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Drug Design, often Mentioned as Rational Drug Design or Just Rational Design

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Description

Drug design, often mentioned as rational drug design or just rational design, is that the inventive process of finding new medications supported the knowledge of a biological target. The drug is most ordinarily an organic small molecule that activates or inhibits the function of a biomolecule like a protein, which successively leads to a therapeutic benefit to the patient. In the most elementary sense, drug design involves the planning of molecules that are complementary in shape and charge to the bio molecular target with which they interact and thus will bind to it. Drug design frequently but not necessarily relies on computer modeling techniques. The phrase "drug design" is to some extent a misnomer. A more accurate term is ligand design (i.e., design of a molecule which will bind tightly to its target). Although design techniques for prediction of binding affinity are reasonably successful, there are many other properties, like bioavailability, metabolic half-life, side effects, etc., that first must be optimized before a ligand can become a secure and efficacious drug. The phrase "drug design" is to some extent a misnomer. A more accurate term is ligand design (i.e., design of a molecule which will bind tightly to its target). Although design techniques for prediction of binding affinity are reasonably successful, there are many other properties, like bioavailability, metabolic half-life, side effects, etc., that first must be optimized before a ligand can become a secure and efficacious drug.

A bio molecular target (most commonly a protein or a nucleic acid) may be a key molecule involved during a particular metabolic or signaling pathway that's related to a selected disease condition or pathology or to the infectivity or survival of a microbial pathogen. Potential drug targets are not necessarily disease causing but must by definition be disease modifying in some cases, small molecules will be designed to enhance or inhibit the target function in the specific disease modifying pathway. Small molecules for example receptor agonists, antagonists, inverse agonists, or modulators; enzyme activators or inhibitors; or ion channel openers or blockers are going to be designed that are complementary to the binding site of target. Small molecules drugs are often designed so as to not affect the other important "off-target" molecules often mentioned as ant targets since drug interactions with off-target molecules may lead to undesirable side effects.

In contrast to traditional methods of drug discovery known as forward pharmacology, which believe trial-and-error testing of chemical substances on cultured cells or animals, and matching the apparent effects to treatments, rational drug design also called reverse pharmacology begins with a hypothesis that modulation of a selected biological target may have therapeutic value. In order for a biomolecule to be selected as a drug target, two essential pieces of data are required. The first is evidence that modulation of the target is going to be disease modifying. This knowledge may come from, for instance, disease linkage studies that show an association between mutations within the biological target and certain disease states. The most fundamental goal in drug design is to predict whether a given molecule will bind to a target and if so how strongly. Molecular mechanics or molecular dynamics is most frequently wont to estimate the strength of the intermolecular interaction between the tiny molecule and its biological target. These methods also are wont to predict the conformation of the tiny molecule and to model conformational changes within the target which will occur when the tiny molecule binds there to. Semi-empirical, initio quantum chemistry methods, or density functional theory are often used to provide optimized parameters for the molecular mechanics calculations and also provide an estimate of the electronic properties electrostatic potential, polarizability of the drug candidate which will influence binding affinity. A more accurate term is ligand design of a molecule which will bind tightly to its target. Although design techniques for prediction of binding affinity are reasonably successful, there are many other properties, like bioavailability, metabolic half-life, side effects, etc., that first must be optimized before a ligand can become a secure and efficacious drug.

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