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SHORT COMMUNICATION

Utility of immunoinformatics in epitope mapping for vaccine and therapeutic design

Utilidad de la inmunoinformática en el mapeo de epítopos para el diseño de vacunas y terapias

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ABSTRACT

Epitope identification is largely the basis for the development of new vaccine candidates and immunotherapies. However, traditional methods for epitope identification present certain limitations in terms of time and high costs, hence experimentation in this field is targeted and rationalized. The development of omics, as well as the introduction of bioinformatics techniques and tools in biomedical specialties, has allowed the development of immunoinformatics, which has the capacity to speed up the discovery process. The present communication aims to describe the potential of immunoinformatics in epitope mapping for the design of vaccines and therapies.

Keywords: Immunoinformatics; Vaccines; Epitopes; Antigens; Computational Biology; Vaccine Development.

RESUMEN

La identificación de epítopos constituye en gran medida las bases para el desarrollo de nuevos candidatos vacunales e inmunoterapias. Sin embargo, los métodos tradicionales para la identificación de epítopos presentan ciertas limitaciones en cuanto tiempos y elevados costos, de ahí que la experimentación en este campo sea orientada y racionalizada. El desarrollo de las ómicas, así como la introducción de técnicas y herramientas de bioinformática en las especialidades biomédicas ha permitido el desarrollo de la inmunoinformática, la cual posee la capacidad de agilizar los procesos de descubrimiento. La presente comunicación tiene como objetivo describir las potencialidades de la inmunoinformática en el mapeo de epítopos para el diseño de vacunas y terapias.

Palabras clave: Inmunoinformática; Vacunas; Epítopos; Antígenos; Biología Computacional; Desarrollo de Vacunas.

INTRODUCTION

Epitope mapping—the precise identification of regions of an antigen recognized by the immune system—is a cornerstone of modern immunology and its application in the development of therapeutics.

These regions, called epitopes, interact with antibodies, B-cell receptors (BCR), and T-cell receptors (TCR), activating the immune response.[1]

Knowing the structure of the antigen and the epitope-paratope interactions is essential for the rational conception, design, and development of effective and safe vaccines, as well as for the creation of immunotherapies and advanced diagnostic tools.

Peptide and subunit vaccines are developed based on identifying immunodominant epitopes of B and T lymphocytes. These vaccine strategies aim to induce particular and potent immune responses targeting the essential pathogen components for protection while minimizing unnecessary antigenic load and the possible biological implications attributable to the use of whole pathogens.[2]

In this context, the application of bioinformatics techniques has led to the development of a new subspecialty, immunoinformatics, which is based on the application of bioinformatics tools to provide efficient and rapid solutions to problems encountered in professional practice in the field of immunology and vaccinology.

This subspecialty has provided adequate tools for identifying proteins with potential therapeutic use, modeling their immunogenic activity, and thus exponentially accelerating the initial phases of vaccine discovery and development.[3]

The present communication aims to describe the potential of immunoinformatics in epitope mapping for the design of vaccines and other therapies**.**

DEVELOPMENT

Literature analysis suggests that epitope-based vaccines developed by applying bioinformatics techniques and tools can elicit a robust and potentially long-lasting immune response by targeting specific antigens with high precision.[4]

This approach brings a paradigm shift in vaccine design, moving from a more empirical 'isolate, inactivate, and inject' approach to a rational and molecularly informed paradigm.

With these tools, the goal shifts from finding an antigen that meets the desired objective to understanding why or how it works at the molecular level. This allows for the deliberate selection of relevant antigenic regions to achieve the desired protective immune response.[1] New-generation vaccines will be developed based on this deep understanding of host-pathogen interactions.

Limitations of traditional methods

It is no secret that traditional methods for selecting epitopes for vaccine development have limitations. Techniques such as deep mutational scanning, phage displays, and synthesizing and screening overlapping peptide libraries are powerful. Still, they require considerable time, financial resources, and highly qualified personnel.

Furthermore, it is impossible to guarantee the ability to screen a high volume and diversity of proteins or to define epitopes, especially conformational ones, precisely. An example of this is the identification of linear epitopes through synthesizing all possible peptides covering an antigenic protein, which is costly and time-consuming.

Another key point lies in the disadvantages of traditional vaccines, whether inactivated or live attenuated. Inactivated vaccines require adjuvants to enhance the immune response; similarly, they may offer short-lived immunity. Although characterized by greater immunogenicity, live attenuated vaccines can suffer from a reversion to virulence, specifically in immunocompromised individuals. They also require a rigorous cold chain for storage and transport and are not immune to the risk of instability. Furthermore, although recombinant or synthetic vaccines are considered safer, they are often low in immunogenicity.

These barriers slow the pace of innovation and development and, in turn, limit the scope of scientific exploration. Given the costs of experimental processes and their duration, selecting antigens or vaccine candidates for study must be targeted and rational. This means that promising epitopes or antigens may be overlooked due to infrastructure and resource limitations.

Potential advantages of immunoinformatics tools

A possible solution to the barriers inherent in traditional experimental methods lies in the application of immunoinformatics. This emerging area of science integrates different disciplines, such as computer science, mathematics, biochemistry, and the so-called omics (genomics, proteomics, transcriptomics, immunogenomics, and others). This enables large-scale analysis of immune system functions and immune data.

Immunoinformatics methods can exponentially reduce the time and costs associated with vaccine development, thanks to the possibility of mapping and analyzing the evolution of biological components in silico before their study in vitro or in vivo.[10] It can also accelerate the identification of antigens and the selection of epitopes capable of inducing a robust and specific immune response.[3]

These tools can potentially develop rational, systemic, and highly parallel analyses with the capacity for large-scale operation, which is complex with traditional methods.[9] One example is screening complete pathogen genomes to select new antigens, which opens the door to developing vaccine strategies against diseases for which there are currently no practical solutions.[11]

The in silico predictive capacity of peptide and protein immunogenicity has become one of this field's central and distinctive objectives.[12]

Another advantage of these techniques and tools is that they not only accelerate discovery but also lead to the democratization of information and access to the early stages of vaccine research. Many predictive tools and biological databases are publicly available and free of charge,[13] allowing laboratories with limited resources to generate hypotheses and select candidates for future validation. While experimental validation is known to be costly,[14] this ability to filter candidates in silico reduces the initial experimental

burden.

Limitations of immunoinformatics tools

Despite their advantages, these tools are not without limitations.

Given that their use is based on information, the availability of biological data is one such limitation. Despite the existence of biological databases, they can sometimes be limited to a specific disease, gene, or protein.[7] Hence, as data collection, mapping, and digital storage increase, so will their scope of application.

Similarly, data is not enough; it must be high-quality, widely diverse, and interoperable, which results in other limitations. As these limitations are overcome, the training of those involved in these tools will expand, they will be better trained, and, as a result, they will lead to more effective solutions**.**

FINAL CONSIDERATIONS

Immunoinformatics accelerates research into vaccine development and allows the biological complexity of the immune response and its relationships to be modeled and analyzed. These tools and techniques, confined to the diversity of pathogens, open up new avenues for efficiently and rationally addressing situations that have long been complex.

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