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Opinion Article

Bioinformatics of Antibody Drug Conjugates: Drug Delivery

David Ewa*

Department of Oncology, University of Warmia, Olsztyn, Poland

DESCRIPTION

Immunoglobulins, also known as antibodies, are members of the "gamma globulin" protein family and are primarily found in the blood of vertebrates. The immune system of vertebrates with jaws uses antibodies as its main line of defence to recognize and destroy potentially harmful invaders like bacteria, viruses, fungi and parasites. The mechanism underlying our immune system's ability to specifically recognize and fight invading organisms or to trigger an autoimmune response and disease is still unknown. As reaction times are "key" to the effective elimination of the foreign pathogen, the number, condition and availability of antibodies have a significant impact on how effectively our immune system reacts to all types of invaders. On the other hand, antibodies are an inappropriate and offensive immune system reaction to the body's normal tissues. In essence, the immune system attacks its own cells because it misidentifies them as potential pathogens. Most often, this reaction will only affect a small portion of a particular organ or a particular type of tissue that is present in multiple human body organs. Immunosuppression, which aims to reduce the reactive immune response, is currently the most widely used clinical treatment for immune system diseases.

Two identical heavy chains and two identical light chains, each with a variable domain at the N-terminal end, make up an antibody. In order to recognize an equally diverse range of antigens, antibodies have variable domains that are composed of structurally hyper variable regions, also referred to as complementarity-determining regions. The CDRs, three per domain, make up the recognition site. There is a huge variety of antibodies because the CDR3 is the result of the rearrangement of two genes for the light chain (kappa or lambda) and three genes for the heavy chain. These antibodies can recognize an enormous variety of antigens. The structural interaction between the three CDRs and the antigen's shape and size is what gives the antibody variable domains their flexibilit. The CDRs essentially control the antibody's specificity and affinity for a given antigen. The area of an antibody that interacts with the corresponding epitope of an antigen is called a paratope. The two molecules can structurally form a complex conformation thanks to the recognition sites on the antibody and antigen. Invaders that need to be neutralized or removed are marked by antibodies through this binding interaction.

A key characteristic of an antibody is specificity, which describes the antibody's capacity to recognize and bind to a particular antigenic determinant. High-resolution structural knowledge of antibodies is required due to the significance of these substances in biotechnology and medical fields. These details can be used to identify an antibody's specific epitope, modify the antigens' binding affinity and engineer new antibodies.

The widely used, albeit tedious and time-consuming, X-ray crystallography is being replaced by computational methods because they are less expensive and quicker. Available immunogenetics data can be used to model antibody variable domains computationally. Standardized amino acid positions and properties can aid in the development of homology models that predict the successful docking of antibodies with their specific antigen, also in optimizing the relationship between the orientation of light and heavy chains.

CONCLUSION

Drug conjugation with antibodies is a promising technique for targeted drug delivery in which the antibody acts as a carrier to transport the medication to a specific place in the body. Bioinformatics can help in the production of such drug conjugates by providing information about the properties and characteristics of the antibodies utilised in the conjugation.The analysis of antibody sequences is a critical part of bioinformatics in this setting. Antibodies are proteins made by the immune system that have millions of distinct sequences that can recognise and bind to a specific target. Antibody sequence analysis can provide information on binding capabilities, structural features, and potential immunogenicity. This study can be used to choose the best antibodies for drug conjugation and to optimise the conjugation process.

Correspondence to: David Ewa, Department of Oncology, University of Warmia, Olsztyn, Poland, E-mail: dawidwa@gmail.com

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