**Legends to Table**

**Supplementary Table S1** Predicted discontinuous B-cell epitopes in the final vaccine construct.

**Supplementary Table S2** Intermolecular interaction details between TLRs and vaccine of the docked complexes.

**Legends to figure**

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| **Supplementary Figure S1 Class combined** population **coverage of predicted T-cell epitopes (A)** World and **(B)** Indian population.  **Supplementary Figure S2** Structure prediction and modelling of the vaccine construct **(A)** 2D structure prediction and **(B)** 3D structure of the modelled vaccine.  **Supplementary Figure S3** Interacting residues of different TLR receptors with vaccine **(A)** TLR-2 with vaccine **(B)** TLR-4 with vaccine **(C)** TLR-7 with vaccine **(D)** TLR-9 with vaccine.  **Supplementary Figure S4.** Normal mode analysis of docked complex. **(A)** NMA mobility of the vaccine-TLR-2 complex with affine-model arrows, **(B)** Deformability plot, **(C)** B-factor plot, **(D)** Eigenvalue plot, **(E)** Normal mode variance plot, **(F)** Covariance map and **(G)** Elastic network.  **Supplementary Figure S5.** Normal mode analysis of docked complex. **(A)** NMA mobility of the vaccine-TLR-9 complex with affine-model arrows, **(B)** Deformability plot, **(C)** B-factor plot, **(D)** Eigenvalue plot, **(E)** Normal mode variance plot, **(F)** Covariance map and **(G)** Elastic network. |

**Supplementary Table S1** Predicted discontinuous B-cell epitopes in the final vaccine construct.

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| **S. No.** | **Discontinuous B-cell epitopes** | **Number of residues** | **Score** |
| 1 | DPLPPPLAPDFLSPPAE | 18 | 0.963 |
| 2 | GEAPPVPVAYSVNWDAIAQCESGGNWSINTGNGYYGGLRFTAGTWRANGGSGSAANASREEQIRVAENVLRSQGIRAWPVCGRR | 84 | 0.753 |
| 3 | MLRLVVGALLLVLAFAGGYAVAACKTVTLTVDGTAMRVTTMKSRVIDIVEENGFSVDDRDDLYPAAGVQVHDADTIVLRRSRPLQISLDGHDAKQVWTTASTVDEALAQLAMTDTAPASRASRVPLSGMALVSAKTVVHPVEGM | 144 | 0.741 |
| 4 | GEAAKSSAHVQELYAAYSPEKIFHVIAAYSSAGSADAPMKNARTTLIAAAGTVTTSPAGIANADDAGLDPAVGFDPNLPPAPDAAPVDTPPAPEDAGF | 99 | 0.683 |

**Supplementary Table S2** Intermolecular interaction details between TLRs and vaccine of the docked complexes.

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| **Complex** | **No. of salt bridges** | **No. of Hydrogen bonds** | **No. of Non-bonded contacts** |
| TLR-2- vaccine | - | - | 140 |
| TLR-4- vaccine | 8 | 24 | 311 |
| TLR-7- vaccine | 8 | 16 | 225 |
| TLR-9- vaccine | 4 | 24 | 258 |

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| **A graph with a line and a line  Description automatically generated with medium confidence** |
| **(A)** |
| **A graph with a line and a line  Description automatically generated with medium confidence** |
| **(B)** |
| **Supplementary Figure S1. Class combined** population **coverage of predicted T-cell epitopes (A)** World and **(B)** Indian population. |

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| A screenshot of a crossword puzzle  Description automatically generated |
| **(A)** |
| A colorful lines of wires  Description automatically generated with medium confidence |
| **(B)** |
| **Supplementary Figure S2.** Structure prediction and modelling of the vaccine construct **(A)** 2D structure prediction and **(B)** 3D structure of the modelled vaccine. |

|  |  |
| --- | --- |
| A diagram of a number of numbers  Description automatically generated with medium confidence | |
| **(A)** | |
| A diagram of a dna model  Description automatically generated with medium confidence | A screen shot of a chart  Description automatically generated |
| A diagram of a chain c vaccine  Description automatically generated | A diagram of a number system  Description automatically generated with medium confidence |
| **(B)** | |
| A diagram of a number of numbers  Description automatically generated with medium confidence | A diagram of a network  Description automatically generated |
| **(C)** | |
| A screen shot of a computer  Description automatically generated | |
| **(D)** | |
|  | |
| **Supplementary Figure S3.** Interacting residues of different TLR receptors with vaccine **(A)** TLR-2 with vaccine **(B)** TLR-4 with vaccine **(C)** TLR-7 with vaccine **(D)** TLR-9 with vaccine. | |

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| **A colorful structure of a cell  Description automatically generated with medium confidence** | | | | | |
| **(A)** | | | | | |
| A picture containing text, screenshot, plot, line  Description automatically generated | | | A picture containing text, screenshot, plot, line  Description automatically generated | | |
| **(B)** | | | **(C)** | | |
| A picture containing text, screenshot, plot, line  Description automatically generated | | | A picture containing text, diagram, plot, line  Description automatically generated | | |
| **(D)** | | | **(E)** | | |
| A picture containing text, screenshot, colorfulness, line  Description automatically generated | | | A picture containing text, diagram, line, parallel  Description automatically generated | | |
| **(F)** | | | **(G)** | | |
| **Supplementary Figure S4.** Normal mode analysis of docked complex. **(A)** NMA mobility of the vaccine-TLR-2 complex with affine-model arrows, **(B)** Deformability plot, **(C)** B-factor plot, **(D)** Eigenvalue plot, **(E)** Normal mode variance plot, **(F)** Covariance map and **(G)** Elastic network. | | | | | |
| **A colorful spiral of wires  Description automatically generated with medium confidence** | | | | | |
| **(A)** | | | | | |
| **A picture containing text, screenshot, plot, line  Description automatically generated** | | | **A picture containing text, screenshot, plot, line  Description automatically generated** | | |
| **(B)** | | | **(C)** | | |
| **A picture containing text, plot, screenshot, line  Description automatically generated** | | | **A picture containing text, diagram, plot, line  Description automatically generated** | | |
| **(D)** | | | **(E)** | | |
| **A picture containing text, screenshot, colorfulness, line  Description automatically generated** | | | **A picture containing text, diagram, line, map  Description automatically generated** | | |
| **(F)** | | | **(G)** | | |
| **Supplementary Figure S5.** Normal mode analysis of docked complex. **(A)** NMA mobility of the vaccine-TLR-9 complex with affine-model arrows, **(B)** Deformability plot, **(C)** B-factor plot, **(D)** Eigenvalue plot, **(E)** Normal mode variance plot, **(F)** Covariance map and **(G)** Elastic network. | | | | | |
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