Supplementary file 1

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Designing a novel therapeutic candidate vaccine for HPV16 using immunoinformatics approach: Targeting E6 and E7 epitopes with TLR4 agonist integration

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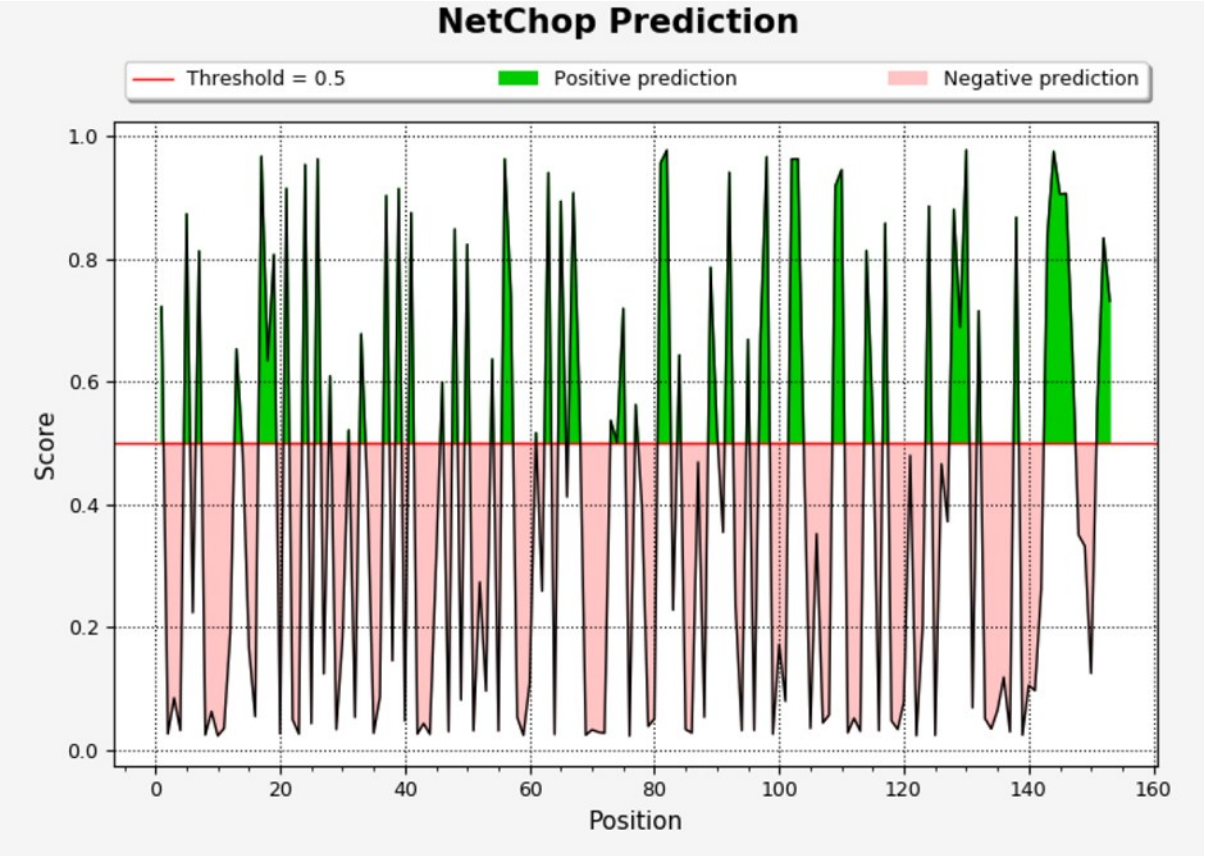

Fig S1. Proteasomal cleavage prediction by NetChop IEDB tool. The x-axis shows the amino acid sequence position and the y-axis shows the proteasomal cleavage score. The threshold was 0.5. The green regions above the threshold are proteasomal cleavage sequences, which are E6 and E7 epitopes.

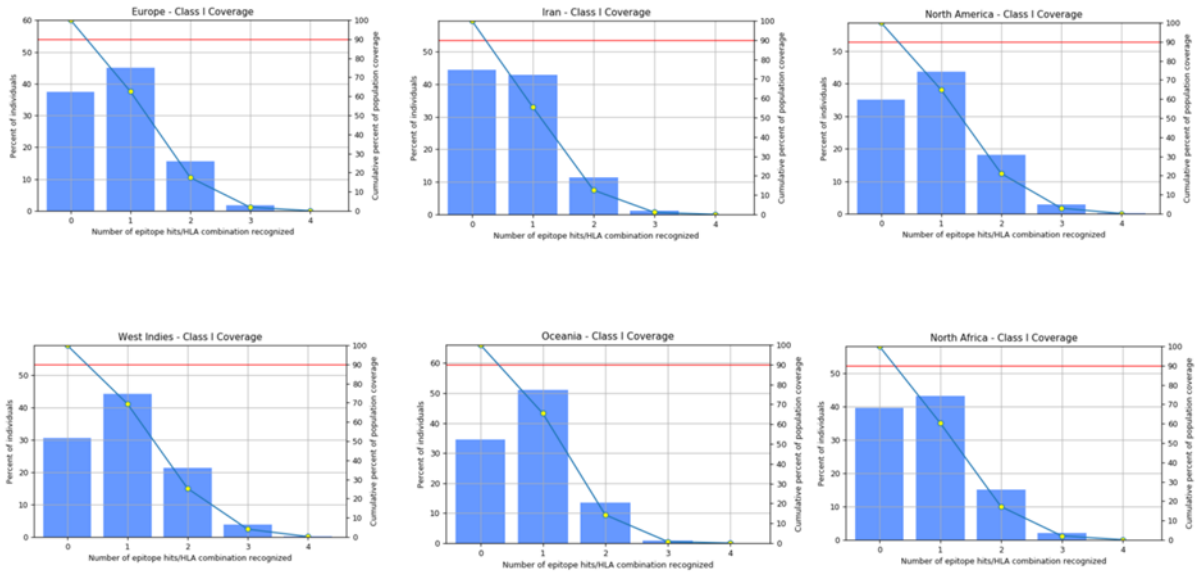

Fig. S2. Population coverage based on MHC-I data. Different HPV-affected regions were selected for assessment of the population coverage of the platform E6 and E7 epitopes. In the graphs, the line (-o- as shown in yellow color) shows the cumulative percentage of population coverage of the epitopes; the bars show the population coverage for platform epitopes. PC90 as shown in the red line is 90% population coverage.

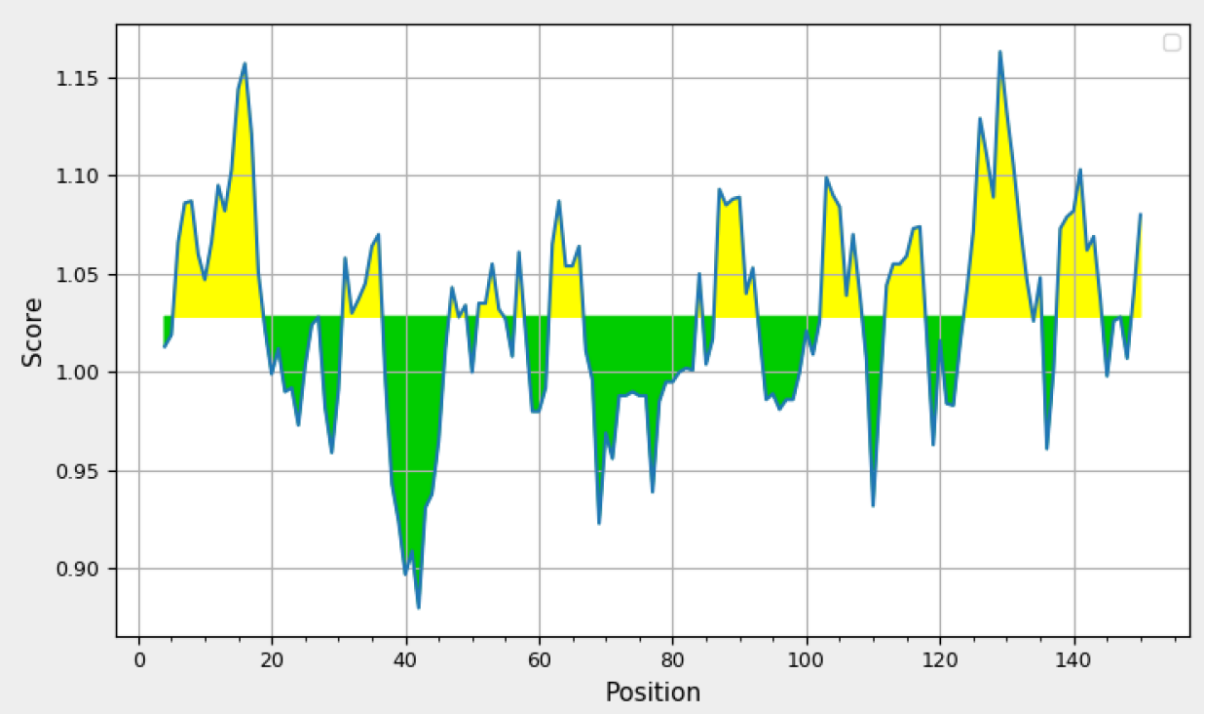

Fig. S3. Antigenicity prediction by Kolashkar and Tongaonkar IEDB tool. The x-axis shows the amino acid sequence position and the y-axis shows the antigenicity score. The threshold was 1.028. The yellow regions above the threshold are antigenic sequences, which are E6 and E7 epitopes.

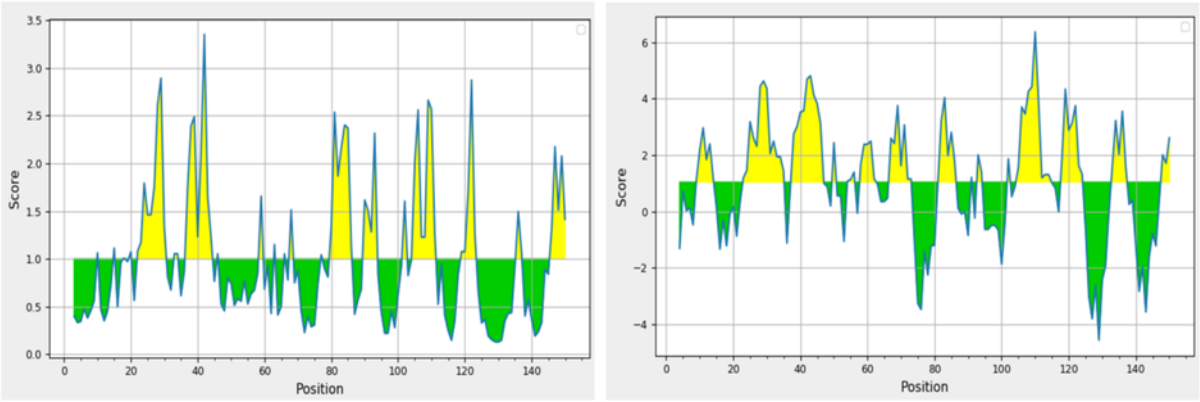

Fig. S4. Surface accessibility of pneumolysin peptide. A) Surface-accessible epitopes are yellow regions above the threshold. The x-axis shows the amino acid sequence position and the y-axis shows the surface accessibility score. The threshold was 1.000. B) Parker hydrophilicity prediction of the pneumolysin peptide. The x-axis and y-axis show the position and score, respectively. The threshold was 1.046. The regions of the protein above the threshold value are hydrophilic and are shown in yellow.

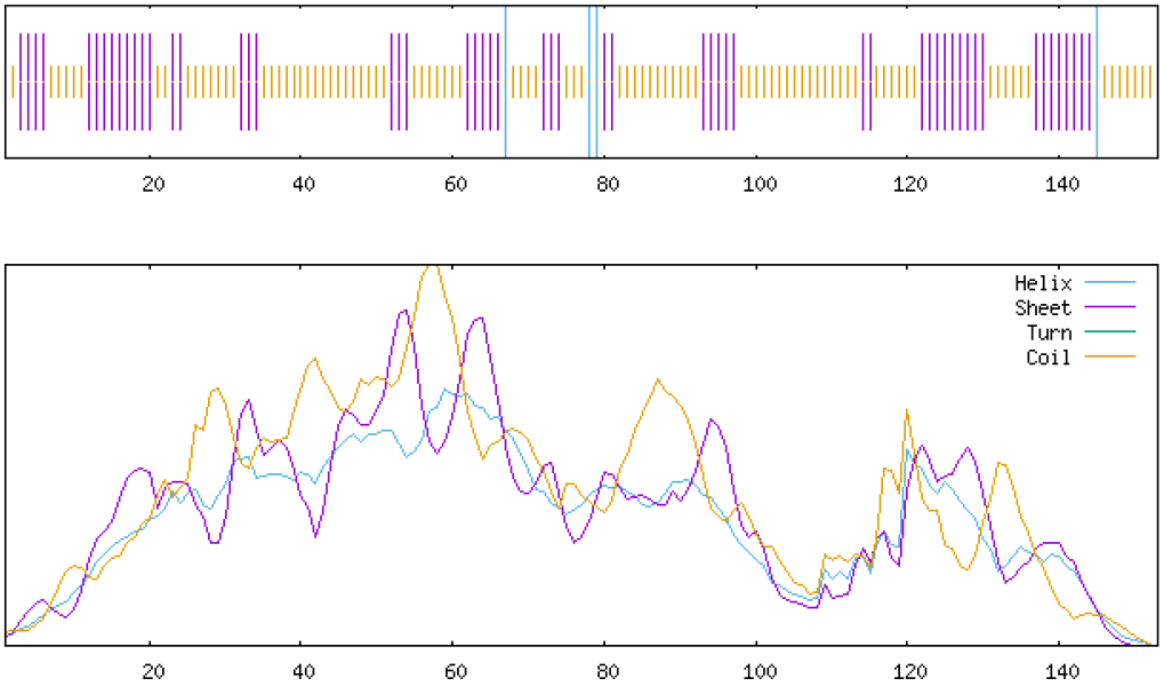

Fig. S5. Secondary structure prediction of platform construct. Secondary structure prediction of platform construct using the SOMPA server having (0%) α-helix, (35.95%) extended strand, and (60.78) % random coil.

Table S1. Population coverage based on MHC-I data.

No.	Population	Coverage[a]	Average Hit[b]	PC90[c]
1	Europe	62.52%	0.82	0.27
2	Iran	55.51%	0.69	0.22
3	North America	64.87%	0.89	0.28
4	West Indies	69.53%	0.99	0.33
5	Northeast Asia	46.32%	0.55	0.19
6	Oceania	65.43%	0.81	0.29
7	East Africa	57.99%	0.75	0.24
8	Southwest Asia	45.84%	0.56	0.18
9	East Asia	66.30%	0.85	0.30
10	North Africa	60.37%	0.80	0.25

a) Projected population coverage

b) Averaged number of epitope Hits/ HLA combinations recognized by the population

c) Minimum number of epitope Hits/ HLA combinations recognized by 90 % of the population