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ANALYSIS OF THE 3D VIEW OF SOME PROTEINS

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Abstract
Today, as we are at the stage of development of science and development, the emergence of bioinformatics has made it possible for us to study macromolecules even more deeply. Conditions have been created for us to see the 3D view of proteins in clear images. We can use different tools and databases for this. Using the information obtained and placed in the bases, we will get to know the 3D view of some types of proteins.

Keywords: 3D structure, protein, database, tool, bioinformatics.

Introduction

Each protein molecule in a living organism is characterized by a certain sequence of amino acids, which is determined by the sequence of nucleotides in the structure of the gene encoding the protein. Thus, proteins with a well-defined chemical structure are synthesized in the body, they were selected to perform certain functions in the course of evolution. The sequence of amino acid residues in a protein molecule determines its primary structure, that is, its chemical formula. With 20 amino acids, you can create an almost unlimited variety of proteins.

Protein Structures

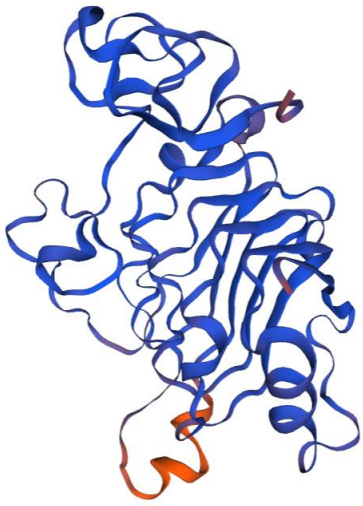
The amino acid sequence of a protein determines its three-dimensional shape. The structure of a protein can be described at several levels. Primary structure is a linear sequence of residues (amino acids) in a polypeptide chain. Secondary structure - the arrangement of the polypeptide chain in more or less regular hydrogen-bonded structures - has two main elements - Alpha helix - a helical configuration of the polypeptide chain with 3.6 residues (amino acids) in each turn. The spiral can be left-handed or right-handed, the latter being more common (Alberts B, 2022). Beta chain - two adjacent polypeptide strands connected to each other. Two or more strands can interact to form a beta sheet. Tertiary structure is the level of protein structure in which the entire polypeptide chain is folded into a three-dimensional structure. In multichain proteins, the term tertiary structure refers to individual chains. Quaternary structure is the fourth order of complexity of the structural organization exhibited by protein molecules and refers to the spatial arrangement of the complete protein regardless of the internal geometry of the subunits. Quaternary structure is obtained only when the molecule consists of at least two distinct subunits.

The three-dimensional structure of a protein is determined by methods such as X-ray crystallography and nuclear magnetic resonance (NMR).

Scientists who determine the structure of proteins enter their data into a database such as the Protein Data Bank (PDB). Structural notation shows the three-dimensional coordinates of each atom in a molecule.

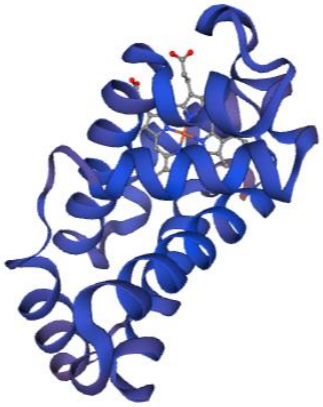
The Molecular Modeling Database (MMDB) at NCBI is derived from the PDB and contains the three-dimensional coordinates of each atom, as well as a precise chemical graph showing which atom is bonded to which atom. Structure records can be imported into a 3D structure viewer such as Cn3D, Rasmol, or Kinemage, where the molecule can be rotated and viewed in different views.

View 3D structure on Swiss Model



1. Picture. Structure of the receptor tyrosine-protein kinase erbB-2

This gene encodes a member of the receptor family of epidermal growth factor (EGF) receptor tyrosine kinases. This protein has no specific ligand binding domain. At the same time, it binds tightly to other members of the ligand-bound EGF receptor family to form a heterodimer, stabilizes ligand binding, and induces downstream signaling including mitogen-activated protein kinase and phosphatidylinositol-3 kinase. enhances kinase-mediated activation of signaling pathways. Allelic variations have been reported at amino acid positions 654 and 655 of the A isoform (positions 624 and 625 of the β isoform), with the most common allele Ile654/Ile655 shown here. Amplification and/or overexpression of this gene has been reported in many cancers, including breast and ovarian tumors. Alternative splicing gives rise to several additional transcript variants, some encoding different isoforms and others not fully characterized (NCBI, 2022)



2. Picture. Hemoglobin subunit beta

The crystal structure of recombinant human adult hemoglobin

The alpha (HBA) and beta (HBB) loci determine the structure of 2 types of polypeptide chains in adult hemoglobin, Hb A. A normal adult hemoglobin tetramer consists of two alpha chains and two beta chains. Mutant beta globin causes sickle cell anemia. Absence of the beta chain results in beta-null-thalassemia. A decrease in detectable beta globin results in beta-plus-thalassemia (NCBI, 2022).

Proteins are synthesized relatively easily compared to nucleic acids, and the RNA world may have been preceded by a stage that could be called the protein world. Some of the three-dimensional (3D) peptide structures in these proteins, we believe, may constitute the oldest surviving biological remains from that time. We focus on 3D peptide motifs of eight or more amino acid residues. The best known of these is the "nest," a three- to seven-residue protein motif that functions to bind anionic atoms or groups of atoms. 10% of the amino acids in normal proteins belong to the nest, so it is a common motif. A five-residue nest is found as part of the well-known P-loop, a repetitive feature of many ATP- or GTP-binding proteins, which has the function of binding the phosphate moiety of these ligands. A synthetic hexapeptide, ser-gly-ala-gly-lys-thr, designed to resemble the P-loop, has been shown to bind inorganic phosphate. Another type of nest connects iron-sulfur centers. A number of other simple motifs appear with various interesting 3D structures; others bind cations or form channels that transport potassium ions; other peptides form catalytically active heme-like or lamellar structures with certain transition metals. Amyloid peptides are also discussed. It appears that the earliest polypeptides were far from non-functional stretches and had binding and catalytic properties (Milner-Uayt, 2019).

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