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MDPI

Supplementary Information

Potential immunogenic activity of computationally designed Spike-RBD epitopes based prophylactic vaccine against MERS, SARS-CoV and SARS-CoV-2, A reverse vaccinology approach

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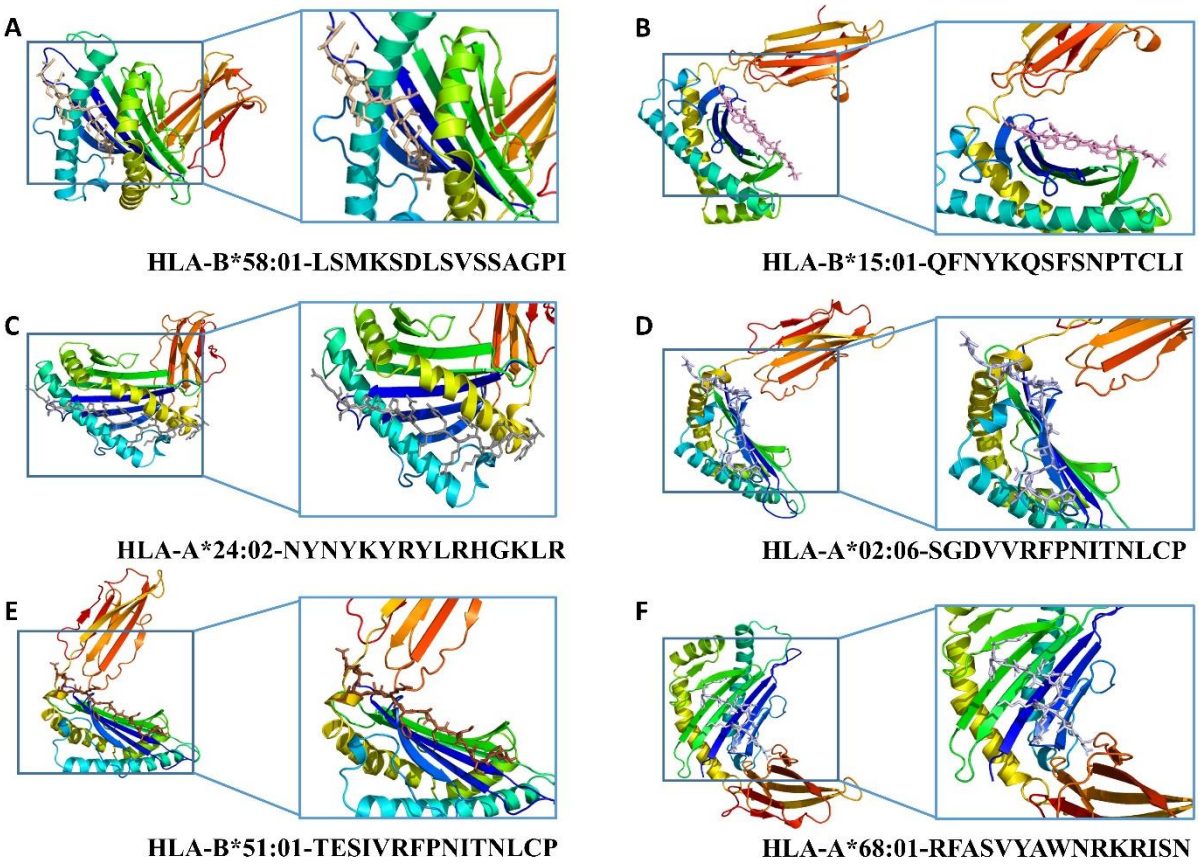

Figure S1. Showing docking complexes of HTL epitopes for each CoV specie with respective HLAs.

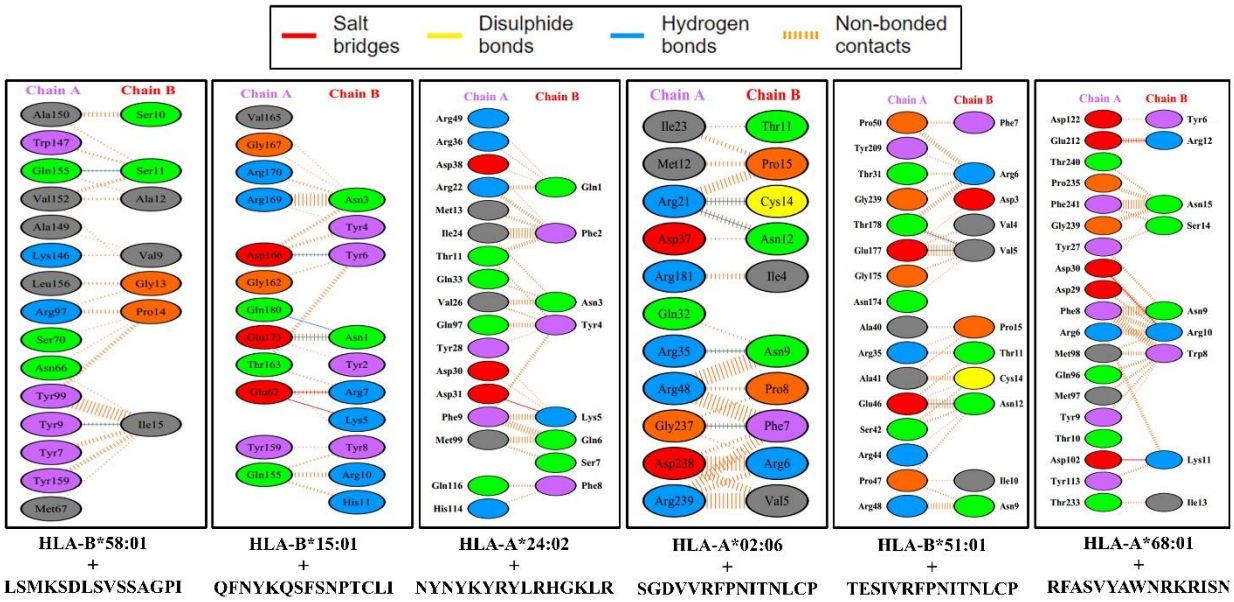

Figure S2. Showing interaction patterns of individual HTL epitopes with respective HLAs.

Table S1. Showing details of binding scores and identified interaction patterns between the different immune epitopes and respective HLAs.

Epitope + HLA complex	Epitope position in the RBD domain	hCOV specie	Docking Score	Binding free energy	Number of Hydrogen Bonds	Number of Salt Bridges	Number of non-bonded contacts
MTEQLQMGF + HLA-B*57:01	183-191	MERS-CoV	-2244.26	-27.86 kcal/mol	5	-	92
NATKFPSVY + HLA-B*35:01	25-33	SARS-CoV	-2426.57	-20.65kcal/mol	3	-	140
VGGNYNYLY + HLA-A*01:01	127-135	SARS-CoV-2	-2945.07	-21.87kcal/mol	5	-	142
LSMKSDLSVSSAGPI + HLA-B*58:01	70-84	MERS-CoV	-2334.26	-37.1kcal/mol	2	-	105
QFNYKQSFSNPTCLI + HLA-B*15:01	86-100	MERS-CoV	-2785.36	-31.49 kcal/mol	3	2	132
NYNYKYRYLRHGKLR + HLA-A*24:02	130-144	SARS-CoV	-3279.04	-33.44 kcal/mol	-	1	141
SGDVVRFPNITNLCP + HLA-A*02:06	5-19	SARS-CoV	-2602.58	-35.7 kcal/mol	4	-	141
TESIVRFPNITNLCP + HLA-B*51:01	5-19	SARS-CoV-2	-2728.46	-29.69 kcal/mol	3	-	118
RFASVYAWNRKRISN + HLA-A*68:01	28-42	SARS-CoV-2	-3669.67	-46.27 kcal/mol	-	3	189

Table S2. Showing details free energy calculations for the different CTL and HTL epitopes and respective HLAs.

Complex name	Epitope position in the RBD Domain	VDW	ELE	GB	SA	TOTAL
MTEQLQMGF + HLA-B*57:01	183-191	-48.52	-59.59	87.51	-7.26	-27.86
NATKFPSVY + HLA-B*35:01	25-33	-62.66	-255.21	305.77	-8.55	-20.65
VGGNYNYLY + HLA-A*01:01	127-135	-52.34	-12.09	49.95	-7.39	-21.87
LSMKSDLSVSSAGPI + HLA-B*58:01	70-84	-40.5	-36.04	46.18	-6.75	-37.1
QFNYKQSFSNPTCLI + HLA-B*15:01	86-100	-60.45	-161.38	198.28	-7.94	-31.49
NYNYKYRYLRHGKL R + HLA-A*24:02	130-144	-65.9	-723.97	765.14	-8.72	-33.44
SGDVVRFPNITNLCP + HLA-A*02:06	5-19	-60.84	-134.77	168.83	-8.92	-35.7
TESIVRFPNITNLCP + HLA-B*51:01	5-19	-54.92	-127.72	160.74	-7.79	-29.69
RFASVYAWNRKRISN + HLA-A*68:01	28-42	-74.1	-602.08	640.31	-10.41	-46.27

Table S3. Showing physiochemical properties including of the proposed MEVC.

Complex name	Epitope position in the RBD Domain	VDW	ELE	GB	SA	TOTAL
MTEQLQMGF + HLA-B*57:01	183-191	-48.52	-59.59	87.51	-7.26	-27.86
NATKFPSVY + HLA-B*35:01	25-33	-62.66	-255.21	305.77	-8.55	-20.65
VGGNYNYLY + HLA-A*01:01	127-135	-52.34	-12.09	49.95	-7.39	-21.87
LSMKSDLSVSSAGPI + HLA-B*58:01	70-84	-40.5	-36.04	46.18	-6.75	-37.1
QFNYKQSFSNPTCLI + HLA-B*15:01	86-100	-60.45	-161.38	198.28	-7.94	-31.49
NYNYKYRYLRHGKL R + HLA-A*24:02	130-144	-65.9	-723.97	765.14	-8.72	-33.44
SGDVVRFPNITNLCP + HLA-A*02:06	5-19	-60.84	-134.77	168.83	-8.92	-35.7
TESIVRFPNITNLCP + HLA-B*51:01	5-19	-54.92	-127.72	160.74	-7.79	-29.69
RFASVYAWNRKRISN + HLA-A*68:01	28-42	-74.1	-602.08	640.31	-10.41	-46.27