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Advances in Computational Vaccinology: From Antigen Discovery to Immune Simulation

Shiying Yu
Biotechnology Research Center, Cuixi Academy of Biotechnology, Zhuji, 311800, China
Corresponding author: shiying.yu@cuixi.org

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Abstract Computational vaccinology, as an emerging interdisciplinary subject integrating bioinformatics, immunology and systems biology, is profoundly transforming the vaccine research and development process. This study systematically reviews the key advancements in the field of computational vaccinology, covering theoretical foundations, core technologies, and practical application scenarios. It examines the background of the shift in vaccine development from traditional methods to computational strategies, and introduces genomic-based antigen screening methods (reverse vaccinology), epitope prediction algorithms, and the application of structural bioinformatics in antigen design The integrated application of immunoinformatics tools and databases was explored, especially the value of multi-omics data in refined antigen analysis. The practical value of computational vaccinology was demonstrated through multiple actual cases (such as AI-assisted COVID-19 vaccine development, multi-epitope vaccine design for tuberculosis and malaria, as well as tumor neoantigen prediction and clinical transformation). This study reveals the crucial role of computational vaccinology in enhancing the efficiency of vaccine development, reducing costs, responding to emerging infectious diseases, and achieving personalized immunization strategies. At the same time, it provides theoretical basis and technical prospects for the future construction of AI-driven automated vaccine platforms.

Keywords Computational vaccinology; Reverse vaccinology; Epitope prediction; Immune simulation; Vaccine design

1 Introduction

How were vaccines made in the past? Most of the time, it relies on experience - detoxification, inactivation, and then trying bit by bit (Li et al., 2024). Although these methods are indeed effective, the process is slow, the cost is considerable, and they are often inadequate in dealing with new pathogens (He and Wang, 2024). In recent years, computational vaccinology has gradually come to the fore, not because it is "high-end and sophisticated", but because it is indeed more practical in saving time and costs. After the integration of genomic, proteomic and immune data, antigen screening is no longer a blind exploration. New methods such as reverse vaccinology and immunoinformatics have begun to provide precise targets, especially in dealing with infectious diseases and cancers, and have been proven to have obvious advantages (Basmenj et al., 2025).

However, no matter how good the tools are, it still depends on how they are used. The computing platforms that many researchers rely on nowadays are no longer merely analytical tools; they are more like the "experimental front desk" for vaccine development. Platforms like iVAX package epitope localization, antigen construction, and immune simulation, and also come with data visualization and resource databases. As long as the models are reasonable and the data are reliable, they can even preliminarily determine which antigens have potential before the vaccines enter the laboratory (Moise et al., 2015). Of course, computational models are not omnipotent, especially when it comes to new variant strains. Whether the algorithm can keep up is a question. However, from the overall trend, the progress of AI algorithms and structural modeling has indeed greatly compressed the time of the prediction work that originally took several years to complete. Therefore, computational vaccinology is regarded as the "standard tool" for the next stage of vaccine research and development (Nag et al., 2025; Tang et al., 2025).

This study reviews the latest advancements in the field of computational vaccinology, with a focus on the entire process from antigen discovery to immune simulation. It also explores the challenges and future development

directions of integrating multi-omics data and artificial intelligence to enhance vaccine efficacy and safety. Through a comprehensive analysis of existing research and tools, this paper emphasizes the transformative impact of computational methods on the fields of immunology and public health, highlighting their significant role in the rapid response to infectious disease outbreaks and personalized vaccine design, with the aim of accelerating vaccine development.

2 Computational Approaches for Antigen Discovery

2.1 Genome-based vaccine target identification (reverse vaccinology)

Traditionally, finding suitable vaccine targets often requires step-by-step screening through experiments, but this method is time-consuming and limited. Reverse vaccinology bypasses this. It does not cultivate bacteria but directly starts from the genome, screening for genes that encode surface or secreted proteins, which are usually virus-related and more easily recognized by the immune system. Of course, this strategy is not applicable to every pathogen, but it has been proven in multiple cases to identify potential antigens (Rawal et al., 2021). When screening, it is not only necessary to look at antigenicity, but also to consider whether these proteins have homology with the host. If they are too similar to human proteins, they may instead cause immune side effects. These computational processes are like multi-layer filters, sifting out candidate antigens layer by layer and laying the foundation for subsequent immunoinformatics analysis.

2.2 Epitope prediction algorithms (B-cell and T-cell epitopes)

Predicting epitopes may sound highly technical, but the logic is actually quite simple: it's about identifying which fragments can be recognized by the immune system. B-cell epitopes are usually regions that antibodies can directly recognize, while T-cells pay more attention to whether peptides can bind to MHC molecules. The problem is that there are too many combinations of TCR and MHC, and it is difficult to exhaust all possibilities relying on experience. For this reason, more and more algorithms have introduced machine learning models, especially performing well in identifying T-cell epitopes. Many tools have been able to balance affinity and specificity prediction (Zhang et al., 2021; Gao et al., 2023). Although the accuracy rate still cannot be compared with that of experiments, in the early screening stage, it can greatly improve efficiency and also help to find some conserved regions that are not easily detectable but have strong immunogenicity.

2.3 Applications of structural bioinformatics in antigen design

Vaccine design without structural information is like picking a key to unlock with eyes closed. Structural bioinformatics is precisely the toolbox for solving this problem. It can tell us how antigens and antibodies "adhere", which epitopes are stereoscopically exposed and which may be hidden. By means of computational simulation and docking technology, it is possible to predict in advance whether the antigen design is reasonable. In recent years, some models have incorporated machine learning algorithms, which can predict antibody affinity and binding sites more accurately (Mason et al., 2021; Wilman et al., 2022). Of course, all of this is based on a reliable structural template. If the pathogen is a "structural blind box", modeling will be limited. Even so, integrating structural information with sequence prediction results can still provide a more realistic conformational basis for vaccine design and enhance its immune effect in vivo.

3 Immunoinformatics and Data Integration

3.1 Vaccine development databases and resources (e.g., IEDB, VaxiJen)

Often, the first step in vaccine design is not in the laboratory but in the database. Platforms like IEDB contain tens of thousands of verified B-cell and T-cell epitope information. It is more like a constantly updated "immune map", and researchers can hardly do without it. On the other side, tools like VaxiJen simply do not even consider the structure and directly predict antigenicity based on the sequence, enabling the screening of potential vaccine candidate proteins without the need for comparative analysis. Although these databases and tools cannot replace experimental verification, they do indeed speed up the antigen screening process significantly. Especially when the research is confronted with a large number of candidate proteins, having a system that can automatically prioritize them is much more efficient than relying solely on intuition (Oli et al., 2020). Of course, the prerequisite is that these databases should be updated in a timely manner and have friendly entry points; otherwise, no matter how good the resources are, they won't be able to play their role.

3.2 Sequence alignment, motif search, and homology modeling techniques

Identifying key regions on proteins does not always rely on experience. Sometimes, a fragment that is conserved across species often conceals crucial immune information. At this point, sequence alignment and motif search tools come in handy. They help identify stable fragments that may trigger immune responses, and are particularly suitable for designing vaccines with high coverage rates of multiple strains. However, if these tools alone are not accurate enough, homologous modeling can fill the gap at the structural level. Even without complete structural data, as long as there is a similar template, a rough three-dimensional conformation can be pieced together. This is crucial for determining which epitopes can be exposed to the "field of view" of the immune system (Zaher et al., 2025). These tools can be used separately, but when combined, the effect is even better. They are an indispensable "intermediate stop" in many vaccine research and development processes.

3.3 Integration of multi-omics data for comprehensive antigen profiling

It is difficult to describe the full picture of an antigen through a single data source. The genome tells us "what components there are", the transcriptome says "who is being expressed", and the proteome and immunopeptide group involve "who is really at work". Relying solely on a set of data, it is very easy to miss the key links in the immune response. Although it is not easy to integrate these multi-omics data, as the data formats, analysis dimensions, and sampling time points may all be inconsistent, once they are connected, a complete picture of the interaction between pathogens and hosts can be presented. Nowadays, many new algorithms and machine learning models are being used to solve the problem of data heterogeneity. Although they are not fully automated yet, the trend is already very clear: Whoever can integrate better is likely to find new vaccine targets in advance (Anderson et al., 2025; Kamali et al., 2025). Especially in the design of personalized vaccines, multi-omics analysis can more accurately identify the most effective antigenic loci for a specific population or individual, which is a cutting-edge step in the field of computational vaccines.

4 Computational Modeling of Immune Responses

4.1 Agent-based and mechanistic models of the immune system

There is more than one path for modeling immune responses. Some models revolve around individual cells or molecules, treating them as objects that can "act", while others choose to use a set of differential equations to capture the operational rules of the immune system. Ultimately, the core objective of these methods is the same - to figure out how the immune system reacts step by step in the face of viruses, bacteria, and even vaccines. For instance, some studies have used hybrid modeling methods to investigate how IL-2 and IL-4 regulate lymphocyte activation. The simulated immune cell proliferation pathways have revealed the details of immune behavior during the infection period (Atitey and Anchang, 2022). When facing viral infections like SARS-CoV-2, mechanism models attempt to capture the dynamic interactions among viruses, immune cells, and cytokines, helping us predict the progression of the disease and even the possibility of immune clearance (Leon et al., 2023; Miroshnichenko et al., 2025). Although these models each have their own focuses, the theoretical support they provide remains indispensable for the validation of vaccine strategies or immunotherapies.

4.2 Applications of immune simulation tools (e.g., C-ImmSim, SimuLymph)

Not everyone can build an immune model from scratch. Fortunately, platforms like C-ImmSim and SimuLymph have already set up the "framework". The design concept of C-ImmSim is to string the antigenic epitope information with the characteristics of lymphocyte receptors and predict the formation of immune response and even immune memory through amino acid sequences (Rapin et al., 2010). In fact, it has been able to reproduce some classic experiments quite well, such as the influence of different MHC combinations on immune responses. SimuLymph takes a different approach. It is based on proxy modeling and pays more attention to individualized immune responses - particularly suitable for predicting the responses of certain individuals to specific immunotherapies (Figure 1) (Matalon et al., 2025). Although these tools each have their own mechanisms, they are essentially like a "digital immunity sandbox" that can test vaccine construction or treatment pathways in advance in a virtual environment.

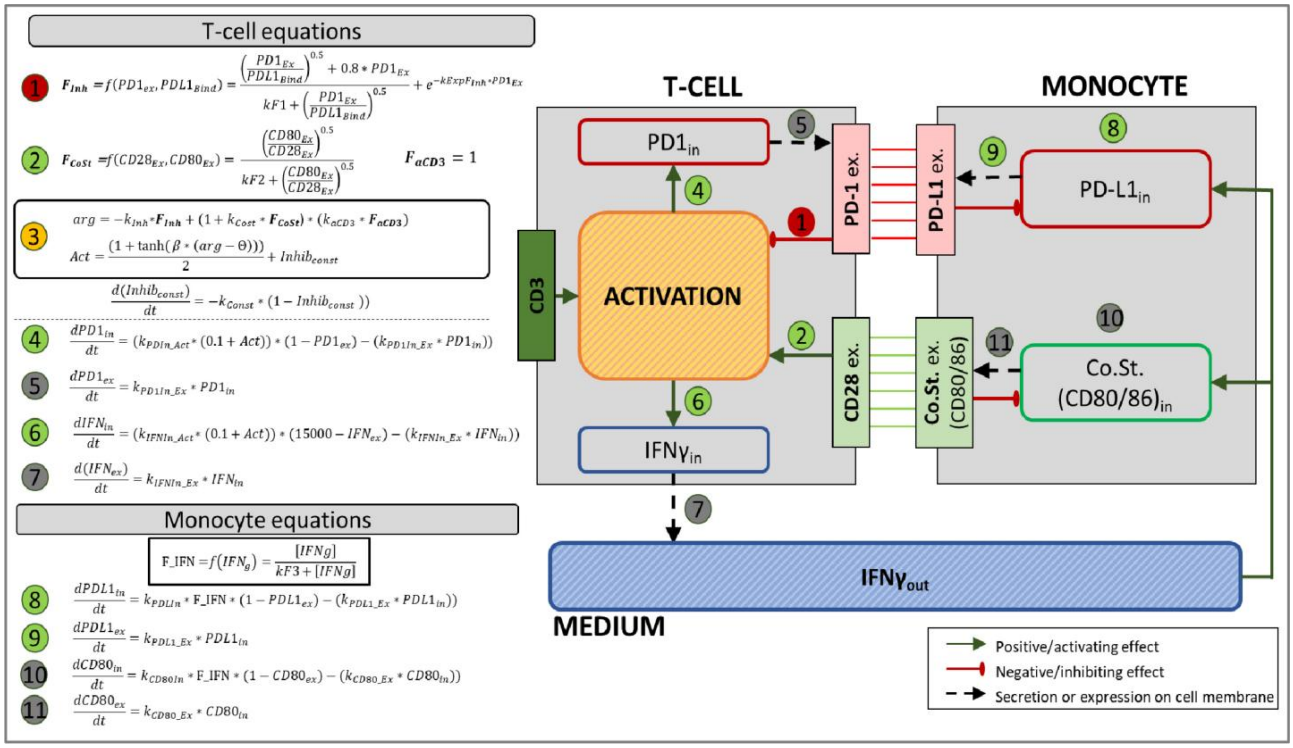

Figure 1 Summary of MLR regulatory network and corresponding equations defining the state machine (Adopted from Matalon et al., 2025)

4.3 Prediction of immunogenicity and population coverage

Designing a vaccine that is effective for the majority of people cannot be achieved merely through experiments. To know in advance which epitopes are more likely to induce immune responses, it is necessary to rely on computational prediction. The model will refer to the specificity of T-cell receptors, analyze the binding affinity of epitopes to MHC molecules, and thereby determine which candidates are more reliable. Interestingly, some machine learning models can handle nonlinear features and integrate a large number of variables - for instance, this advantage is particularly evident in complex tasks such as predicting the pertussis vaccine response (Shinde et al., 2025). As for whether the vaccine is suitable for a wide range of people, it still needs to be considered in combination with the distribution of MHC alleles in the population. Combining these predictive capabilities with immune simulation models can more effectively assess the efficacy of vaccines in advance and also help optimize immunization strategies for different populations.

5 Case Studies in Computational Vaccine Development

5.1 COVID-19: AI-assisted epitope mapping and vaccine candidate design

At the beginning of the outbreak of the epidemic, no one expected that AI would be so quickly involved in vaccine research and development. But in fact, immunoinformatics platforms like iVAX had already begun screening for conserved and immunopotential T-cell epitopes shortly after the SARS-CoV-2 genome was published. These platforms do not rely on "guessing". They predict immune responses by analyzing sequences and can even optimize the construction plan of antigens. Although traditional methods remain important, computational tools have clearly shortened the entire time window from sequencing to candidate vaccine design (De Groot et al., 2020).

5.2 Multi-epitope vaccine design for tuberculosis and malaria

For stubborn and structurally complex pathogens such as tuberculosis and malaria, the intervention of computational methods is not an added bonus; rather, it is more often the key to solving the problem. Researchers first identified antigenic proteins by combining reverse vaccinology with immunoinformatics techniques, and then selected from them the highly immunogenic epitopes that could trigger MHC Class I, II or B-cell responses. After the epitopes are assembled into a structure, linkers and adjuvants are added, somewhat like building with blocks.

This not only ensures stability but also minimizes the risk of allergies as much as possible (Figure 2). Simulation data show that the overall immune-inducing potential is good. Although there is still a way to go before clinical application, the direction is clear (Kardani et al., 2020).

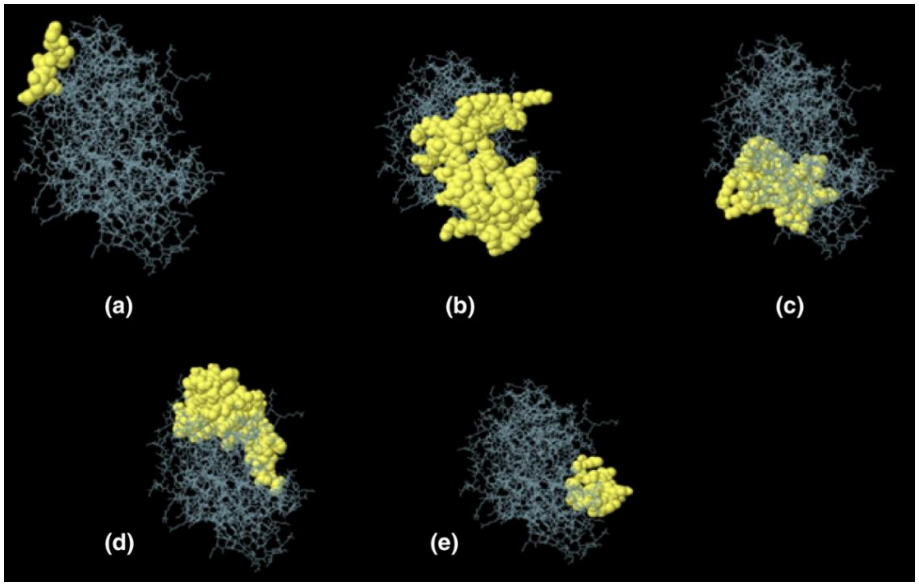

Figure 2 Discontinuous B-cell epitopes predicted by ElliPro. (A-E): 3D representation of conformational or discontinuous epitopes of the most antigenic chimeric protein from *T. cruzi* CL Brenner. Epitopes are shown as yellow surfaces, and the bulk of the protein is represented in grey sticks (Adopted from Rawal et al., 2021)

5.3 Cancer neoantigen vaccines: from prediction to clinical trials

In the field of cancer vaccines, predicting individual-specific neoantigens is becoming increasingly realistic. By using AI to analyze tumor mutation sites, identifying which fragments might become "targets", and then combining structural modeling to confirm whether they can trigger immune attacks, this set of processes is no longer just theoretical. At present, some neoantigen vaccines screened out based on these algorithms have entered the clinical trial stage. Although the mutations of each patient are different, this personalized strategy does provide a breakthrough for the design of tumor vaccines (Guarra and Colombo, 2023).

6 Challenges, Limitations, and Validation Bottlenecks

6.1 Accuracy and generalizability issues in predictive models

Calculating vaccine design is not as "automatic" as it seems. Often, the model works well on a certain type of pathogen at the beginning, but once the target is changed, its performance immediately drops. Especially when the data volume is small and the sources are diverse, many AI algorithms will fall into the trap of overfitting. This situation is not uncommon - for some models, the longer they are trained, the worse their generalization ability becomes. Not to mention that the existing data report formats are diverse. Many times, even the connection between different data becomes a problem, let alone expecting to extract from them which factors are truly meaningful for immune protection (Dalsass et al., 2019; Bravi, 2024). In other words, a model is not a universal key. The more complex the scene is, the more tailor-made algorithms and features selection skills are needed.

6.2 The necessity of experimental validation: bridging the computational-experimental gap

No matter how accurate the calculation is, it still has to pass the test. Many epitope predictions that seemed "promising" ultimately failed to pass the in vivo and in vitro experimental test. Between calculation and reality, it's not something that can be easily bridged with just a few sets of data. This also makes experimental verification the most time-consuming yet indispensable part of the entire process. Although some high-throughput technologies and community standard testing platforms have been established, to be honest, the investment cost is still high and they cannot completely replace traditional verification methods. Unless computational prediction, immune experiments and clinical research are integrated, the entire process can truly succeed. Otherwise, no matter how intelligent AI is, it can only remain at the "hypothesis" stage (Hashim and Dimier-Poisson, 2025).

6.3 Ethical, regulatory, and data privacy concerns related to vaccine AI

Not all challenges stem from technical difficulties. Once AI enters the core process of vaccine development, regulatory and ethical issues become unavoidable. Want the public to trust AI models? First, we need to figure out how these models make judgments. But strangely enough, many of the most effective models are also the most "black box" ones. In addition, the use of an individual's genomic and health data can also easily raise privacy concerns. The more such data is used, the higher the requirements for the governance framework will be. If the model also contains data bias, not only will the results be distorted, but it may also amplify the already existing health inequalities. Therefore, from algorithmic fairness to privacy protection and then to regulatory standards, behind the development of AI vaccines is actually a test of a whole set of social mechanisms (El Arab et al., 2025).

7 Future Perspectives and Technological Innovations

It is no longer news that AI is increasingly involved in vaccine research and development. But interestingly, the efficiency it has demonstrated in antigen and adjuvant screening has indeed changed many of the old methods that relied on feeling and trial in the past. Tools like convolutional neural networks and recurrent neural networks, which were previously mainly used in image and text processing, are now also being brought in to assist in the design of multi-epitope vaccines. By combining omics data and structural information, they can significantly enhance the accuracy of antigen selection. During the outbreak of COVID-19, AI-driven epitope prediction came into its own, and the pace of research and development significantly accelerated. In terms of adjuvant development, many new strategies have also moved away from the traditional trial-and-error model. By relying on the inference of immune pathways through AI models, the discovery efficiency has been accelerated and the hit rate has been improved.

However, when it comes to truly personalized vaccines, we still have to go back to the genetic level. The combination of immunogenomics and computational vaccinology has begun to make "personalized" vaccines possible. As long as the genomic and transcriptomic data of patients can be obtained, the system can predict which new antigens each person may respond to. Combined with the analysis of the immune library, the design can be targeted. This approach is particularly useful in dealing with infectious diseases where the virus mutates rapidly, such as in the direction of cancer vaccines. Some neoantigen vaccines have already shown initial effects in clinical trials. In addition, digital twin simulation and vaccine formulas customized specifically for different populations have made the protection strategies for people with different genetic backgrounds more precise, and both safety and effectiveness are more guaranteed.

Of course, a fully automated vaccine design process sounds ideal, but to be truly successful, many technical barriers still need to be overcome. At present, from antigen screening to epitope prediction and then to immune simulation, many steps can indeed be automatically processed. But the question is - can the model understand it? Is the data standard correct? Can the experiment verify whether it can be connected? All of these are still being resolved. Only when the AI process can be integrated with high-throughput experiments and regulatory frameworks can vaccine research and development truly enter the "closed-loop era". By then, the response speed to sudden infectious diseases and the capacity for large-scale production might indeed undergo a qualitative change.

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Conflict of Interest Disclosure

The author affirms that this research was conducted without any commercial or financial relationships that could be construed as a potential conflict of interest.

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