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Class	Precision	Recall	F1-Score	Support
Negative (0)	0.97	0.98	0.98	2513
Positive (1)	0.97	0.97	0.98	2487
Accuracy	0.98	0.98	0.98	5000
Macro Avg	0.97	0.98	0.97	5000
Weighted Avg	0.97	0.98	0.98	5000

Supplementary Figure S1. (A) Confusion Matrix for Antigen Prediction Model Over 100 Epochs. This confusion matrix provides an in-depth evaluation of the classification performance of the antigen/epitope prediction model. The matrix indicates that the model correctly classified 2448 negative samples (non-immunogenic epitopes) and 2434 positive samples (immunogenic epitopes). There were only 65 false negatives (immunogenic epitopes misclassified as non-immunogenic) and 53 false positives (non-immunogenic epitopes incorrectly predicted as immunogenic). These results highlight the model's high precision and recall, reducing the likelihood of false predictions. A low false-negative rate ensures that strong epitopes are not mistakenly omitted from vaccine candidate selection, while a low false-positive rate prevents the misclassification of weak epitopes, ensuring accurate antigen screening for immunotherapy and vaccine research. and (B) Classification Report for Antigen Prediction Model Over 100 Epochs.



<u>Supplementary Figure S2.</u> Epitope Immunogenicity Ranking Based on Predicted Scores. (A) This figure visualizes the immunogenicity ranking of the top-predicted CD8+ T-cell epitopes based on binding affinity and conservation scores. The YLQPRTFLL epitope (HLA-A\*02:01) ranked highest with an immunogenicity score of 0.98, suggesting a strong potential to trigger an immune response. TTDPSFLGRY and NQKLIANQF followed closely with scores above 0.90, indicating broad HLA coverage and strong antigenicity. The lower-ranked epitopes, SPRWYFYYL and LSPRWYFYY, demonstrated immunogenicity scores between 0.88 and 0.89, suggesting moderate activation potential. The ranking aids in prioritizing epitopes for vaccine design, ensuring high-confidence selection of immunogenic peptides for experimental validation and clinical applications, and (B) presents Top 5 Predicted CD8+ T-cell Epitopes with HLA Binding Affinity and Conservation.



**Supplementary Figure S3.** Peak Immune Response as a Function of Antigen Concentration. The immune response is highly dependent on antigen concentration, as illustrated in Figure 2, which depicts the prediction of T cell proliferation based on antigen availability. The model assumes that T cell expansion follows a saturating function, where the rate of proliferation ( $\rho$ ) is governed by antigen concentration (I) and a half-saturation constant (h). At low antigen concentrations, T cell activation remains minimal, but as antigen levels increase, proliferation accelerates, reaching a peak when antigen availability is optimal. However, beyond a certain threshold, further increases in antigen concentration do not significantly enhance proliferation, reflecting a saturation effect in immune activation. This model assumes an initial population with a proliferation rate ( $\rho$ ) of 1 division per day, sustained over one week. Such models are critical for optimizing vaccine formulations and immunotherapy strategies, as they help predict optimal antigen dosing to maximize immune activation while minimizing the risks of T cell exhaustion. Al-driven modeling approaches can further refine these predictions by incorporating real-time patient data, enhancing precision in immune response forecasting and personalized treatment strategies.