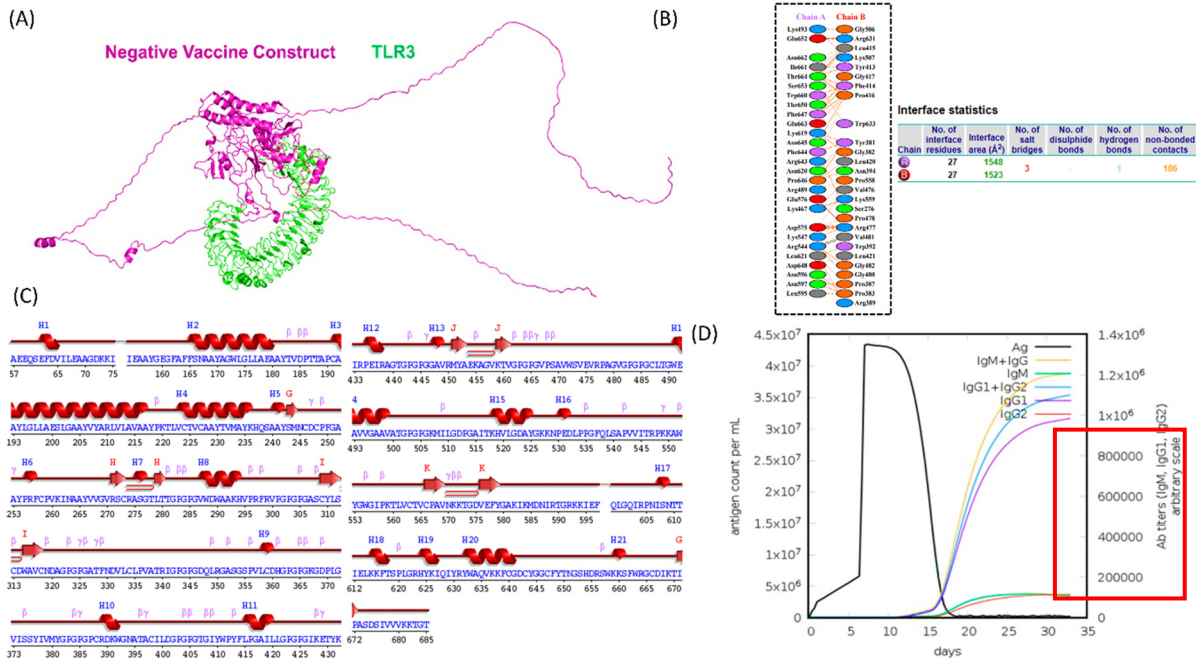


Figure S1: Molecular Docking, secondary structure and Immune simulation results for the negative vaccine construct. (A) show the docking results of the negative vaccine construct which reflects that though the vaccine interacts with correct binding site but most of the residues are modelled as loop region thus question the validity. (B) show the interaction pattern, (C) shows the secondary structural elements distribution while (D) display the antibodies titer production over the days.

>Negative Control Vaccine Sequence

MAKLSTDELLEDAFKEMTLLELSDFVKKFEETFEVTAAPVAVAAAGAAPAGAAVEAAEEQSEFDVI
LEAAGDKKIGVIVKVVREIVSGLGLKEAKDLVDGAPKPLLEKVAKEAADEAKAKLEAAGATVTVKE
AAKCSIRSKTEGAAAYRSKTEGRIEAAAYGEGFAFFSNAAYAGWLGLLAEAAAYTVDPTTAPCAAYLGL
LAESLGAAYVYARLVLAAYPKTLVCTVCAAYTMAYKHQSAAYSMNDCDPFGAAYPRFCPVK
INAAAYVVGVRSCASGTLTTGPGPGVWDWAAKHVPRFRVPGPGPGASCYLSCDWAVCNDAGPG
PGATFNDVLCLPVATRIGPGPGDQLRGASGSPVLCDHGPGPAGAVRMYAEKAGVKTGPGPGVPS
AVWSVEVRPAGVGPGPCLTGWEAVVGAATGPGPGKMLGDPGAITKHVLGDAYGKKNPED
LPPGFQLSAPVVITRPPKAWYGWGIPTLVCTVCPAVNKTGDFEYGAIKMDNIRTGRKKIEFV
QLGQIRPNISNTTIELKKFTSPLGRHYKIQIYRYWAQVKKFCGDCYGGCFYTNGSHDRSWKKSFWR
GCDIKTIPASDSIVVVKK