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Review Article

Artificial Intelligence in Vaccine Design and Optimisation for Infectious Diseases: A Review

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Abstract

The integration of artificial intelligence (AI) into vaccine development has revolutionised the traditional paradigm of vaccinology, significantly accelerating the timeline from pathogen identification to clinical deployment. This review examines the transformative role of AI technologies, including machine learning, deep learning, and neural networks, in various stages of vaccine design and optimisation for infectious diseases. We conducted a comprehensive literature search of PubMed, Scopus, Web of Science, and Google Scholar databases for publications from 2020 to 2025 using keywords: artificial intelligence, machine learning, deep learning, vaccine design, epitope prediction, infectious diseases, and immunoinformatics. Studies focusing on AI applications in vaccine development pipeline stages were included. We explore AI applications in antigen selection, epitope prediction, immunogen design, adjuvant identification, clinical trial optimisation, and manufacturing processes. Recent advances in graph neural networks, transformer-based architectures, and generative models have enhanced prediction accuracy and enabled the discovery of previously overlooked immunogenic epitopes. Despite these remarkable achievements, challenges persist in data quality, model interpretability, regulatory frameworks, and equitable global implementation. This review synthesises current evidence from 2020-2025 and provides insights into future directions for AI-driven vaccine development against emerging infectious threats.

Keywords: Artificial Intelligence; Machine Learning; Vaccine Design; Epitope Prediction; Infectious Diseases; Immunoinformatics

Introduction

Vaccine development represents one of humanity's most significant public health achievements, preventing millions of deaths annually from infectious diseases. However, traditional vaccine development is notoriously protracted, resource-intensive, and costly, typically requiring 10-15 years and approximately $900 million to bring a candidate from concept to market [1,2]. The COVID-19 pandemic dramatically demonstrated both the urgent need for rapid vaccine development and the potential of artificial intelligence (AI) to accelerate this process, with mRNA vaccines progressing from viral sequence to regulatory approval in less than one year [3,4].

AI encompasses a broad spectrum of computational approaches, including machine learning (ML), deep learning (DL), natural language processing (NLP), and neural networks, which can analyse vast datasets to identify patterns, make predictions, and optimize complex biological processes [5,6]. In vaccinology, AI has emerged as a transformative tool that expedites antigen discovery, enhances immunogen design, predicts immune responses, and optimizes clinical trial designs [7,8]. The integration of AI with multi-omics technologies, structural biology, and systems immunology has created unprecedented opportunities to design safer, more effective vaccines against both established and emerging infectious threats [9,10].

This narrative review examines the current state and future prospects of AI applications across the vaccine development pipeline, focusing on infectious diseases. We synthesize recent literature from 2020-2025 to provide a comprehensive overview of AI methodologies, achievements, challenges, and emerging trends in computational vaccinology.

AI technologies in vaccine development

Machine learning approaches

Machine learning algorithms form the foundation of AI-driven vaccine discovery, employing various statistical and computational methods to learn from immunological data. Traditional ML techniques, including random forests (RF), support vector machines (SVM), gradient boosting, and logistic regression, have been extensively applied to antigen prioritisation, epitope scoring, and immunogenicity prediction [11,12]. These algorithms excel at processing structured data from experimental assays, genomic sequences, and protein structures to predict vaccine candidates with optimal safety and efficacy profiles [13]. Table 1 presents the AI-Technologies and Computational Approaches in Vaccine Development.

Deep learning architectures

Deep learning has revolutionised vaccine design by leveraging neural network architectures capable of learning hierarchical representations from complex, high-dimensional biological data [14,15]. Convolutional neural networks (CNNs) have been successfully applied to analyse protein sequences and structures, identifying spatial patterns associated with epitope regions. Recurrent neural networks (RNNs) and long short-term memory (LSTM) networks excel at capturing sequential dependencies in amino acid sequences, essential for predicting T-cell epitopes and MHC binding affinity [16].

Recent advances include transformer-based architectures, such as EpiBERTope, which leverage pre-trained language models to predict both linear and conformational B-cell epitopes with improved accuracy and interpretability [17]. Graph neural networks (GNNs) represent a paradigm shift by modelling protein structures as three-dimensional interaction graphs, enabling more accurate prediction of conformational epitopes. Models like GraphBepi and EpiGraph have demonstrated substantial improvements over traditional methods, achieving ROC-AUC scores exceeding 0.75 for B-cell epitope prediction [18].

Generative models

Generative adversarial networks (GANs) and variational autoencoders (VAEs) have opened new frontiers in rational immunogen design by generating novel protein sequences and structures optimised for immunogenicity [19]. These models can create diverse multi-epitope vaccine constructs that maximise population coverage while minimising autoimmunity risks. The Linear Design AI tool exemplifies this approach, optimising mRNA vaccine sequences to enhance stability and translational efficiency, reportedly increasing antibody responses up to 128-fold compared to conventional designs [20]. Figure 1 presents the AI-powered vaccine development pipeline.

Comprehensive illustration of the AI-powered vaccine development pipeline showing integration of computational

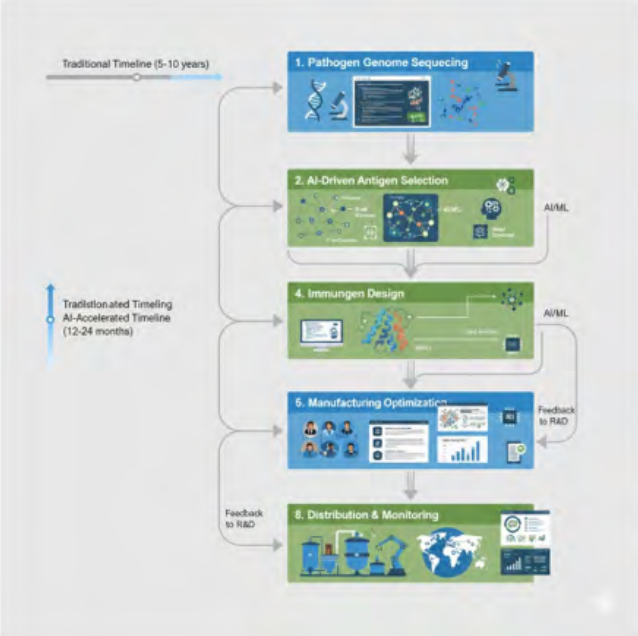

Figure 1: AI-Powered Vaccine Development Pipeline.

Sources: Adapted from references [4,5].

approaches from pathogen identification through to vaccine deployment and post-marketing surveillance. The diagram displays eight key stages: (1) Pathogen Genome Sequencing, (2) AI-Driven Antigen Selection, (3) Epitope Prediction with neural networks processing B-cell and T-cell epitopes, (4) Immunogen Design showing 3D protein structure optimization, (5) In Silico Testing with computer simulations, (6) Clinical Trials with patient cohorts and data analytics, (7) Manufacturing Optimization with bioreactor illustrations, and (8) Distribution and Monitoring with global map and surveillance dashboard. Each stage shows AI/ML integration with timeline comparisons between traditional (10-15 years) and AI-accelerated approaches (2-5 years).

AI applications across the vaccine development pipeline

Antigen selection and epitope prediction

The initial challenge in vaccine development is identifying which pathogen components will elicit protective immunity. Reverse vaccinology uses computational approaches to screen entire pathogen genomes for potential vaccine targets [21]. AI has dramatically enhanced this process by integrating diverse data types to prioritise antigens based on predicted immunogenicity, accessibility, and conservation across strains [22,23].

Machine learning models like Vaxign-ML integrate multiple algorithms to rapidly evaluate vaccine candidates based on antigenicity and host-pathogen interactions, successfully applied to emerging pathogens including Nipah and Ebola viruses [17]. For B-cell epitopes, traditional methods achieved modest accuracy (ROC-AUC ≈0.66-0.75), but graph neural networks have substantially improved performance by capturing spatial relationships in protein structures. GraphBepi, which integrates AlphaFold2-predicted structures with edge-enhanced GNN and BiLSTM encoders, outperforms previous methods by over 5.5% in ROC-AUC and 44% in precision-recall metrics [18].

T-cell epitope prediction focuses on peptide-MHC binding and T-cell receptor recognition. Models like GraphMHC simulate MHC-peptide complexes as 3D atomic interaction graphs, achieving ROC-AUC scores of approximately 0.92, significantly surpassing sequence-based approaches [18]. Table 2 shows the performance comparison of AI-based epitope prediction tools.

Prediction Tool	Year	Epitope Type	Methodology	Performance Metrics	Key Innovation
GraphBepi	2023	B-cell (conformational)	Edge-enhanced GNN + BiLSTM + AlphaFold2 structures	ROC-AUC: 0.75; PR-AUC: +44% vs. previous	Integration of predicted structures with GNN architecture
EpiGraph	2024	B-cell (conformational)	GAT + ESM embeddings	ROC-AUC: 0.73	Combined structural and sequence embeddings
GraphMHC	2024	T-cell (MHC-I and II)	3D atomic interaction graphs + attention	ROC-AUC: 0.92	Attention mechanism identifies critical residues

HeteroTCR	2024	T-cell (TCR binding)	Heterogeneous graph networks	Improved ROC-AUC across multiple datasets	Multi-hop message passing for TCR-peptide interactions
Vaxign-ML	2020	Vaccine candidate	Multiple ML algorithms + DNN	Applied to Nipah, Ebola pathogens	Integrates antigenicity with host-pathogen features
DiscoTope 2.0	Traditional	B-cell (conformational)	Geometric heuristics	ROC-AUC: 0.66	Baseline traditional method
SEPPA 3.0	Traditional	B-cell (conformational)	Propensity scales	ROC-AUC: 0.75	Baseline traditional method

Table 2: Performance Comparison of AI-Based Epitope Prediction Tools.

Sources: *Author's methodology based on references [1,17,18].*

Schematic representation of graph neural network architecture for structure-based epitope prediction, demonstrating the conversion of 3D protein structures into graph representations and subsequent prediction of immunogenic regions. The diagram shows three main components: (1) Left panel displays a 3D protein structure (antibody-antigen complex) being converted into a molecular graph with nodes representing amino acid residues and edges representing spatial interactions, (2) Center panel illustrates GNN layers with message passing between nodes, attention mechanisms highlighted with glowing connections showing critical residues, and feature aggregation processes, (3) Right panel presents the output showing predicted epitope regions highlighted in red on the protein surface with confidence scores and statistical metrics. The diagram includes mathematical notations for graph convolution operations and a small inset showing AlphaFold2 predicted structure integration.

Immunogen design and clinical trial optimisation

Beyond epitope identification, AI facilitates the rational design of complete immunogens with optimal structural and immunological properties [24]. Deep learning models predict protein folding, stability, and immunogenicity, enabling the design of novel antigens that do not exist in nature but elicit desired immune responses. Multi-epitope vaccine design benefits significantly from AI, which can combine multiple T-cell and B-cell epitopes with appropriate linkers and adjuvants to create chimeric constructs that provide broad population coverage [25,26].

AI has transformed clinical trial design through predictive analytics that optimise patient recruitment, identify suitable cohorts based on genetic and immunological markers, and simulate trial outcomes [27,28]. Adaptive trial designs powered by AI enable real-time data analysis, allowing researchers to modify protocols based on interim results, potentially reducing trial duration and costs. Machine learning algorithms can predict adverse events by analysing safety databases and clinical records, enhancing pharmacovigilance during vaccine development [29]. Figure 2 shows the graph of the neural network architecture for epitope prediction, and Figure 3 shows the AI-enhanced clinical trial optimisation framework.

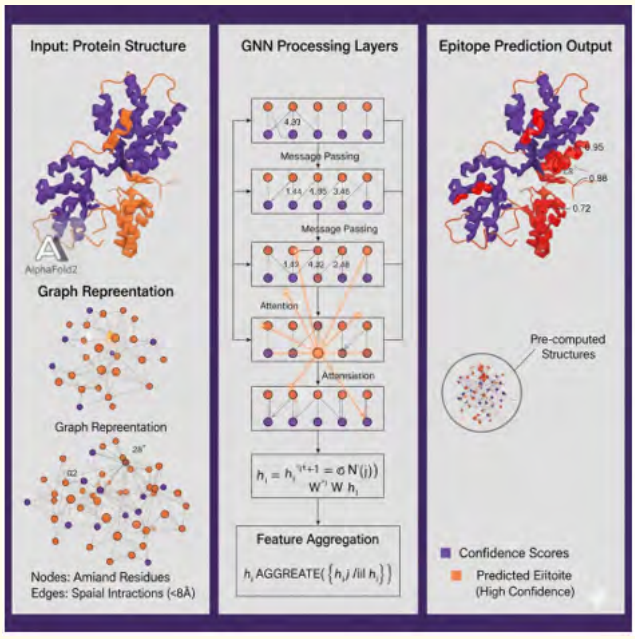

Figure 2: Graph Neural Network Architecture for Epitope Prediction.

Sources: *Author's methodology based on references [1,18].*

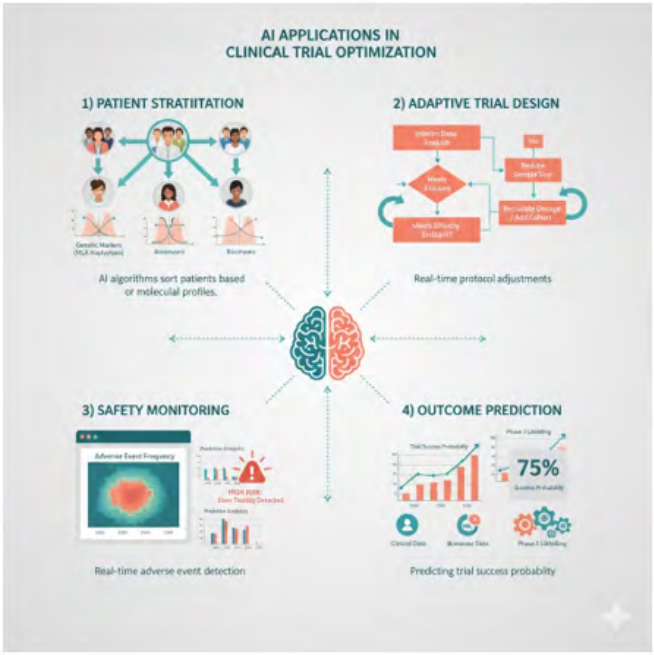

Figure 3: AI-Enhanced Clinical Trial Optimisation Framework.

Sources: *Author's illustrations based on references [12,27-28].*

Integrated framework showing artificial intelligence applications in clinical trial optimisation, including patient stratification based on genetic markers (HLA haplotypes) and biomarkers, adaptive trial design with real-time protocol adjustments based on interim data analysis, safety monitoring through predictive analytics with warning indicators and alert systems for adverse events, and outcome prediction using machine learning models processing clinical data. The framework demonstrates how AI reduces trial duration by 20-30% while improving safety profiles and patient outcomes. The diagram features four interconnected quadrants centred around an AI brain icon, with data visualisation elements including bar charts showing patient stratification, flowcharts for adaptive design decision nodes, real-time monitoring dashboards, and probability curves for outcome predictions.

Manufacturing and distribution

AI extends beyond discovery and development to manufacturing and distribution. Predictive models optimise bioreactor conditions, monitor product quality in real-time, and forecast yield variations. For temperature-sensitive vaccines like mRNA formulations, AI-driven supply chain logistics ensure optimal cold-chain management, critical for global vaccine distribution (30). Table 3 gives the AI-applications across the vaccine development lifecycle, and Figure 4 illustrates the multi-epitope vaccine design using generative AI.

Development Stage	AI Application	Specific Tasks	Impact on Timeline	Success Examples
Discovery and Antigen Selection	Reverse vaccinology, genome screening	Pathogen genome analysis, antigen prioritisation, conserved epitope identification	Reduces from 5-15 years to 1-2 years	Vaxign-ML for Nipah/Ebola; NERVE 2.0 platform
Epitope Prediction	ML/DL models, GNNs	B-cell and T-cell epitope identification, MHC binding prediction	Months saved in experimental screening	GraphBepi (5.5% improvement); GraphMHC (ROC-AUC 0.92)
Immunogen Design	Generative models, structural prediction	Multi-epitope constructs, sequence optimisation, stability enhancement	Weeks to months for design iteration	Linear Design (128x antibody response); AlphaFold2 integration
Clinical Trials	Predictive analytics, adaptive design	Patient stratification, cohort selection, outcome prediction, and real-time monitoring	20-30% reduction in trial duration	COVID-19 adaptive trial designs

Manufacturing	Process optimization, quality control	Bioreactor optimisation, yield prediction, contamination detection	15-25% efficiency improvement	mRNA vaccine scale-up optimization
Distribution and Monitoring	Supply chain optimisation, pharmacovigilance	Cold-chain logistics, demand forecasting, and adverse event detection	Improved distribution efficiency	COVID-19 vaccine distribution planning

Table 3: AI Applications Across the Vaccine Development Lifecycle.

Sources: *Author's compilations based on references [1,17,18,20,22-24,27-30].*

ML: Machine Learning; DL: Deep Learning; GNN: Graph Neural Network; MHC: Major Histocompatibility Complex; ROC-AUC: Area Under the Receiver Operating Characteristic Curve.

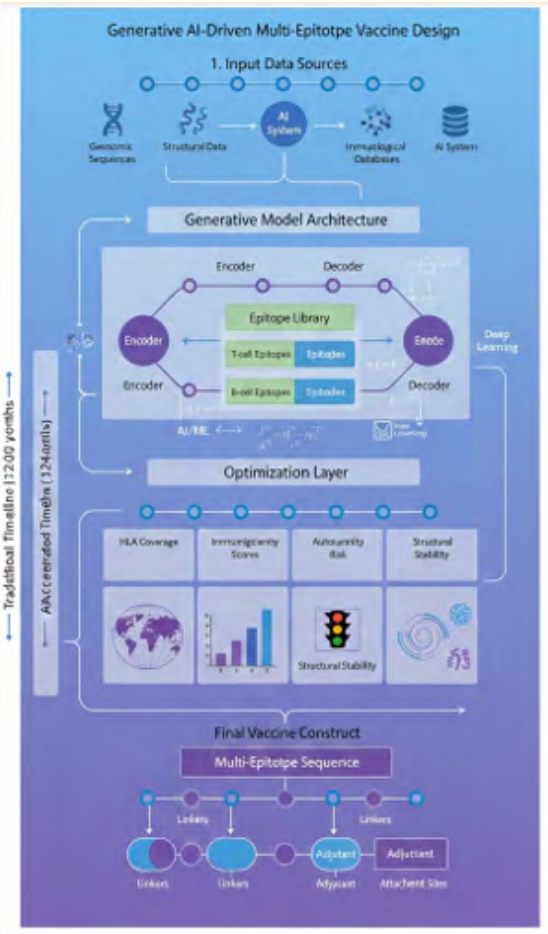

Figure 4: Multi-Epitope Vaccine Design Using Generative AI.

Sources: *Author's illustration Based on concepts from references [19,20,25].*

Generative artificial intelligence workflow for designing multi-epitope vaccine constructs, showing integration of epitope selection, optimisation parameters including HLA coverage and immunogenicity scores, and final construct assembly. The workflow demonstrates how generative models (GAN/VAE architecture) combine T-cell epitopes (shown in green boxes) and B-cell epitopes (shown in blue boxes) with appropriate linkers and adjuvant attachment sites to maximise population coverage while minimising autoimmunity risks. The diagram includes four main sections: input data sources (pathogen genomic sequences, structural data, immunological databases), generative model architecture with encoder-decoder structure, optimization layer showing selection criteria with world maps for HLA coverage percentages, immunogenicity bar charts, autoimmunity risk indicators (red/yellow/green traffic light system), and structural stability folding simulations, culminating in the final vaccine construct showing the assembled multi-epitope sequence with molecular detail.

Recent achievements and case studies

COVID-19 vaccines

The COVID-19 pandemic provided the most dramatic demonstration of AI's potential in vaccine development. AI algorithms rapidly identified the spike protein receptor-binding domain as the optimal antigen target, analysed epitope conservation across viral variants, and optimised mRNA sequences for stability and expression [3,4]. Companies like Moderna and Pfizer-BioNTech leveraged AI platforms to accelerate antigen design, reducing development timelines from years to months.

Emerging infectious diseases

AI-driven reverse vaccinology has been applied to numerous emerging pathogens, including the dengue virus, Zika virus, and multidrug-resistant bacteria. Rapid computational screening enables researchers to design vaccine candidates within days of pathogen genome sequencing, dramatically improving pandemic preparedness [22,23]. Figure 5 timeline Comparison and Global Impact of AI in Vaccine Development.

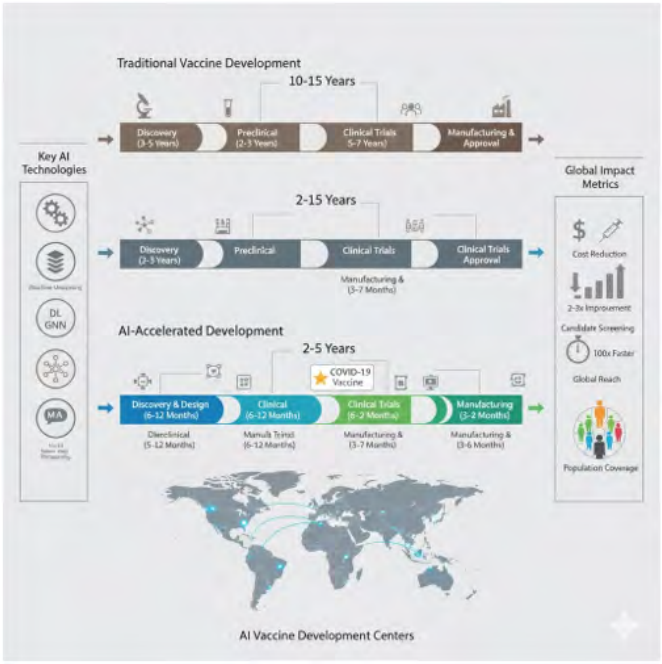

Figure 5: Timeline Comparison and Global Impact of AI in Vaccine Development.

Sources: *Data compiled from references [3,4,8].*

Comparative analysis of traditional versus AI-accelerated vaccine development timelines, demonstrating dramatic reductions in development duration from 10-15 years to 2-5 years (with COVID-19 achieving <1 year as a breakthrough case study highlighted with a gold star). The figure shows two parallel timeline tracks: the top track displays traditional vaccine development in grey/brown tones with major milestones (Discovery 3-5 years, Preclinical 2-3 years, Clinical Trials 5-7 years, Manufacturing 1-2 years), while the bottom track shows AI-accelerated development in vibrant blue/green with compressed durations for the same milestones. Side panels display key AI technologies employed (Machine Learning, Deep Learning, Graph Neural Networks, Natural Language Processing) on the left, and global impact metrics on the right showing cost reduction (50-70%), success rate improvement (2-3x), and candidate screening acceleration (100x faster) with icons and visualisations. A world map illustrates the global distribution of AI-enabled vaccine research centres, highlighting international collaboration and technology adoption.

Challenges and limitations

Despite remarkable progress, several challenges impede the full realisation of AI's potential in vaccine development [7,8].

Data quality and model interpretability

AI models require large, high-quality datasets for training, but immunological data is often fragmented, heterogeneous, and biased toward well-studied pathogens and populations. Many epitope databases lack standardisation in assay conditions and outcome measures, complicating model development and validation. Deep learning models often function as "black boxes," providing predictions without mechanistic explanations, posing challenges for scientific understanding and regulatory acceptance.

Overfitting and Regulatory Considerations

Recent benchmarking studies reveal that many epitope prediction models suffer from overfitting to training datasets, limiting their performance on novel pathogens [18]. Prospective validation using blinded predictions for emerging diseases remains critical to assess true model generalizability. Current regulatory frameworks lack clear guidelines for AI-driven vaccine development, requiring collaboration between AI developers, immunologists, regulators, and ethicists to establish standardised performance metrics and approval pathways.

Global equity

AI infrastructure, computational resources, and expertise are concentrated in high-income countries, potentially exacerbating vaccine inequity. Ensuring that AI-accelerated vaccine development benefits low- and middle-income countries requires capacity building, technology transfer, and sustained funding.

Future Directions

The future of AI in vaccine development lies in several promising directions. Integration of multi-omics data (genomics,

transcriptomics, proteomics, metabolomics) with single-cell technologies will provide unprecedented resolution of immune responses, enabling more precise vaccine design. Explainable AI (XAI) methods will enhance model interpretability, building trust among scientists and regulators. Prospective validation studies, where AI predictions are tested before experimental results are available, will better demonstrate model utility. The convergence of AI with synthetic biology and automated laboratories promises to create closed-loop systems where computational predictions are rapidly validated experimentally, iteratively refining vaccine designs.

Conclusion

Artificial intelligence has emerged as a transformative force in vaccine development, offering unprecedented speed, accuracy, and innovation in the fight against infectious diseases. From antigen discovery and epitope prediction to clinical trial optimization and manufacturing, AI technologies have demonstrated their capability to accelerate every stage of the vaccine pipeline. The COVID-19 pandemic showcased both the potential and limitations of these approaches, highlighting the critical need for continued investment in data infrastructure, methodological development, and regulatory harmonization.

As AI technologies continue to evolve, their integration with emerging fields like structural biology, systems immunology, and synthetic biology promises to revolutionize our approach to preventing infectious diseases. However, realizing this potential requires addressing persistent challenges in data quality, model interpretability, equitable access, and regulatory acceptance. Through interdisciplinary collaboration and sustained commitment to both technological innovation and global health equity, AI-driven vaccine development can substantially reduce the burden of infectious diseases worldwide.

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Conflict of Interest

The authors declare no competing interests.

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