Supplementary file 1

Designing multi-epitope based peptide vaccine candidates against SARS-CoV-2 using immunoinformatics approach

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Table S1. Molecular docking of MHC Class I epitope with HLA-A*11-01 allele

Protein	MHC allele	Epitope	Global Energy	Hydrogen Bond
Spike		GVYYHKNNK	-50.28	-5.02
		GVLTESNKK	-23.40	-2.69
		KSTNLVKNK	-8.40	-1.75
Nucleocapsid	HLA-A*11-01 allele (PDB ID: 5WJL)	QQQGQTVTK	-22.71	-2.91
		FTALTQHGK	-39.02	-0.85
		LIRQGTDYK	-38.59	-2.31
ORF1a		ASMPTTIAK	-41.96	-1.40
		KTIQPRVEK	-10.93	-0.66
		AVLQSGFRK	-58.65	0.00

Table S2. Molecular docking of MHC Class II epitope with HLA DRB1*04-01 allele

Protein	MHC allele	Epitope	Global Energy	Hydrogen Bond
Spike		DLFLPFFSNVTW	-1.46	0.00
		QSLLIVNNATNV	-10.79	-0.36
	HLA DRB1*04-01 (PDB ID: 5JLZ)	QDLFLPFFSNVT	-3.99	-0.35
Nucleocapsid		PNFKDQVILLNK	0.26	0.00
		AQFAPSASAFFG	-19.47	-1.25
		IAQFAPSASAFF	-6.82	-1.11
ORF1a		SHFVNLDNLRAN	-0.97	0.00

| | SSFLEMKSEKQV | -1.80 | -0.75 |
| | HFVNLDNLRANN | -1.00 | 0.00 |

Table S3. Vaccine constructed by two different adjuvants including HABA named CVCoV1 and L7/L12 ribosomal CVCoV2.

Name of Vaccine	Vaccine Constructs	Length of Amino Acid
CVCoV1 (HABA)	**EAAAK**MAENPNIDDLPAPLLAALGAADLALATVNDLIANLRERAEETRAETRTRVEERRARLTKFQEDLPEQFIELRDKFTTEELRKAAEGYLEAATNRYNELVERGEAALQRLRSQTAFEDASARAEGYVDQAVELTQEALGTVASQTRAVGERAAKLVGIEL**EAAAK**AKFVAAWTLKAAA**GGGS**GVYYHKNNK**GGGS**GVLTESNKK**GGGS**KSTNLVKNK**GGGS**QQQGQTVTK**GGGS**FTALTQHGK**GGGS**LIRQGTDYK**GGGS**ASMPTTIAK**GGGS**KTIQPRVEK**GGGS**AVLQSGFRK**GPGPG**DLFLPFFSNVTW**GPGPG**QSLLIVNNATNV**GPGPG**QDLFLPFFSNVT**GPGPG**PNFKDQVILLNK**GPGPG**AQFAPSASAFFG**GPGPG**IAQFAPSASAFF**GPGPG**SHFVNLDNLRAN**GPGPG**SSFLEMKSEKQV**GPGPG**HFVNLDNLRANN**KK**SQCVNLTTRTQLPPAYTNSFTRGVY**KK**MDLEGKQGNFKNL**KK**KHTPINLVRDLPQGFS**KK**KSFTVEKGIYQTSNFRVQP**KK**FPNITNLCPFGEVFNATRFASVYAWNRKRISNCVA**KK**NGPQNQRNAPRI**KK**FGGPSDSTGSNQNGERSGARSKQRRPQGLPNN**KK**HGKEDLKFPRGQGVPINTNSSPDDQIGYYRATRRIRGGDGKMKDLS**KK**GALNTPKDHIGTRNPANNAAIVLQLPQ**KK**RLNQLESKMSGKGQQQQGQTVTKKSAAEASKKPRQKRTATKA**KK**HNESGLKTILRKGGR**KK**CGETSWQTGDFVKAT**KK**KKFDTFNGECPNFVFPLNSIIKTIQPRVEKKKLDGFMG**KK**PLECIKDLLARAGKASCTLS**KK**KNGNKGAGGHSYGADLKSFDLGDELGTDPYEDFQENWNTKHSSGV**KK**AKFVAAWTLKAAA**GGGS**	902
CVCoV2 (L7/L12 ribosomal)	**EAAAK**MAKLSTDELLDAFKEMTLLELSDFVKKFEETFEVTAAAPVAVAAAGAAPAGAAVEAAEEQSEFDVILEAAGDKKIGVIKVVREIVSGLGLKEAKDLVDGAPKPLLEKVAKEAADEAKAKLEAAGATVTVK**EAAAK**AKFVAAWTLKAAA**GGGS**GVYYHKNNK**GGGS**GVLTESNKK**GGGS**KSTNLVKNK**GGGS**QQQGQTVTK**GGGS**FTALTQHGK**GGGS**LIRQGTDYK**GGGS**ASMPTTIAK**GGGS**KTIQPRVEK**GGGS**AVLQSGFRK**GPGPG**DLFLPFFSNVTW**GPGPG**QSLLIVNNATNV**GPGPG**QDLFLPFFSNVT**GPGPG**PNFKDQVILLNK**GPGP G**AQFAPSASAFFG**GPGPG**IAQFAPSASAFF**GPGPG**SHFVNLDNLRAN**GPGPG**SSFLEMKSEKQV**GPGPG**HFVNLDNLRANN**KK**SQCVNLTTRTQLPPAYTNSFTRGVY**KK**MDLEGKQGNFKNL**KK**KHTPINLVRDLPQGFS**KK**KSFTVEKGIYQTSNFRVQP**KK**FPNITNLCPFGEVFNATRFASVYAWNRKRISNCVA**KK**NGPQNQRNAPRI**KK**FGGPSDSTGSNQNGERSGARSKQRRPQGLPNN**KK**HGKEDLKFPRGQGVPINTNSSPDDQIGYYRATRRIRGGDGKMKDLS**KK**GALNTPKDHIGTRNPANNAAIVLQLPQ**KK**RLNQLESKMSGKGQQQQGQTVTKKSAAEASKKPRQKRTATKA**KK**HNESGLKTILRKGGR**KK**CGETSWQTGDFVKAT**KK**KKFDTFNGECPNFVFPLNSIIKTIQPRVEK	873

KKLDGFMG**KK**PLECIKDLLARAGKASCTLS**KKK**KNGNKGAGGH
SYGADLKSFDLGDELGTDPYEDFQENWNTKHSSGV**KK**AKFVAA
WTLKAAA**GGGS**

Table S4. Physicochemical properties, allergenicity, antigenicity of two different vaccines constructed with adjuvant, CVCoV1 and CVCoV2.

Name	Amino acid	Anti genicity	Allergenicity	MW	Theore-tical pI	Ext. coefficient (M−1 cm−1)	Aliphatic index	GRAVY	Stability
CVCoV1	902	Antigenic (0.7234)	NonAllergen	96631	10.09	54235	61.20	-0.732	34.90 (Stable)
CVCoV2	873	Antigenic (0.7505)	NonAllergen	92443	10.04	49765	62.10	-0.639	31.07 (Stable)

Table S5. Ramachandran and ERRAT characterization of 3D structure of constructed vaccine

Vaccine	Quality Factor ERRAT	Most Favored region	Additional Allowed regions	Generously allowed Region	Disallowed regions
CVCoV1	90.75	79%	16.8%	2.5%	1.8%
CVCoV2	71.43	83.2%	14.5%	1.8%	0.4%

Table S6. Results of molecular Docking of vaccine construct with TLR 3 and TLR8

Vaccine	Name of Target	PDB ID	Representative	Weighed Score	Global Energy	Hydrogen Bond	Attractive VdW	Repulsive VdW
CVCoV1	TLR-3	1ziw	Center	-1027.3	2.24	0.00	-4.74	1.72
			Lowest Energy	-1324.9				
	TLR-8	3w3m	Center	-1155.4	-10.38	-0.55	-25.84	10.33
			Lowest Energy	-1431.5				
	TLR4	4g8a	Center	-1084.6	2.60	-2.65	-30.93	38.10
			Lowest Energy	-1234.1				
	ACE2	1r42	Center	-1147.4	-0.79	0.00	-7.46	0.00
			Lowest Energy	-1477.5				
CVCoV2	TLR-3	1ziw	Center	-1096.1	4.29	0.00	-6.47	17.95
			Lowest Energy	-1206.2				
	TLR-8	3w3m	Center	-1120.9	2.68	0.00	-0.20	0.00
			Lowest Energy	-1256.3				
	TLR4	4g8a	Center	-1289.2	-20.00	-1.26	-27.10	12.18
			Lowest Energy	-1346.0				
	ACE2	1r42	Center	-969.1	-0.80	0.00	-15.73	10.63
			Lowest Energy	-1296.8				