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Application of artificial intelligence in vaccine development against infectious diseases

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Abstract

Vaccine and vaccination are important components for the control of infectious diseases and reducing global mortality and morbidity. Vaccine development through existing traditional methods is often laborious, time-consuming and costly affair. However, the artificial intelligence (AI) and machine learning (ML) techniques offer unprecedented opportunities to expedite the vaccine development process. AI/ML can offer the selection and design of immunogen, epitope prediction, adjuvant identification, immune simulation, and optimisation of vaccine delivery process. AI assisted computational approaches are capable of simulating the host's immune system under different conditions and create predictive models to determine the novel targets for vaccine developments. Nevertheless, various challenges such as data heterogeneity, AI-model interpretation, and regulatory harmonization must be addressed to realise the full utilization of AI in new-generation vaccine development. Besides, the AI-aided vaccine designs must be considered for further *in vitro* and *in vivo* studies for their efficacy evaluation.

1. Introduction

Vaccine has been the most powerful invention in the history of science and medicine, playing a vital role in saving millions of both human and animal lives. A vaccine is a biological formulation designed to stimulate an immune response specific to a pathogen, aiming to reduce, prevent, and ultimately eradicate the disease it causes. The primary objective of vaccination is to induce either humoral or cell-mediated immunity, thereby stimulating the production of immunological memory that can provide protection against future infections. Vaccination is the most cost-effective and practical solution for preventing and controlling both emerging and re-emerging diseases in human and animals. However, the tradition method of vaccine development is a time-consuming process from pathogen isolation and identification of antigen to the clinical trials of the developed vaccine. In addition, the traditional methods have been associated with many challenges that hinder the efficacy and efficiency of the vaccine. The high prevalence of infectious diseases and recent emergence of new viral disease sparked the development of novel vaccine candidate using artificial intelligence (AI). In the recent years. AI and associated computational techniques completely transformed the landscape of vaccine development against infectious diseases. AI methods such as deep neural networks, artificial neural network, machine learning tools and gradient-boosting decision trees have been leveraged to predict immunogenic epitopes and that can effectively activate the host's immune system. In addition, AI has been effectively used in the analyses of immunological data, immune response prediction for vaccine efficacy, large-scale immunological data analyses and discovery of disease related biomarkers. These cutting-edge AI-based technologies along with the tried-and-tested laboratory methods offer unprecedented opportunities to accelerate vaccine design, optimize immunogen formulations, and predict immune responses with greater precision and efficiency.

2. Genesis of Artificial Intelligence

AI is the state-of-the-art and most complex scientifically developed technique under the broad discipline of computer science. Therefore, AI is a branch of computer science in which computer systems are designed to perform the tasks that mimics human intelligence. The idea of AI originated in the 1950s, when the British computer scientist Alan Turing was the first to introduce the concept of computers performing intelligent tasks. The term *Artificial Intelligence* was coined by John McCarthy in 1955 (Andresen, 2002). Although some of the current applications of AI have been in the works during the last 10-years, but the concept and ideas were developed at least 70 years back. With the dramatic increase in computational processing power, mass acquisition and digitization of data, AI has taken off with the turn of the millennium. Computational understanding of the machine has been made possible by integrating cognitive and biological data sets to develop the inventive machine learning (ML). Although there is a close relationship between AI and ML owing to their supervised learning procedure, there is a conceptual difference between AI and ML. AI is the broad concept of building devices or systems that are capable of carrying out activities that typically require human intelligence, whereas ML is a subset of AI that focuses on enabling machine to learn from data without specific programming (Gorki & Medhi, 2024). An important application of AI in the medical field and health sciences is the development of vaccine candidates against emerging and remerging pathogens. By utilizing AI-driven algorithm for vaccine antigen selection, epitope prediction, adjuvant identification and optimization strategies, vaccine candidates can be quickly designed and synthesized to address the current and emerging infectious diseases.

3. Vaccine development through traditional methods

Traditional methods in vaccine development typically involve several sequential steps such as pathogen isolation, antigen identification, scaling-up the pathogen, inactivation/live-attenuation, formulation, pre-clinical testing and clinical trials. These steps are inherently time-consuming, costly, labour-intensive and can take several years to decades to develop a vaccine from conception to market. Therefore, the traditional method of vaccine development is costly, with estimates ranging from millions to billions of dollars per vaccine (Snyder et al., 2023). The high cost is primarily attributed to R &D expenses, pre-clinical and clinical testing, regulatory approval and scaling-ups. Therefore, there is a limitation for investment in vaccine candidates for disease prevalent in low-income countries or those with limited market potential. In addition, traditional method of vaccine development often relies on empirical approaches such as selection of either whole antigen or well-characterised protein antigen which may not always yield optimal immunogenicity or safety profiles (Chen et al., 2023). Furthermore, traditional method also struggles to address the antigenic diversity of pathogen and broad-antigenic coverage. Finally, the regulatory approval for the safety, efficacy and manufacturing process of traditional vaccine may be lengthy and a costly affair (Bollaerts et al., 2024). During the recent years, emerging technologies such as genomics, bio-informatics, synthetic biology, AI-integrated reverse vaccinology offers promising opportunities to overcome the issues associated with traditional vaccine development and to accelerate the vaccine development timelines.

4. AI driven vaccine development

4.1 Design of the immunogen

Recently AI has emerged as a powerful tool for the selection and design of vaccine immunogen thereby revolutionizing the traditional vaccine development process. AI-driven algorithms can analyse vast amounts of genomic data, protein structure and immune system interaction and can lead into the rapid identification of potential vaccine candidate, this has been witnessed for the COVID-19 vaccine, where the AI algorithms played a pivotal role in identifying the novel vaccine antigens (Sharma et al., 2022). ML methodology such as deep learning and random forest can facilitate the prediction of antigenic epitopes and access the immunogenicity of selected antigen with unprecedented accuracy and efficiency (Bravi, 2024). These algorithms analyse various features of the antigen such as sequence motifs, physiochemical properties, and structural characteristics to identify the region of the pathogen that can elicit robust immune response. For example, deep learning and random forest algorithms have been used to prediction/identification of Zika virus and malaria vaccine antigen (Wistuba-Hamprecht et al., 2024) which significantly accelerated the experimental validation process. In addition, AI-driven generative models and molecular dynamics simulations empowered the rational design of immunogen with enhanced stability, immunogenicity and broad antigenic coverage for pathogens like influenza virus and SARS-CoV2. Therefore, by integrating AI algorithms with experimental validation, researchers can accelerate the vaccine development process in order to address the global health challenges on emergence of infectious diseases and antimicrobial resistance (Federico et al., 2023).

4.2 Epitope identification

Epitope identification and vaccine target represent the critical component of vaccine design, as they are essential to identify the specific region of the pathogen that can stimulate the desired immune response. AI-based algorithm has significantly accelerated the epitope prediction and prioritization of epitopes, thereby enabling the precise identification of antigenic determinants on a particular pathogen that can be recognised by the host's immune system (Ward et al., 2021). ML algorithm such as neural network, hidden Markov models and support vector machines has been commonly employed to predict the B-cell epitopes, T-cell epitopes and MHC-binding motifs. In addition, AI-driven epitope prediction algorithms can identify conserved epitopes that are shared amongst different antigenically divergent strains of the same virus, facilitating the development of broad-spectrum vaccines with cross-protective efficacy as in case of Influenza and HIV (Shanthappa et al., 2024). Therefore, with the continuous evolution of AI and computational resources, the potential for AI-driven epitope prediction to revolutionize vaccine development is unlimited.

4.3. AI-based adjuvant identification

Adjuvants are indispensable component of vaccine which augments the immune response to the antigen, thereby, enhances the overall efficacy of the vaccine. The ability of adjuvant to promote the antigen presentation, immune activation and memory response is crucial for inducing robust and long-lasting immunity to vaccine (Hemmati et al., 2024). In the recent years AI has revolutionized the process of adjuvant identification from a vast library of chemical and biological compounds and therefore, offering unique opportunity to select novel adjuvants with optimum safety and efficacy. Various machine learning models enable the identification of adjuvant candidate with desirable properties such as low toxicity, high stability and optimum immunomodulation. Through virtual screening and docking simulation, AI-driven adjuvant discovery methodologies allow the researchers to expedite the

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identification and optimization of vaccine-adjuvant formulation (Hemmati et al., 2024). In addition, AI-driven structure-activity relationship models can analyse the structure-function relationships of adjuvant molecules, as a result of which new adjuvant molecules with enhanced efficacy and safety can be synthesized for their incorporation into the final vaccine formulation.

4.4. AI-based assistance in pre-clinical and clinical trials of vaccine

AI technologies have the potential to complement lab-based experimentation, pre-clinical and clinical studies. AI can streamline various aspects of the clinical trials such as patient selection, trial design, monitoring and clinical data analyses. Based on the electronic health record and genomic data, AI-can select suitable population for clinical trials (Olawade et al., 2023). In addition, AI can optimise the clinical trial protocols by simulating various trial scenarios and predicting potential outcomes, which can help to reduce the time and costs associated with the clinical trial methods. Nevertheless, it is crucial to emphasize that AI-based methodologies are not intended to completely replace the clinical testing systems, rather it is meant to supplement the traditional clinical trials protocol, ensuring the safety, efficacy and regulatory requirements for a vaccine. Therefore, by combining AI-technologies with the existing trial methodology the vaccine development process can became more efficient, robust and time-saving in nature.

5. Challenges of AI-driven vaccine development

Although AI-driven vaccine development holds tremendous potential to transform the landscape of global health by enabling the rapid development of precision vaccine, there are several challenges associated with the technical, regulatory, ethical and practical aspect of the vaccine development. Those challenges are (i) availability of complete and heterogenous data, (ii) biological complexity, (iii) hardware requirements for running the AI-models, (iv) validation and integration of AI-methods with traditional methods, (v) intellectual property (IP) and collaboration.

Vaccine developments through AI-methodologies relies on large and high-quality diverse dataset encompassing genomic sequences, protein structures, immune response profiles and clinical outcomes. However, in-complete, noisy, biased and lack of standardised dataset can lead to unreliable predictions. In addition, handling of sensitive health and genomic data often raises privacy concerns with respect to data-sharing.

The host's immune system is highly variable and complex amongst the individual and species, making it difficult for the AI-driven vaccine construct to predict the immune response

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accurately. Furthermore, pathogen variability and frequent genetic mutations also poses challenges to AI to predict future strain and mutations and vaccines against these variants.

Additionally, the computational hardware requirements for running the AI-generated models pose a significant challenge for vaccine development as advanced algorithm often requires substantial computational power. Therefore, access to high-performance computer infrastructure is crucial for running the AI-models which may not be always available in all the research settings.

AI-driven vaccine candidates must be validated through rigorous laboratory validation and clinical trials. Although regulatory agencies have a well-established framework for evaluating the traditional vaccines based on the laboratory and clinical data, they don't have standardized regulatory framework for AI-driven vaccines such as algorithm bias and model uncertainty.

Finally, there has been no clear guideline on the IP landscape for the AI-driven vaccine. Therefore, AI-generated vaccine may fall into the legal grey areas with respect to the ownership and patentability.

6. Future Directions

By harnessing the power of AI and interdisciplinary collaboration, researchers can overcome the long-standing issues with vaccine development through the traditional methods. AI can identify the antigenic signature, predict immunogenic epitopes and optimize the vaccine formulation for enhanced safety and efficacy. AI driven models have been successful for identifying potential vaccine candidates for important infectious diseases such as HIV, tuberculosis, malaria and SARS-Cov2. During the COVID-19 pandemic, AI had played a significant role in accelerating the mRNA vaccine developments. Due to the recent advancements in genome sequencing technologies high-resolution sequence data have been generated and are plentily available in public-domain databases. These data including virus proteomes could be used as input for novel vaccine designing. Though the present AI vaccine tools heavily rely on traditional ML models for various tasks including epitope prediction, physicochemical analyses, etc. Further, generative, foundation, multi-modal AI-models have been recently successfully employed in multiple biomedical tasks. Thus, their utility can be harnessed and tested in designing novel vaccines against emerging and re-emerging infectious diseases.

Using AI, personalized vaccine tailored to individual immune systems and disease susceptibilities can be developed. By integrating omics data with machine learning pipelines

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researchers can identify biomarkers, immune signatures and genetic marker associated with vaccine-induced response variability. Therefore, personalized vaccine would be useful to improve vaccine efficacy and simultaneously reducing adverse reaction in geriatric and immunocompromised patients. AI-driven approach would also be useful for the development of cross-protective universal vaccine capable of providing broad protection against antigenically divergent strains of a pathogen. Furthermore, ML approaches can analyse viral evolution pattern to design futuristic cross-protective vaccine. In future, capacity building initiatives, training and technology transfer can empower low- and medium-income countries (LMIC) to harness the power of AI for vaccine development, there by promoting equitable access to AI driven vaccine-innovations and public health benefits.

References

Andresen, S. L. (2002). John McCarthy: father of AI. IEEE Intelligent Systems, 17(5), 84–85. https://doi.org/10.1109/MIS.2002.1039837

Bollaerts, K., Wyndham-Thomas, C., Miller, E., Izurieta, H. S., Black, S., Andrews, N., Rubbrecht, M., Van Heuverswyn, F., & Neels, P. (2024). The role of real-world evidence for regulatory and public health decision-making for Accelerated Vaccine Deployment- a meeting report. Biologicals : Journal of the International Association of Biological Standardization, 85, 101750. https://doi.org/10.1016/j.biologicals.2024.101750

Bravi, B. (2024). Development and use of machine learning algorithms in vaccine target selection. Npj Vaccines, 9(1), 15. https://doi.org/10.1038/s41541-023-00795-8

Chen, S., Quan, D. H., Sam, G., Ozberk, V., Wang, X. T., Halfmann, P., Pandey, M., Good, M. F., Kawaoka, Y., Britton, W. J., & Rehm, B. H. A. (2023). Assembly of Immunogenic Protein Particles toward Advanced Synthetic Vaccines. Small, 19(8). https://doi.org/10.1002/smll.202205819

Federico, L., Malone, B., Tennøe, S., Chaban, V., Osen, J. R., Gainullin, M., Smorodina, E., Kared, H., Akbar, R., Greiff, V., Stratford, R., Clancy, T., & Munthe, L. A. (2023). Experimental validation of immunogenic SARS-CoV-2 T cell epitopes identified by artificial intelligence. Frontiers in Immunology, 14. https://doi.org/10.3389/fimmu.2023.1265044

Gorki, V., & Medhi, B. (2024). Use of artificial intelligence in vaccine development against pathogens: Challenges and future directions. Indian Journal of Pharmacology, 56(2), 77–79. https://doi.org/10.4103/ijp.ijp_259_24

Hemmati, S., Saeidikia, Z., Seradj, H., &Mohagheghzadeh, A. (2024). Immunomodulatory Peptides as Vaccine Adjuvants and Antimicrobial Agents. Pharmaceuticals, 17(2), 201. https://doi.org/10.3390/ph17020201

Olawade, D. B., Wada, O. J., David-Olawade, A. C., Kunonga, E., Abaire, O., & Ling, J. (2023). Using artificial intelligence to improve public health: a narrative review. Frontiers in Public Health, 11. https://doi.org/10.3389/fpubh.2023.1196397

Shanthappa, P. M., Verma, N., George, A., Dhar, P. K., &Athri, P. (2024). Computational Prediction of Potential Vaccine Candidates From tRNA Encoded peptides (tREP) Using a Bioinformatic Workflow and Molecular Dynamics Validations. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 21(3), 439–449. https://doi.org/10.1109/TCBB.2024.3371984

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Sharma, A., Virmani, T., Pathak, V., Sharma, A., Pathak, K., Kumar, G., & Pathak, D. (2022). Artificial Intelligence-Based Data-Driven Strategy to Accelerate Research, Development, and Clinical Trials of COVID Vaccine. BioMed Research International, 2022(1). https://doi.org/10.1155/2022/7205241

Snyder, C. M., Hoyt, K., &Gouglas, D. (2023). An optimal mechanism to fund the development of vaccines against emerging epidemics. Journal of Health Economics, 91, 102795. https://doi.org/10.1016/j.jhealeco.2023.102795

Ward, D., Higgins, M., Phelan, J. E., Hibberd, M. L., Campino, S., & Clark, T. G. (2021). An integrated in silico immuno-genetic analytical platform provides insights into COVID-19 serological and vaccine targets. Genome Medicine, 13(1), 4. https://doi.org/10.1186/s13073-020-00822-6

Wistuba-Hamprecht, J., Reuter, B., Fendel, R., Hoffman, S. L., Campo, J. J., Felgner, P. L., Kremsner, P. G., Mordmüller, B., & Pfeifer, N. (2024). Machine learning prediction of malaria vaccine efficacy based on antibody profiles. PLOS Computational Biology, 20(6), e1012131. https://doi.org/10.1371/journal.pcbi.1012131

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