

Appendix 1. The selection of HTL epitopes and their immunological properties investigated using the ABCpred, BcePred and IEDB. All the epitopes were non-toxicogenic, non-allergen, non-mutant, and contained to induce IFN-gamma. Most of them could induce IL-4. The amino acid sequence of selected immuno-dominant epitopes of OprF, OprI, and PopB has indicated red, green, and blue colors.

No.	Peptide Sequence	Mutation	Allergenicity	Toxicity	Prediction		Hydrophobicity	Hydropathicity	Hydrophilicity	Charge	Mol wt
					IFN- γ	IL-4 inducer					
1	DAIYHFGTPGVGLRP	NO	NO	NO	+	+	-0.00	-0.03	-0.35	0.50	1600.03
2	LDAIYHFGTPGVGLR	NO	NO	NO	+	+	0.04	0.33	-0.47	0.50	1616.08
3	HFGTPGVGLRPYVSA A	NO	NO	NO	+	+	0.02	0.13	-0.51	1.50	1557.99
4	VELALSYGEYHDVRR G	NO	NO	NO	+	+	-0.11	-0.31	0.01	-1.50	1708.08
5	GGRVNAVGYGESRPV V	NO	NO	NO	+	+	-0.17	-0.46	0.15	1.00	1517.88
6	GRVNAVGYGESRPVA A	NO	NO	NO	+	+	-0.17	-0.31	0.11	1.00	1531.90
7	RVNAVGYGESRPVAD D	NO	NO	NO	+	+	-0.22	-0.52	0.31	0.00	1589.93
8	NAVGYGESRPVADNA A	NO	NO	NO	+	+	-0.17	-0.61	0.19	-1.00	1519.79
9	ELALSYGEYHDVRRG T	NO	NO	NO	+	+	-0.16	-0.63	0.08	-1.50	1710.05
10	VEGGRVNAVGYGESR R	NO	NO	NO	+	+	-0.21	-0.59	0.35	0.00	1549.88
11	EGGRVNAVGYGESRP P	NO	NO	NO	+	+	-0.25	-0.97	0.45	0.00	1547.86
12	TPGVGLRPYVSAGLA A	NO	NO	NO	+	-	0.05	0.53	-0.47	1.00	1457.91
13	GTPGVGLRPYVSAGL L	NO	NO	NO	+	-	0.05	0.38	-0.43	1.00	1443.89
14	LDAIYHFGTPGVGLRP P	NO	NO	NO	+	+	0.03	0.21	-0.44	0.50	1713.21
15	VGYESRPVADNATAE AE	NO	NO	NO	+	+	-0.17	-0.62	0.33	-2.00	1635.92
16	VELALSYGEYHDVRRG GT	NO	NO	NO	+	+	-0.11	-0.33	-0.02	0.75	1809.20
17	GCSHSHKETEARLTA	NO	NO	NO	+	+	-0.29	-0.86	0.52	0.50	1576.90
18	ATGCSHSHKETEARL	NO	NO	NO	+	+	-0.29	-0.86	0.52	0.50	1576.90

19	LATGCSSSHKETEAR	NO	NO	NO	+	+	-0.29	-0.86	0.52	0.50	1576.90
20	TGCSSSHKETEARLTA	NO	NO	NO	+	+	-0.29	-0.85	0.46	0.94	1678.02
21	DVESLRVERLAAPAA	NO	NO	NO	+	+	-0.18	0.09	0.45	-1.00	1597.00
22	VQESRADLTTLQGV	NO	NO	NO	+	+	-0.12	0.08	-0.00	-1.00	1630.06
23	ESRADLTTLQGVIER	NO	NO	NO	+	+	-0.27	-0.50	0.49	-1.00	1688.09
24	ALGRPVARDVESLRV	NO	NO	NO	+	+	-0.24	0.03	0.41	1.00	1638.11

Appendix 2. The selection of CTL epitopes and their immunological properties investigated using the NetCTL 1.2 server and IEDB. All the epitopes were non-toxicogenic, non-allergen, and non-mutant. The amino acid sequence of selected immune-dominant epitopes of OprF, OprI, and PopB has indicated red, green, and blue colors.

No.	Peptide Sequence	Mutation	Allergenicity	Toxicity	Hydrophobicity	Hydrophaticity	Hydrophilicity	Charge	Mol wt
1	LTDDVELAL	NO	NO	NO	0.02	0.69	0.13	-3.00	988.23
2	VRDVLVNEY	NO	NO	NO	-0.17	0.01	0.07	-1.00	1106.37
3	NLTSLDAIY	NO	NO	NO	0.03	0.46	-0.57	-1.00	1009.25
4	HTDSVGTDA	NO	NO	NO	-0.17	-0.76	0.33	-1.50	902.00
5	CSDSNDGV	NO	NO	NO	-0.29	-1.03	0.81	-3.00	910.97
6	GTDAYNQKL	NO	NO	NO	-0.26	-1.24	0.16	0.00	1009.21
7	KSKVKENSY	NO	NO	NO	-0.50	-1.93	1.00	2.00	1082.34
8	AQARADEAY	NO	NO	NO	-0.31	-1.01	0.54	-1.00	994.13
9	MTASLASKV	NO	NO	NO	0.00	0.81	-0.27	1.00	907.21

Appendix 3. The result of five refined models generated via the GalaxyWeb server.

<i>Model</i>	<i>GDT-HA</i>	<i>RMSD</i>	<i>MolProbity</i>	<i>Clash score</i>	<i>Poor rotamers</i>	<i>Rama favored</i>
<i>Initial</i>	1.0000	0.000	2.467	7.3	2.9	81.2
<i>1</i>	0.9751	0.333	2.748	27.2	2.0	88.1
<i>2</i>	0.9745	0.338	2.629	26.6	1.4	88.1
<i>3</i>	0.9714	0.354	2.504	26.6	0.6	88.3
<i>4</i>	0.9730	0.350	2.598	24.6	1.4	88.1
<i>5</i>	0.9719	0.354	2.735	26.6	2.0	88.3