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Bioinformatics Analysis of Immunoglobulin ε (IgE) Heavy Chain

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Abstract: Immunoglobulin ε is a key immunoglobulin that plays an important role in the immune system. IgE is usually associated with allergic reactions such as food allergies, allergic rhinitis, and allergic dermatitis. In this project, this article Use NCBI or *https://www.uniprot.org/* Website to obtain immunoglobulins ε Heavy chain related nucleotide sequences. Using relevant websites and software to analyze and predict immunoglobulins using bioinformatics methods ε Bioinformatics analysis of heavy chains includes physical and chemical properties, structural functions, positional expression, phylogenetic relationships, protein interactions, etc. Understanding the bioinformatics analysis of IgE can help reveal its function in the immune system and its relationship with allergies and other diseases, promote the improvement of diagnosis and treatment methods for allergic diseases, and advance in the field of immunotherapy.

Keywords: IgE; Bioinformatics Analysis; Biostatistics; Biopharmaceuticals.

1. Introduction

Immunoglobulin ε Our research has a long history internationally. Numerous studies both domestically and internationally have been devoted to revealing its molecular structure and critical role in immune responses, especially its FcεRI binding region and its function in immune response. IgE plays a crucial role in immune responses, especially in type I hypersensitivity reactions. This immune response process can be divided into three stages: sensitization, stimulation, and utility. [1] Firstly, specific antigens are ingested, degraded, and presented to antigen presenting cells (APCs). APC then transmits signals to Th2 cells and ultimately to B cells, causing plasma cells to release specific antibody IgE. Free IgE antibodies and receptor FcεRI binding sensitizes cells or the body [2].

2. Materials and Methods

2.1. Materials

Obtain IgE heavy chain related nucleotide sequences using https: //www.uniprot. org /website [3], and modify the obtained nucleotide sequences using https: //reverse completion. com /website (see Figure 1)

>sp|P0DOX4.1|IGE_HUMAN RecName: Full=Immunoglobulin epsilon heavy chain; AltName: Full=Immunoglobulin epsilon heavy chain ND
QVQLVQSGAEVRKPGASVRVSCKASGYTFIDSYVGWIRQAPGHGLEWIHWINPNSGGTNYAP
RFQGRVTM
TRDASFSTAYMDLRSLRSDDSAVFYCAKSDPFWSDYNFDYSSSEEGTEVTYTVSGAWTLPSVF
PLTRCCK
NIPSNATSVTLGCLATGYFPEPVMVTWDTGSLNGTTLPATTLTLSGHYATISLLTVSGAWAKQM
FTCRVA
HTPSSTVDNKTFSVCSRDFTPPTVKILQSSCDGLGHFPPTIQLCLVSGYTPGTINITWLEDGQVM
DVDLS
TASTESQGELASTESQLTLSQKHWLSDRTYTCQVTYQGHTFQDSTKKCADSNPRGVSAYLSRP
SPFDLFI
RKSPTITCLVVDLAPSKGTVNLTWSRASGKPVNHSTRKEEKQRNGTLTVTSTLPVGTRDWIEG
ETYQCRV
THPHLPRALMRSTTKTSGPRAAPEVYAFATPEWPGSRDKRTLACLIQNFMPEDISVQWLHNEV
QLPDARH
STTQPRKTKGSGFFVFSRLEVTRAEWQEKDEFICRAVHEAASPSQTVQRAVSVNPGK

Figure 1. Immunoglobulin ε Heavy chain amino acid sequence

2.2. Method:

Obtain immunoglobulins using https://web. expasy. org/protparam/ ε The amino acid sequence of the heavy chain was analyzed using https:///web. expasy.org/protscale/for immunoglobulins ε The hydrophilicity and hydrophobicity of the heavy chain were predicted using https: //www.cbs. dk /services /SignalP to predict the protein signal peptide. The structure of the protein was visualized using http: //wlab. ethz. ch /protocol /start /and http: //npsa prabi. ibcp. fr /cgi bin /npsa_ Automat.pl? Page=npsa_ SOPM AHTML on Human Immunoglobulin ε Predicting the secondary structure of. The results showed that immunoglobulins were analyzed and predicted through bioinformatics methods ε Bioinformatics analysis of heavy chains: physical and chemical properties, structural functions, positional expression, phylogenetic relationships, protein interactions, etc [4].

3. Results and Discussion

3.1. Human Immunoglobulin ε Analysis of Physical and Chemical Properties of Heavy Chains

Physical and chemical properties analysis of human immunoglobulins using the website https:///web. expasy. org/ protparam/ ε the heavy chain contains 547 amino acids with a relative molecular weight of 60322.73. The total number of negatively charged residues (Asp+Glu) is 48, and the total number of positively charged residues (Arg+Lys) is 52. The molecular formula is C2659 H4117N741O822S22. Its lipid solubility coefficient is 66.11, and the total average hydrophobicity (GRAVY) is -0.382, which is negative. The predicted results indicate that human immunoglobulin ε It is a hydrophilic protein. Its instability coefficient is 41.84, with a value greater than 40. The analysis results indicate that human immunoglobulin ε Not very stable.

Human immunoglobulin ε The hydrophilicity/ hydrophobicity of the protein was predicted, as shown in Figure 2. Among them, V (Val) at position 360 had the strongest hydrophobicity (+2.289), and E (Glu) at position 390 had the strongest hydrophilicity (-3.500). Based on the K-D method, the protein hydrophobicity was determined; A score higher than 0 indicates hydrophobic amino acids, while a score lower than 0 indicates hydrophilic amino acids. As can be analyzed from Figure 2, immunoglobulin ε The number of hydrophilic amino acids is significantly higher than that of hydrophobic amino acids, indicating that they are hydrophilic proteins, consistent with the results of physicochemical analysis.

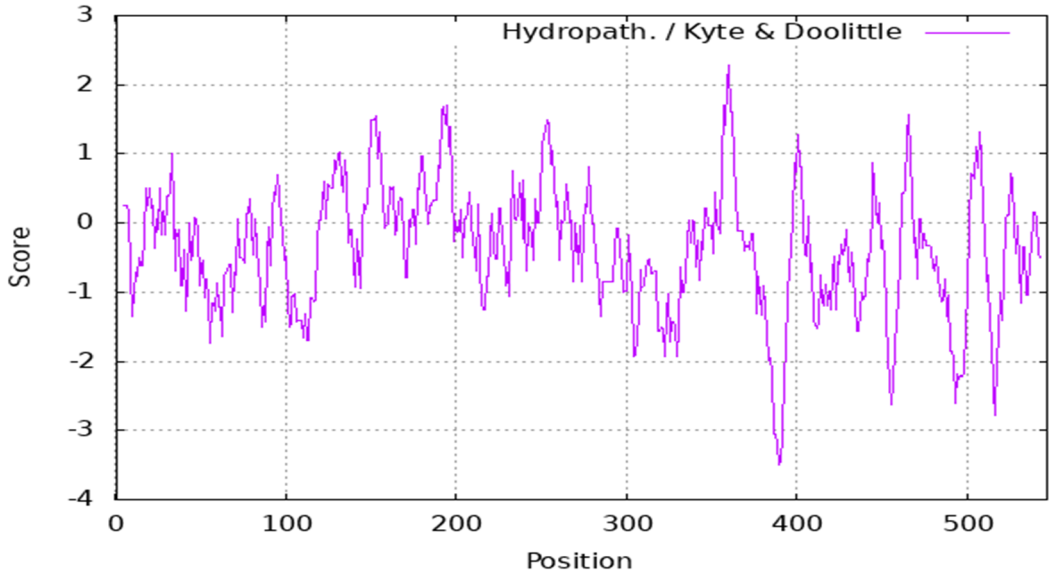


Figure 2. Human immunoglobulin ε Prediction of hydrophobicity/hydrophilicity of heavy chain amino acid sequences

The presence or absence of signal peptides often provides important information about the subcellular localization and function of proteins. The prediction of the signal peptide of this protein using SignalP5.0 online software howed that the likelihood of the protein having a signal peptide was 0.0046, and the absence of a signal peptide sequence meant that the protein did not possess secretory properties [5]. Its function within the cell may be related to biological processes within the cell, rather than interaction or secretion outside the cell. The presence or absence of signal peptides often provides important information about the subcellular localization and function of proteins. Visualize the structure of proteins, including transmembrane regions, through http: //wlab. ethz. ch /protocol /start /(Figure 3). We can conclude that the main function or location of this protein does not need to cross the cell membrane, and there is no transmembrane region.

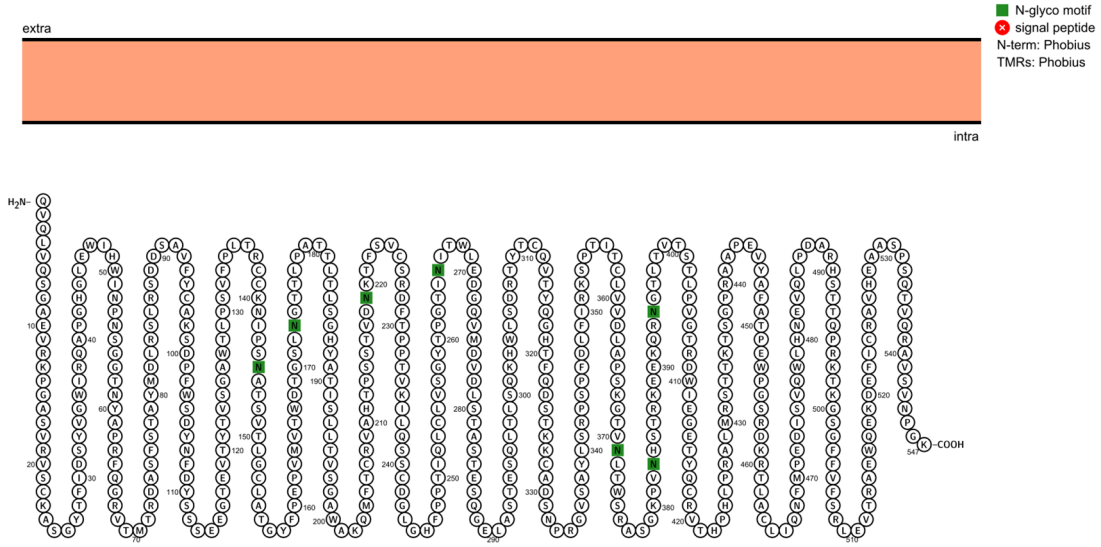


Figure 3. Human immunoglobulin ε Prediction of Topological Structure of Heavy Chains

3.2. Human Immunoglobulin ε Structure and Function Prediction of Heavy Chains

Human immunoglobulin detection through website Prabi ε The secondary structure is predicted, with the blue part being α- Spiral, green part is β- Corner, red represents the extended chain, and yellow represents irregular bending. The protein has 286 irregularly bent chains, accounting for 52.29%, and 169 extended chains, accounting for 30.90%, α- There are 51 spirals, accounting for 9.32%, β- Corner 41 chapters 7.50%. It can be seen that the protein is mostly irregularly bent and extended chains, which may allow the protein to interact with various different molecules, thereby performing various biological functions. The secondary structure is shown in Figure 4

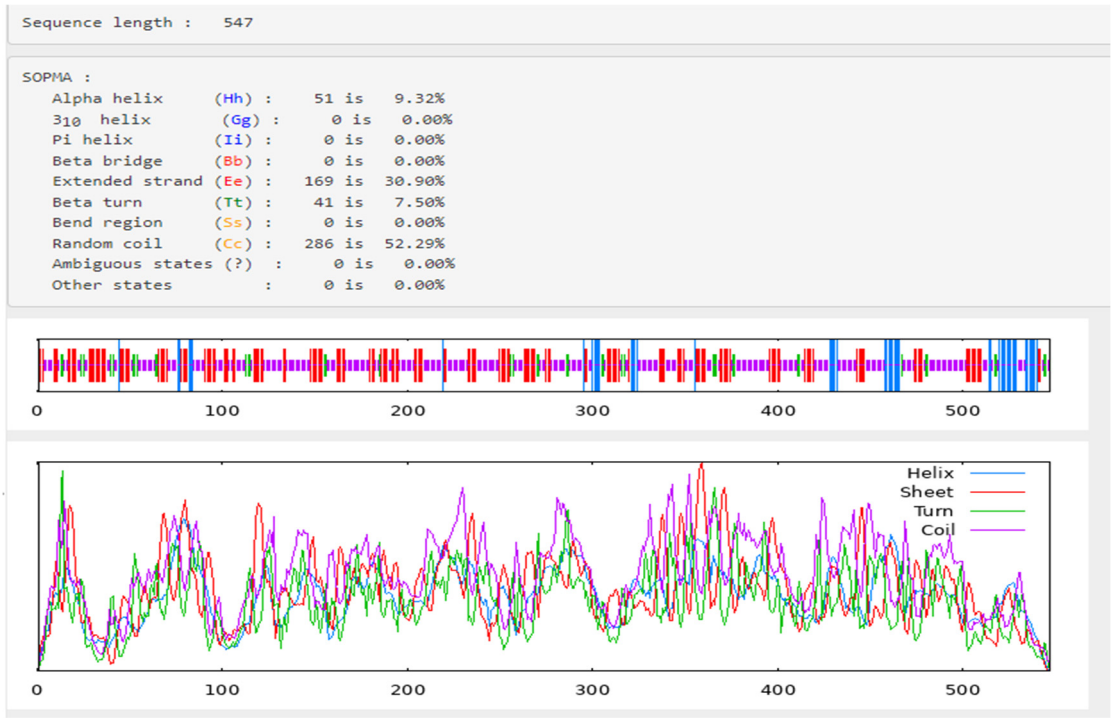


Figure 4. Human immunoglobulin ε Prediction of the Secondary Structure of Heavy Chains

By targeting human immunoglobulins ε By predicting the tertiary structure of the protein, we can find that the main components of the protein structure are irregularly bent and extended chains, which is consistent with the predicted results of the secondary structure. The three-level structure is shown in Figure 5.

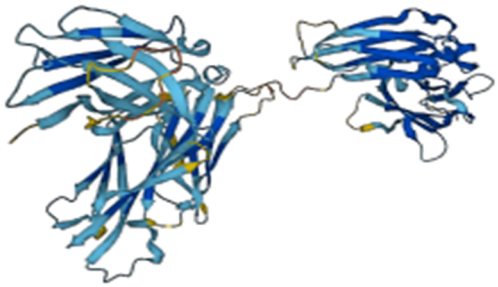
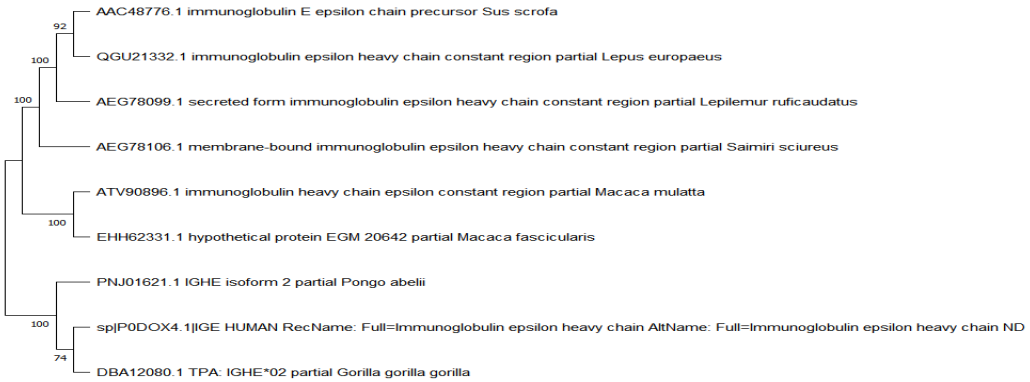


Figure 5. Human immunoglobulin ε Prediction of the tertiary structure of heavy chains

3.3. Human Immunoglobulin ε Homology Analysis of Heavy Chains

Searching the NCBI database for human immunoglobulins ε The similarity between heavy chain and homologous proteins in gorillas, macaques, macaques, crab eating monkeys, Semir squirrels, wild boars, European rabbits, and red tailed foxes is 94.09%, 92.20%, 82.55%, 81.84%, 74.35%, 47.66%, 56.34%, and 56.74%. Using DNAMAN software to perform homology alignment of protein sequences from 9 species, and constructing human immunoglobulins using the neighbor joining (NJ) method based on sequence homology in MEGA11 software ε Genetic evolution relationship tree (see Figure 6). According to the evolutionary tree, it can be seen that during the evolutionary process, humans have the closest genetic relationships with gorillas and macaques. Macaques and crab eating monkeys are closely related and grouped together, while wild boars and European rabbits are closely related and grouped together. According to the evolutionary distance analysis results (see Table 1), the minimum genetic distance between humans and chimpanzees is 0.055, followed by Abbe monkeys and macaques, and the farthest genetic distance between humans and wild boars is 0.511.



P0DOX4.1 Human; DBA12080.1 Gorilla; PNJ01621.1 Abbe Monkey; ATV90896.1 Macaque mulatta; EHH62331.1 Macaque fascicularis; AEG78106.1 Semir Squirrel; AAC48776.1 Wild boar; QGU21332.1 European Rabbit; AEG78099.1 Red tailed fox;

Figure 6. Different species of immunoglobulins ε Phylogenetic tree

Table 1. Protein Evolution Distance of Immunoglobulins ε from Different Species

Species	Human	Gorilla	Abbe Monkey	Macaque mulatta	Macaque fascicularis	Semir Squirrel	Wild boar	European Rabbit	Red tailed fox
Human	0								
Gorilla	0.055	0							
Abbe Monkey	0.076	0.042	0						
Macaque mulatta	0.170	0.138	0.152	0					
Macaque fascicularis	0.177	0.145	0.159	0.007	0				
Semir Squirrel	0.254	0.238	0.242	0.264	0.273	0			
Wild boar	0.511	0.483	0.482	0.475	0.480	0.489	0		
European Rabbit	0.428	0.411	0.417	0.436	0.441	0.429	0.387	0	
Red tailed fox	0.425	0.412	0.417	0.433	0.438	0.422	0.424	0.384	0

4. Summary

This article uses different bioinformatics tools to study human immunoglobulins ε by analyzing and predicting heavy chains, we have identified human immunoglobulins ε It may be a hydrophilic protein with specific molecular weight and amino acid composition. The protein lacks a signal peptide sequence, indicating that it does not possess secretory properties and is mainly related to intracellular biological processes. Immunoglobulin ε The heavy chain structure is mainly composed of irregularly bent and extended chains, and there is no transmembrane region. By targeting immunoglobulins from different species ε Comparison of its coding sequence revealed that human immunoglobulin ε The high homology with certain primates such as gorillas and macaques reveals their conservatism in evolution.

In the current research field, it has not been found that there is a significant impact on immunoglobulin ε Research on bioinformatics analysis. By analyzing its sequence and structure, it will contribute to a deeper understanding of immunoglobulins ε the functions of immunoglobulins and their differences from other immunoglobulins are of great significance for the development of immunotherapy. In future research, we can rely on the obtained immunoglobulins ε Relevant information can be obtained by measuring the IgE concentration level in allergic patients using detection techniques such as ELISA. Develop more effective drugs and improve treatment methods for allergic diseases based on the knowledge of biostatistics.

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