

Table Supplementary 1. Selected Cytotoxic T Lymphocytes (CTL) epitopes from mutational spike protein SARS-CoV2

Epitopes	Length	Immunogenicity	No. Sequence	Antigenicity	Score	Allergenic	Toxicity	Percentile	Alleles
QYIKWPWYI	9 mer	0.21624	1206-1214	Antigenic	1.4669	Nonallergenic	Nontoxic	0.01	HLA-A*24:02, HLA-A*23:01, HLA-A*32:01
NTQEVFAQV	9 mer	0.17889	775-783	Antigenic	0.5244	Nonallergenic	Nontoxic	0.01	HLA-A*68:02, HLA-A*02:06, HLA-A*02:01, HLA-A*26:01, HLA-A*68:02, HLA-A*26:01
DISGINASV	9 mer	0.04027	1166-1174	Antigenic	0.5358	Nonallergenic	Nontoxic	0.02	HLA-A*02:01, HLA-A*02:06, HLA-A*32:01, HLA-A*68:02, HLA-A*30:02, HLA-A*26:01, HLA-A*11:01, HLA-A*68:01, HLA-A*31:01, HLA-A*33:03, HLA-A*03:01, HLA-A*30:01, HLA-A*26:01,
SVLNDILSR	9 mer	0.03075	973-981	Antigenic	0.7875	Nonallergenic	Nontoxic	0.06	HLA-A*68:02, HLA-A*02:01, HLA-A*26:01,
NTQEVFAQV	9 mer	0.17889	777-785	Antigenic	0.5244	Nonallergenic	Nontoxic	0.01	HLA-A*24:02, HLA-A*23:01, HLA-A*32:01,
QYIKWPWYI	9 mer	0.21624	1208-1216	Antigenic	1.4669	Nonallergenic	Nontoxic	0.01	HLA-A*02:01, HLA-A*32:01, HLA-A*68:02, HLA-A*30:02, HLA-A*26:01,
VLNDILSR	9 mer	0.03	976-984	Antigenic	0.8746	Nonallergenic	Nontoxic	0.03	HLA-A*24:02, HLA-A*23:01, HLA-A*11:01, HLA-A*68:01, HLA-A*31:01, HLA-A*33:03, HLA-A*03:01, HLA-A*30:01, HLA-A*26:01,
NYNYLYRLF	9 mer	0.0171	448-456	Antigenic	1.1274	Nonallergenic	Nontoxic	0.04	HLA-A*24:02, HLA-A*23:01, HLA-A*11:01, HLA-A*68:01, HLA-A*31:01, HLA-A*33:03, HLA-A*03:01, HLA-A*30:01, HLA-A*26:01,
SVLNDILSR	9 mer	0.03075	975-983	Antigenic	0.7875	Nonallergenic	Nontoxic	0.06	

Table Supplementary 2. Selected Helper T lymphocytes (HTL) epitopes from mutational spike protein SARS-CoV2

	Score	Order	Antigenic	Antigenic	Allergenic	Percentile	Length	IL-4	IL-10	IFN-γ	Alleles
SFELLHAPATVCGPK	0.09	512-526	0.5224	Antigenic	Nonallergen	0.01	15 mer	Inducer	Noninducer	Noninducer	HLA-DRB1*01:01
TPINLVRDLPQGFS	0.59	206-220	0.848	Antigenic	Nonallergen	0.02	15 mer	Noninducer	Inducer	Noninducer	HLA-DRB1*03:01
PINLVRDLPQGSAL	0.6	207-221	0.8938	Antigenic	Nonallergen	0.03	15 mer	Noninducer	Inducer	Noninducer	HLA-DRB1*03:01
NLLQYGSFCTQLNR	0.75	749-763	0.5145	Antigenic	Nonallergen	0.06	15 mer	Inducer	Inducer	Inducer	HLA-DRB1*15:01
NTLVKQLSSNFGAIS	0.9	958-972	0.4886	Antigenic	Nonallergen	0.11	15 mer	Inducer	Inducer	Noninducer	HLA-DRB1*04:01
GNYNYLYRFRKSNL	1.1378	447-461	1.1378	Antigenic	Nonallergen	0.22	15 mer	Inducer	Non	Inducer	HLA-DRB1*11:01
SNLLQYGSFCTQLN	0.4809	750-764	0.4809	Antigenic	Nonallergen	0.6	15 mer	Inducer	Inducer	Inducer	HLA-DRB1*15:01
NLLQYGSFCTQLNR	0.5145	751-765	0.5145	Antigenic	Nonallergen	0.75	15 mer	Inducer	Inducer	Inducer	HLA-DRB1*15:01
LQYGSFCTQLNRALT	0.4372	754-768	0.4372	Antigenic	Nonallergen	1.3	15 mer	Noninducer	Inducer	Inducer	HLA-DRB1*04:01
LLLQYGSFCTQLNRA	0.4697	752-766	0.4697	Antigenic	Nonallergen	1.8	15 mer	Inducer	Inducer	Inducer	HLA-DRB1*15:01

Table Supplementary 3. Final vaccine construction from selected CTL and HTL epitopes with additional components including adjuvant, PADRE, linkers and 6His-tag

GIINTLQKYYCRVRGGRCVLSCLPKKEEQIGKCSTRGRKCCRRKKEAAAKAKFVAAWT
 LKAAAEAAAKQYIKWPWYIAAYNTQEVFAQVAAYDISGINASVAAAYVLNDILSRLAAY
 SVLNDILSRAAYNTQEVFAQVAAYQYIKWPWYIAAYVLNDILSRLAAYNYNYLYRLFA
 AYSVLNDILSRGPGPGSFELLHAPATVCGPKGPGPGTPINLVRDLPQGFSAGPGPGPINL
 VRDLPQGFSALGPGPGNLLLQYGSFCTQLNRGPGPGNTLVKQLSSNFGAISGPGPGGN
 YNYLYRLFRKSNLGPGPSNLLLQYGSFCTQLNGPGPGNLLLQYGSFCTQLNRGPGPG
 LQYGSFCTQLNRALTGPGPGLLLQYGSFCTQLNRAHHHHHH

Table Supplementary 4. Results of refinement of the final vaccine construction using GalaxyRefine

Model	GDT-HA	RMSD	MolProbity	Clash score	Poor rotamers	Rama favored
Initial	1	0	1.409	4.5	0.3	96.9
MODEL 1	0.9783	0.308	1.664	13.9	0	97.9
MODEL 2	0.9776	0.33	1.694	13.1	0.3	97.7
MODEL 3	0.9815	0.316	1.729	16.4	0	97.9
MODEL 4	0.9853	0.295	1.664	13.9	0.7	97.9
MODEL 5	0.9789	0.322	1.684	12.8	1	97.7

Note: GDT-HA, global distance test-high accuracy; RMSD, root mean square deviation.

Figure Supplementary 1. Population coverage of both CTL and HTL selected epitopes for construction of multiepitope vaccine.

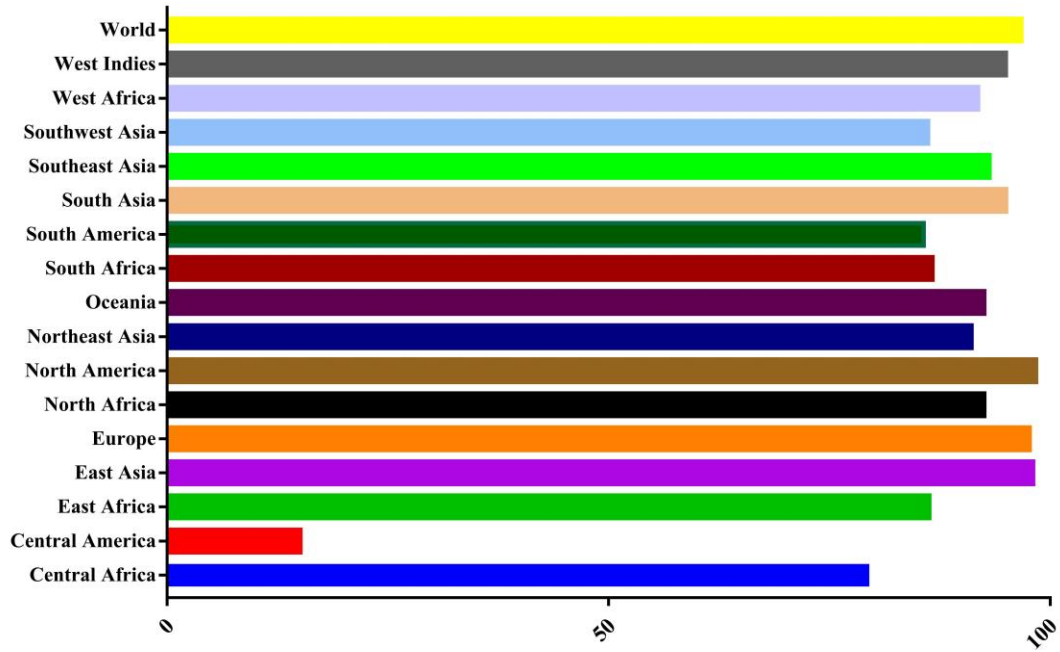


Figure Supplementary 2. Results of secondary structure analysis of vaccine constructed by PSIPRED.

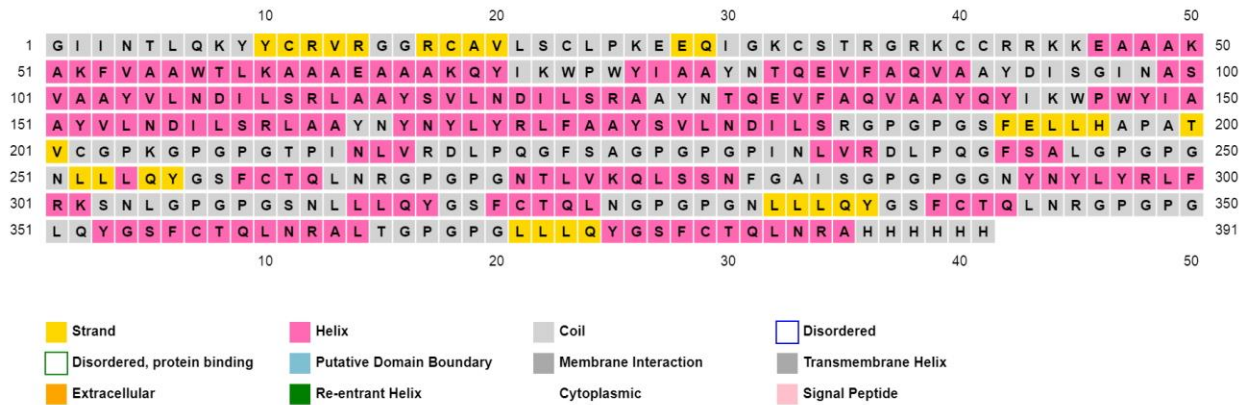


Figure Supplementary 3. Results of secondary analysis of vaccine constructed by SOPMA.

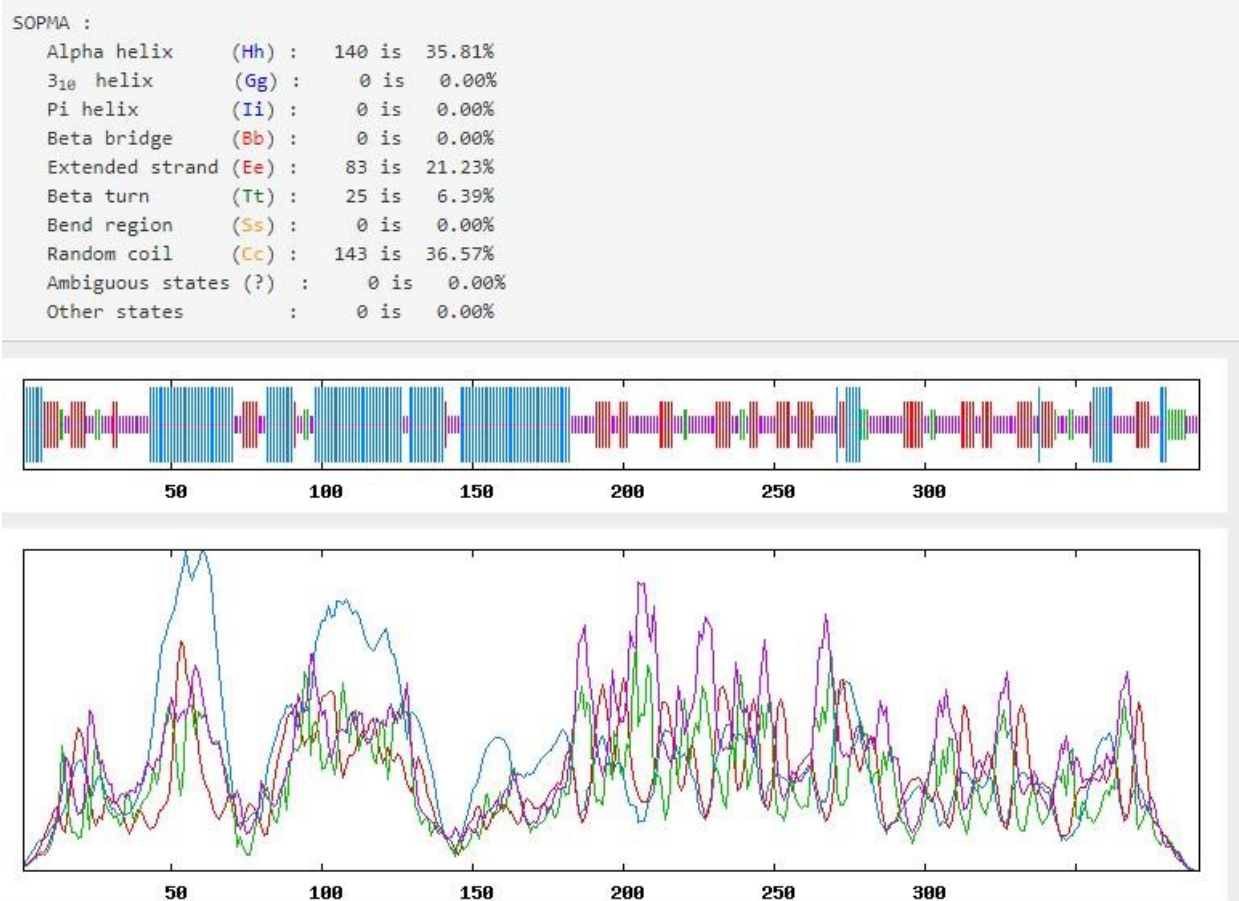


Figure Supplementary 4. Refinement model of vaccine construct.

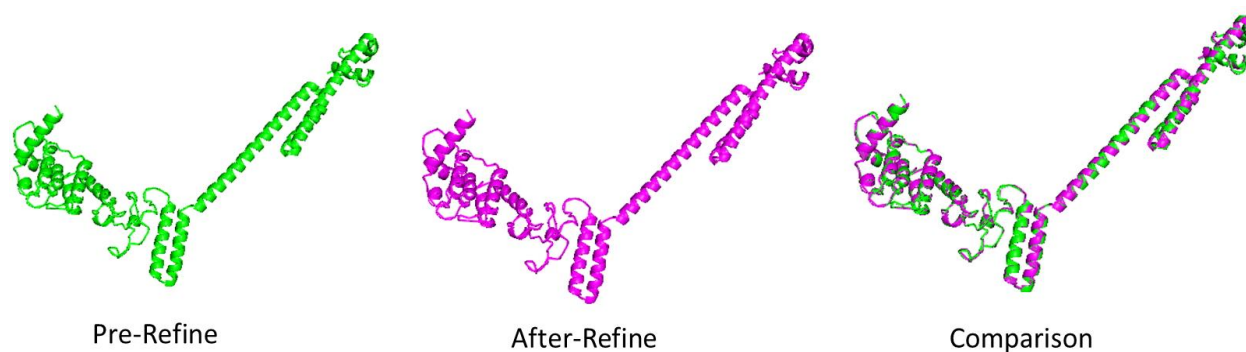


Figure Supplementary 5. Vaccine flexibility results by CABSflex. (A) Depiction of 10 models of the vaccine final model, (B) Interaction/contact map of vaccine residues, and (C) Root Mean Square Fluctuation (RMSF) diagram of vaccine residues.

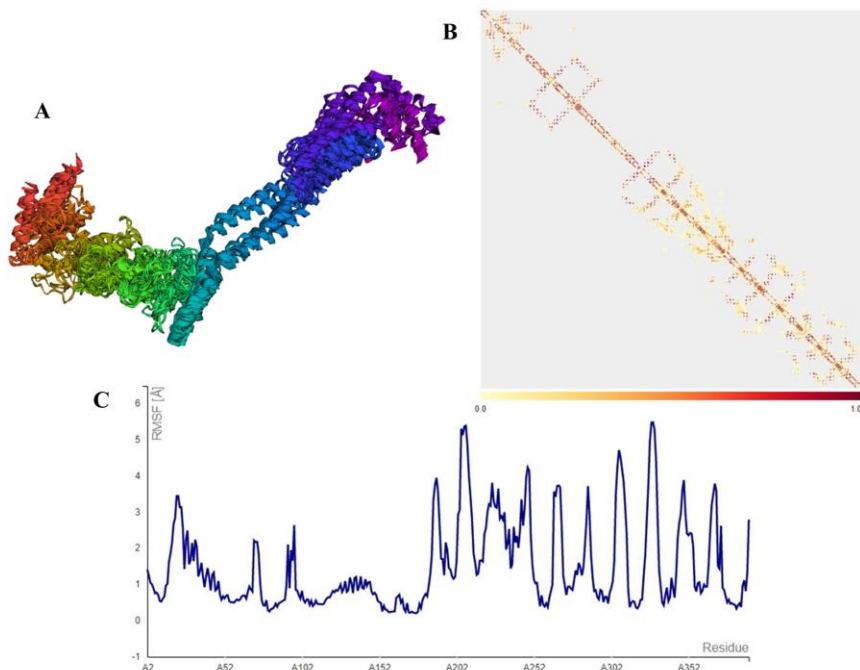


Figure Supplementary 6. Molecular dynamic of complex vaccine-ACE2 using SWAX and iMod server. (A) The radius of gyration of vaccine/ACE2 complex. (B) Eigenvalue, (C) Deformability, (D) Beta factor values, (E) The covariance matrix, and (F) The elastic network

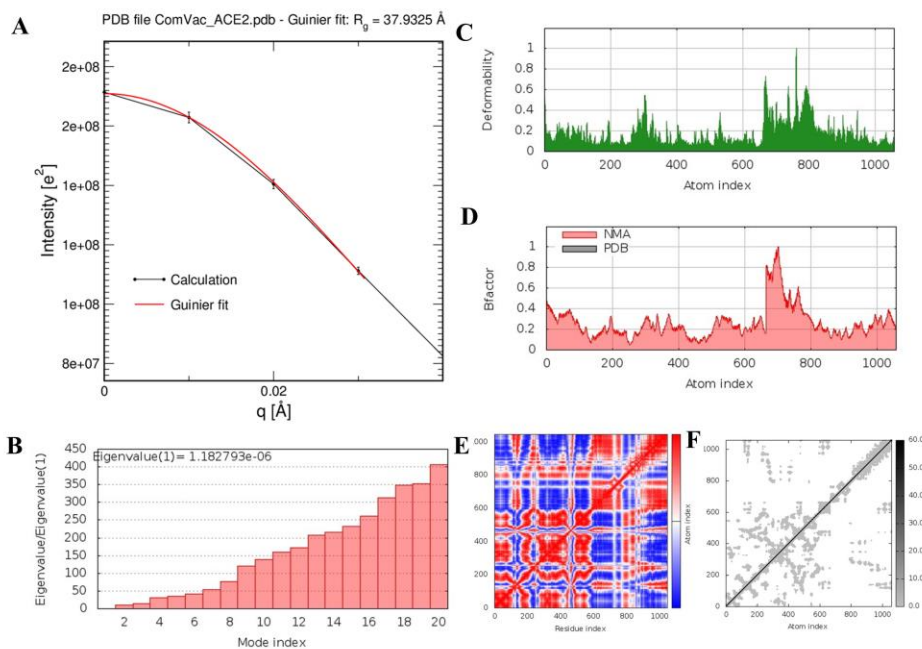


Figure Supplementary 7. Molecular dynamic of complex vaccine-TLR3 using SWAX and iMod server. (A) The radius of gyration of vaccine/TLR3 complex. (B) Eigenvalue, (C) Deformability, (D) Beta factor values, (E) The covariance matrix, and (F) The elastic network

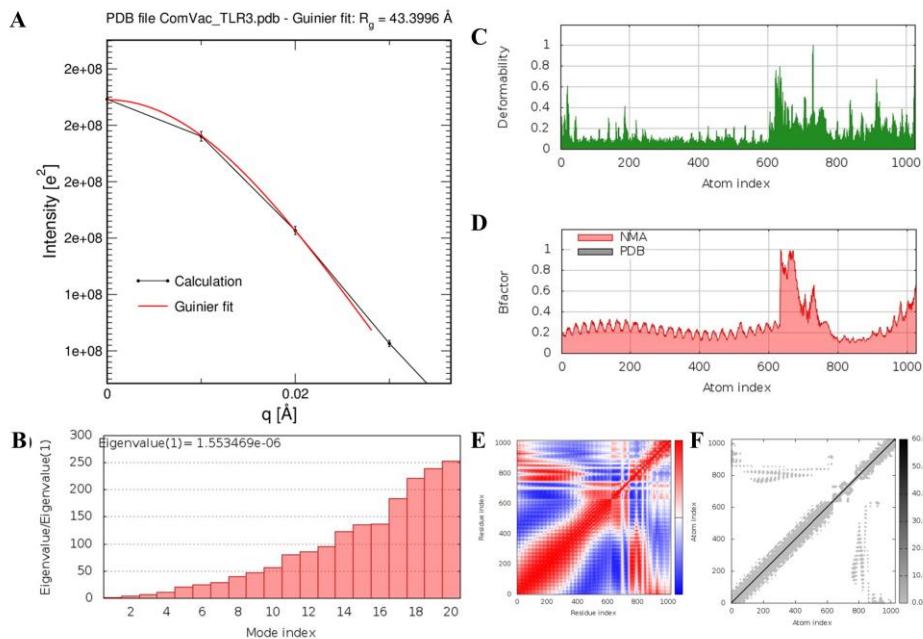


Figure Supplementary 8. Molecular dynamic of complex vaccine-TLR8 using SWAX and iMod server. (A) The radius of gyration of vaccine/TLR8 complex. (B) Eigenvalue, (C) Deformability, (D) Beta factor values, (E) The covariance matrix, and (F) The elastic network.

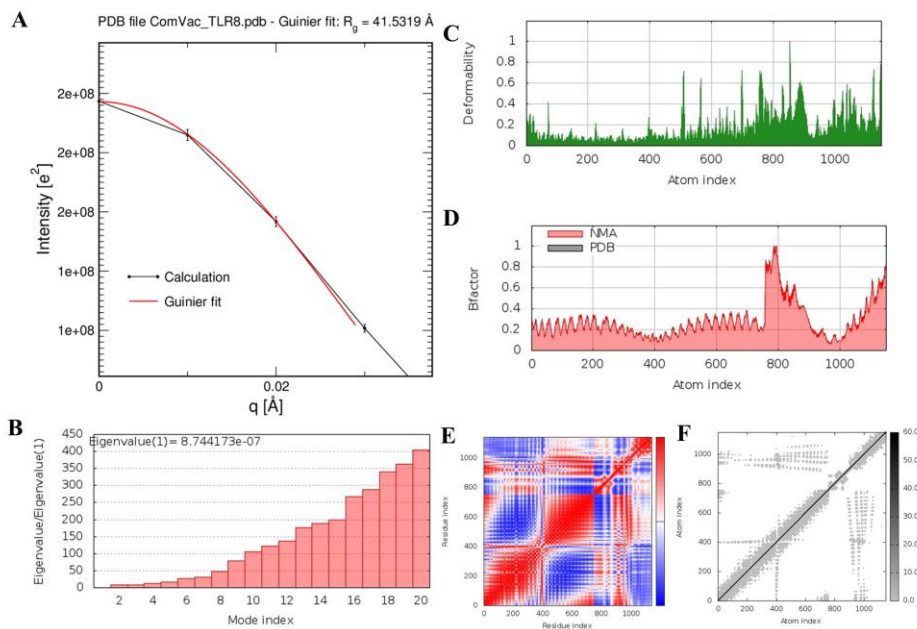


Figure Supplementary 9. Post translation modification prediction results of the vaccine construct

