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Drug Targets and Types of Drug Designing

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Short Communication

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DESCRIPTION

Drug design, often known as rational drug design or simply rational design, is the imaginative process of discovering novel treatments based on understanding of a biological target. The medicine is often an organic small molecule that activates or inhibits the action of a biomolecule such as a protein, resulting in a therapeutic benefit for the patient. In its most basic form, drug design is creating molecules that are complimentary in shape and charge to the biomolecular target with which they interact and therefore bind. Typically, drug design can be made by using computer modelling. This form of modelling is also known as computer-aided medication design. Finally, structure-based drug design refers to drug design that is based on knowledge of the three-dimensional structure of the biomolecular target. Biopharmaceuticals, which include peptides and, in particular, therapeutic antibodies, are an increasingly important class of medications, and computational approaches for boosting the affinity, selectivity, and stability of these protein-based treatments have also been created.

Drug design types

Drug design is typically divided into Ligand based drug design and structure based drug design.

Ligand-based drug design: Ligand-based drug design (also known as indirect drug design) is based on understanding of other compounds will bound to target site. Other additional molecules attached to the drug might be used in pharmacophore modelling, which outlines the minimum structural properties. In other words, based on what binds to the biological target, a model of the target may be developed, and this model can then be used to design new molecular entities that interact with the target. A Quantitative Structure-Activity Relationship (QSAR) can also be derived, which is a correlation between estimated characteristics of molecules and their experimentally determined biological activity. These QSAR relationship in turn may be used to predict the activity of new analogs [1,2].

Structure-based drug design: In Structure based drug design, the molecule containing three dimensional protein structure complements biological and biochemical information having same type of activity as the original one leading to formation of the novel drug. A homology model of the target based on the experimental structure of a related protein may be possible. This is attained by using high through put structural determination pipeline, pipeline technologies, protein expression and fermentation, crystallization, X ray diffraction screening and data collection, Nuclear magnetic resonance, suitability testing, etc [3] .

Drug targets

A bimolecular target (typically a protein or a nucleic acid) is a key molecule involved in a specific metabolic or signaling pathway linked to a specific disease condition or pathology, or to the infectivity or survival of a microbial pathogen. Potential drug targets are not necessarily disease-causing, but must be disease-modifying by definition. Small molecules may be designed to enhance or inhibit the target function in a disease-modifying pathway in some cases. Small molecules that are complementary to the target's binding site will be designed (for example, receptor agonists, antagonists, inverse agonists, or modulators; enzyme activators or inhibitors; or ion channel openers or blockers). Small molecules (drugs) can be designed so that they do not interact with any other important "off-target" molecules (also known as antitargets), because drug interactions with off-target molecules can result in undesirable side effects. Closely related targets identified through sequence homology have the highest chance of cross reactivity and thus the highest side effect potential due to binding site similarities [4,5] .

Drugs are typically organic small molecules created through chemical synthesis, but biopolymer-based drugs (also known as biopharmaceuticals) created through biological processes are becoming more common. Furthermore, gene silencing technologies based on mRNA may have therapeutic applications.

Examples of drug design

- The use of three-dimensional information about biomolecules gained from techniques such as X-ray crystallography and NMR spectroscopy is one example of rational drug design. When there is a high-resolution structure of a target protein attached to a potent ligand, computer-aided drug creation becomes significantly more tractable. This method of drug discovery is also known as structure-based drug design. The carbonic anhydrase inhibitor dorzolamide was approved in 1995 as the first unequivocal example of structure-based drug design leading to an approved medicine [6] .
- Imatinib, a tyrosine kinase inhibitor created particularly targeting the bcr-abl fusion protein seen in Philadelphia chromosome-positive leukemias, is another notable case study in rational drug design (chronic myelogenous leukaemia and occasionally acute lymphocytic leukemia). Imatinib is significantly different from prior cancer medications in which most chemotherapy agents simply target quickly dividing cells without distinguishing between cancer cells and other tissues.

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