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Perspective

Docking Method for the Interaction between Protein and Ligand Molecule

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DESCRIPTION

A molecule is a tiny chemical compound consisting of two or more atoms joined by chemical bonds. Either a single sort of element (like H_2) or a various kinds of elements can form a molecule (e.g. CO_2). Both living things and non-living things contain molecules. A medication is a tiny molecule that can interact, bind and regulate the activity of biological receptors, aiding in the treatment of disease. Proteins called receptors work with other biological substances to maintain a variety of cellular processes in the body. Some significant receptors in human body include enzymes, hormone receptors, cell signalling receptors, neurotransmitter receptors, etc.

The process of creating a therapeutic molecule that can interact with and bind to a target is known as drug designing. Receptors are visible on the surface of cells that receive signals. They are characterised as molecules that detect tiny molecules and, upon binding, start cellular processes. The functionalities of the receptor are quiet in an unbounded state receptor. According to this concept, a receptor will only bind to a certain ligand or vice versa, but in some situations, ligands in high quantities will bind to several receptor sites.

In most cases, drug receptors do not have an endogenous ligand. These medications' molecules can bind to receptors that are enzymes, ion channels, proteins, nucleic acids, etc. As a result, the drug molecule will cross-link DNA and prevent DNA replication. The treatment of malignant cancers uses it. Hormones, neurotransmitters, aracoids, growth factors, cytokines, and other substances are examples of endogenous regulatory ligands that bind to receptors. Therefore, these receptors' purpose is to detect the ligands and start the reaction. For instance, the tiny painkiller medication molecule aspirin has four oxygen atoms, nine hydrogen atoms, and eight carbon atoms. The form and charge of the molecules should complement the target.

Computational methods for modelling molecules are included in molecular modelling. Computer-aided drug design is the term used to describe the process of creating drugs utilising these modelling tools. Drug design with computers is a quick, automatic, and extremely affordable approach. Either ligand-based drug design or structure-based drug design can be used to accomplish this. Structure-based drug design is based on the three-dimensional structure of the target, whereas ligand-based drug design is solely based on the model that is going to bind to the target. Pharmacophoric areas must be defined for the molecule in order for it to bind the target. If there isn't a target available, one can be made through homology modelling. Predict the drug molecules' propensity for attaching to the target using the target's structural information. The computer-aided molecule construction process is a crucial step in the design of pharmaceuticals. For the purpose of creating a molecule, there are so many computational tools available.

Protein ligand interaction

All living cells are made up primarily of proteins, which are essential for many biological processes. Every protein in our bodies has a specialised purpose. As an illustration, haemoglobin, a protein present in Red Blood Cells (RBC), transports oxygen from the lungs to the cells and gathers carbon dioxide to return to the lungs. A protein's function determined by its structure. For a protein to function effectively, it needs to bind to other molecules in a highly particular way. Every protein has a unique structure as a result. A molecule is a microscopic chemical compound consisting of two or more atoms joined by chemical bonds. A medication is a tiny molecule that can interact with, bind to, and regulate the activity of biological receptors, aiding in the treatment of disease.

All processes taking place in living organisms depend on interactions between proteins and their ligands. All living processes depend on ligand-mediated signal transmission through molecular complementarity; these chemical interactions include molecular-level biological recognition. The evolution of specialised binding sites that are intended to bind ligand molecules is essential for protein function evolution. The ability to bind ligands is crucial for the control of biological processes. Protein-ligand interactions take place as a result of conformational changes between low affinity and high affinity states in molecular mechanics. Protein state and function are altered by ligand binding interactions.

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CONCLUSION

After modelling a molecule, it check's the location where the ligand docks onto the receptor, determine whether the ligand suits the target molecule, and then conduct docking tests. Using a technique called docking, it is possible to foretell how two molecules will orient themselves when joined to form a stable complex. The "lock and key" concept can be used to describe molecular docking. Here, the ligand can be thought as the key and the protein as the lock, which indicates the optimum orientation in which the ligand goes to attach to a specific protein. A protein molecule might be needed first in order to accomplish a docking. The inputs for docking are the ligands and protein structures.