AI and bioinformatics for accelerating peptide-based vaccine discovery in infectious diseases response.

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Abstract

Global infectious diseases continue to pose significant threats to public health, highlighting the urgent need for faster, safer, and more adaptable vaccine development strategies. Peptide-based vaccines offer a promising alternative to conventional approaches because they can be designed in silico and synthesised rapidly, reducing reliance on whole-pathogen culture and enabling more agile responses to emerging and re-emerging outbreaks (1). This project explores how artificial intelligence (AI) and immunoinformatic can strengthen and accelerate early-stage peptide vaccine discovery for global infectious disease response (2,3).

Modern in silico vaccine design combines a range of computational approaches, including B-cell and T-cell epitope prediction, antigenicity and immunogenicity assessment, allergenicity screening, population coverage analysis, sequence conservation analysis, structural modelling, molecular docking, molecular dynamics simulation, and immune response simulation (1,3). Together, these methods support the efficient identification, screening, and prioritisation of promising vaccine candidates before laboratory validation and clinical investigation, particularly for emerging, diverse, and complex pathogens (1,3).

Positioned within translational medicine, this project highlights the potential of AI-enabled bioinformatics to bridge the gap between large-scale biological data and clinically relevant vaccine innovation (2,3). It also reflects the broader shift towards precision-focused healthcare by recognising pathogen diversity and host immune variability (1). Overall, the project highlights how computational vaccine discovery advances can improve outbreak preparedness, support personalised approaches to vaccine design, and strengthen future healthcare responses to global infectious disease challenges across diverse populations and health systems.

Reference

1.Shukla P, Pandey P, Prasad B, Robinson T, Purohit R, D'Cruz LG, et al. Immuno-informatics analysis predicts B and T cell consensus epitopes for designing peptide vaccine against SARS-CoV-2 with 99.82% global population coverage. Briefings in bioinformatics 2022;23(1):bbab496.
2.Villanueva-Flores F, Sanchez-Villamil JI, Garcia-Atutxa I. AI-driven epitope prediction: a systematic review, comparative analysis, and practical guide for vaccine development. npj Vaccines 2025;10(1):207.
3.Rawat SS, Keshri AK, Kaur R, Prasad A. Immunoinformatics approaches for vaccine design: a fast and secure strategy for successful vaccine development. Vaccines 2023;11(2):221.