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Drug Design: Types and its Determination

Brian Montes*
Department of Pharmacology, University of Florence, Florence, Italy

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Description

The creative process of discovering novel pharmaceuticals based on the understanding of a biological target is known as drug design, sometimes known as rational drug design or simply rational design. A protein is a common example of a biomolecule whose function is activated or inhibited by the medicine, which benefits the patient therapeutically. In essence, drug design involves the creation of compounds that can interact with and attach to bio-molecular targets in a way that complements their shape and charge. The primary goal is to design a molecule that can strongly bind to the target. While there are methods available for predicting the binding affinity, it is important to ensure that the ligand is optimized to be safe and efficacious before it can be used as a medication. These features include bioavailability, metabolic half-life, side effects, etc. Using rational design methodologies, it can be challenging to forecast these additional properties.

The creative process of developing novel drugs based on an understanding of a biological target is known as drug design. Designing molecules that are complementary in shape and charge to the molecular target with which they interact and bind is the most fundamental aspect of medication development. All areas of drug discovery are covered in the course, including genomics, bioinformatics, structural biology, cheminformatics, molecular modelling, fragment-based drug design, drug target choice, intellectual property, and commercialization. These are the two main categories of medication design. Both are known as structure-based drug design and ligand-based drug design, respectively.

Structure-based drug design

The term structure-based drug design refers to drug development that is based on an understanding of the biomolecular target's three-dimensional structure. Designing and improving a chemical structure with the intention of finding a substance suited for a drug candidate's clinical testing is known as structure-based drug design. In addition to small molecules, biopharmaceuticals, which include peptides and in particular therapeutic antibodies, by growingly significant class of medications. Computational techniques have also been developed to enhance the affinities, selectivities, and stabilities of these protein-based therapeutics. The SBDD process is iterative and involves several cycles before an optimised drug candidate is ready for clinical testing. The discovery phase, development phase, clinical trial phase, and registry phase are the four standard stages of a drug discovery process.

Ligand-based drug design

A strategy called ligand-based drug design, which focuses on understanding of compounds that bind to the desired biological target, is employed in the lack of 3D information about the receptor. Predictive models are generated in de novo drug design using structure and ligand-based approaches. While ligand-based methods are typically utilised when a protein structure is not accessible, structure-based methods exclusively rely on existing knowledge of a protein structure to generate novel ligands.

Drug design is due to high attrition rates, particularly during the clinical phases of drug development, more attention is being paid early in the drug design process to choosing candidate drugs whose physi-

Contact: Brian Montes, E-mail: brianmontes@gmail.com

cochemical properties are predicted to result in fewer complications during development and, therefore, more likely to result in an approved, marketed drug. In early drug discovery, in vitro tests combined with computational techniques are being employed more and more to choose substances with better ADME (Absorption, Distribution, Metabolism, and Excretion) and toxicity profiles.