

Supplementary file 1

A novel therapeutic multiepitope vaccine based on oncoprotein E6 and E7 of HPV 16 and 18: An *in silico* approach

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Table S1. Characteristics of E6 and E7 Oncoproteins of HPV 16 and 18

Virus	Protein	Antigenicity	AA	Molecular weight	Theoretical <i>pI</i>	Ext. coefficient	Est. half-life	Instability index	Aliphatic index	GRAVY
HPV 16 (RefSeq: NC_001526.4)	E6	0,6921	158	19187,28	9,16	1,109; 1,063	Mammalia, in vitro: 30 hours; yeast, in vivo: >20 hours; E. coli, in vivo: >10 hours	76,14 (unstable)	68,48	-0,778
	E7	0,5765	98	11022,32	4,2	0,575; 0,541	Mammalia, in vitro: 30 hours; yeast, in vivo: >20 hours; E. coli, in vivo: >10 hours	63 (unstable)	78,57	-0,405
HPV 18 (GenBank: LC509006.1)	E6	0,5433	158	18871,68	8,95	0,665; 0,632 (not including Trp residues)	Mammalia, in vitro: 30 hours; yeast, in vivo: >20 hours; E. coli, in	66,88 (unstable)	78,99	-0,63

vivo: >
10 hours

E7	0,4846	105	11995,57	4,7	0,490; 0,459	Mammal ia, in vitro: 30 hours; yeast, in vivo: >20 hours; E. coli, in vivo: > 10 hours	72,93 (unstable)	86,38	-0,375
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Table S2. Selected CTL epitopes

No	Protein	Peptide	Location	HLA	Immunogenicity	Antigenicity	AllerTOP	AllergenFP	Toxicity
1	E6 HPV 16	VYDFAFRDL	49 - 57	HLA-A*24:02	0,32994	1,4227	probable non- allergen	probable non- allergen	non-toxin
2		DPQERPRKL	11 - 19	HLA-B*07:02, HLA-B*08:01	0,02079	0,5782	probable non- allergen	probable non- allergen	non-toxin
3	E7 HPV 16	RAHYNIVTF	49 - 57	HLA-A*24:02, HLA-A*26:01, HLA-B*07:02, HLA-B*08:01	0,18328	0,5919	probable non- allergen	probable non- allergen	non-toxin
4		EPDRAHYNI	46 - 54	HLA-B*07:02	0,12093	0,6109	probable non- allergen	probable non- allergen	non-toxin
5	E6 HPV 18	SLQDIEITC	24 - 32	HLA-A*02:01	0,34357	2,722	probable non- allergen	probable non- allergen	non-toxin
6		RFHNIAGHY	126 - 134	HLA-A*03:01, HLA-A*26:01, HLA-B*15:01	0,21792	0,5004	probable non- allergen	probable non- allergen	non-toxin
7		LQRRRETQV	150 - 158	HLA-B*08:01	0,17861	0,9329	probable non- allergen	probable non- allergen	non-toxin
8		FEFAFKDLF	45 - 53	HLA-B*39:01, HLA-B*40:01	0,00061	1,6451	probable non- allergen	probable non- allergen	non-toxin
9		LEKLTNTGL	90 - 98	HLA-B*40:01	0,00311	0,8025	probable non- allergen	probable non- allergen	non-toxin
10	E7 HPV 18	EENDEIDGV	36 - 44	HLA-B*40:01	0,28152	0,7879	probable non- allergen	probable non- allergen	non-toxin

Table S3. Selected HTL epitopes

No	Protein	Peptide	Location	HLA	Antigenicity	AllerTOP	AllergenFP	Toxicity	IFN- γ	IL-4	IL-10
1	E6 HPV 16	VYDFAFR	49 - 63	HLA-DQA1*01:01/	1,715	probable	probable	Non-toxic	0,0196	0,28	0,77829
		DLCIVYR D		DQB1*05:01		non- allergen	non- allergen		7		
2		RHYCYSL	84 - 98	HLA-DPA1*02:01/	0,8311	probable	probable	Non-toxic	0,2623	0,44	0,57041
		YGTTLEQ Q		DQB1*01:01		non- allergen	non- allergen		4		
3	E7 HPV 16	LHEYML	8 - 22	HLA-DQA1*03:01/	1,0181	probable	probable	Non-toxic	0,0393	-0,15	-0,44674
		DLQPETT DL		DQB1*03:06		non- allergen	non- allergen		6		
4	E6 HPV 18	VFEFAFK	44-58	HLA-DPA1*01:03/	0,8872	probable	probable	Non-toxic	0,803	0,31	0,40508
		DLFVVYR D		DPB1*04:01; DQA1*01:01/ DQB1*05:01; DPA1*02:01/ DPB1*05:01		HLA- HLA-	non- allergen		non- allergen		
5		FEFAFKD	45 - 59	HLA-DPA1*01:03/	1,3061	probable	probable	Non-toxic	0,6227	0,31	0,3456
		LFVVYRD S		DPB1*02:01		non- allergen	non- allergen		2		
6	E7 HPV 18	EARIELV	69 - 83	HLA-DQA1*03:01/	0,5472	probable	probable	Non-toxic	-	0,24	-0,31835
		VESSADD L		DQB1*03:02; HLA-DQA1*05:01/ DQB1*02:01		non- allergen	non- allergen		0,4340 3		

Table S4. Selected LBL epitopes

No	Protein	Peptide	Location	Antigenicity	AllerTOP	AllergenFP	Toxicity	IgPred
1	E6 HPV 16	RDLCLVYRDGNPYAVC	55 - 70	1,0221	probable allergen	non-allergen	probable non-allergen	Non-toxic non-epitope
2		YRDGNPYAVCDKCLKF	61 - 76	0,7509	probable allergen	non-allergen	probable non-allergen	Non-toxic non-epitope
3		ISEYRHYCYSLYGTTL	80 - 95	0,9064	probable allergen	non-allergen	probable non-allergen	Non-toxic non-epitope
4		ERPRKLPQLCTELQTT	14 - 29	0,6858	probable allergen	non-allergen	probable non-allergen	Non-toxic non-epitope
5		PLCPEEKQRHLDKKQR	116 - 131	1,1455	probable allergen	non-allergen	probable non-allergen	Non-toxic non-epitope
6	E7 HPV 16	GPAGQAEPDRAHYNI	39 - 54	0,4342	probable allergen	non-allergen	probable non-allergen	Non-toxic IgG epitope
7		STHVDIRTLEDLLMGT	71 - 86	0,7225	probable allergen	non-allergen	probable non-allergen	Non-toxic IgG epitope
8	E6 HPV 18	HKCIDFYRSIRELRHY	66 - 81	0,5118	probable allergen	non-allergen	probable non-allergen	Non-toxic non-epitope
9		CQKPLNPAEKLRLHNE	108 - 123	0,7424	probable allergen	non-allergen	probable non-allergen	Non-toxic non-epitope
10		TCVYCKTVLELTVFE	31 - 46	0,4468	probable allergen	non-allergen	probable non-allergen	Non-toxic non-epitope
11	E7 HPV 18	KATLQDIVLHLEPQNE	5 - 20	1,094	probable allergen	non-allergen	probable non-allergen	Non-toxic non-epitope
12		SDSEEENDEIDGVNHQ	32 - 47	0,6299	probable allergen	non-allergen	probable non-allergen	Non-toxic IgG epitope