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Short Communication

Importance and Future Prospective of Protein Structure Prediction

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DESCRIPTION

The three-dimensional configuration of an amino acid-chain is known as protein structure. Sequences of amino acids, the polymer, monomers are used to create proteins, specifically polypeptides. A single amino acid monomer can also be referred to as a residue, which denotes a polymer repeating unit. Proteins are created when amino acids go through condensation processes, losing one water molecule each time to form peptide bonds with one another. Conventionally, a chain with fewer than 30 amino acids is called a peptide rather than a protein. It is far simpler to create a protein sequence than to figure out its structure. However, a protein's structure offers significantly more information about its function than its sequence. As a result, various techniques for computing protein structure prediction from sequence have been created. Methods for ab initio prediction only employ the protein's sequence [1]. A protein family, or set of related proteins with known experimental structures, can be used to create a three-dimensional model for a protein with unknown structure. With the help of protein structure there is better understanding of how protein works and depending on this feature theories can be devloped about how to influence, regulate or modify it. For instance, understanding the structure of a protein could let you create site-directed mutations with the goal of altering function. Tens to thousands of amino acids can make up a protein structure. Proteins, which range in size from 1 to 100 nm, are characterized as nanoparticles. Protein subunits can combine to generate very massive protein complexes. For instance, a microfilament is formed when thousands of actin molecules come together. When a protein performs a biological function; it typically experiences reversible structural modifications. Different conformations of the same protein are its alternate structures, and transitions between them are known as conformational alterations [2,3]. The configuration of the atoms in the three-dimensional structure of a protein determines its biological function. This may refer to how a protein interacts with other proteins for structural or other regulatory purposes, or it may refer to the configuration of catalytic residues in an active site. For instance, knowing the structure of a protein could let you create site-directed mutations with the goal of altering function. A protein's binding molecules could also be predicted. A proteins biological function is based on how its atoms are arranged in its three-dimensional structure. This could be a statement to how a protein engages in structural or other regulatory interactions with other proteins, or it could be a term to the organization of catalytic residues in an active site. Scientists may build theories about how to impact, regulate, or modify a protein after we have a better comprehension of how it works as a result of its structure. For instance, knowing a protein's structure might enable you to make site-directed changes with the intention of changing function. The compounds that a protein will bind to can also be predicted. Homology modeling is a key component of many protein structure prediction techniques. This works by locating proteins in the Protein Data Bank that have a lot of sequence similarity using sequence alignment. For proteins with at least 70% sequence identity, these techniques are effective. However, relying solely on sequence similarity has drawbacks. It gets harder to choose templates when you reach closer to 50% sequence identity. And because any two random pairs of proteins can have this level of sequence identical, it becomes extremely challenging as you approach near to the 30 percent sequence identity level, sometimes known as the "twilight-zone." Utilizing homology modelling in well-known systems like kinases, predicted models are already employed for drug screening. Structure prediction has attracted a lot of attention as a method of screening for proteins that cannot be determined experimentally. For instance, businesses engaged in the development of antibodies are able to produce tens of thousands different antibody sequences in response to targets [4]. As soon as feasible, they need to screen out antibodies that don't have the desired properties. By predicting a protein fold's features based on its amino acid sequence, structure prediction can help to combat this quick-to-fail mindset. Protein engineering will also make use of these tools.

CONCLUSION

The value of computationally predicted three-dimensional protein structure has been proved in various biomedical fields, from precision drug screening to approximative family designations. But for almost 40 years, the existence of similar structural templates has been a limiting factor in the predictive models' accuracy. Recently, progress has been made in

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developing low-resolution models so that they are more like the original ones. This has been made feasible by merging knowledge-based data from various sources of structural templates and by enhancing the energy funnel of physics-based force fields. Unfortunately, there hasn't been much progress made in the creation of methods for determining unique protein structures and discovering remotely homologous templates.

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