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Perspective

The Molecular Designing of Drugs

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Drug design is referred to as simply rational design or rational drug design.

The main aim in drug design is to forecast that the given molecule will bind to a target and if so, then how strongly it binds?.

Molecular dynamics or Molecular mechanics are the most which are used to estimate the strength of the intermolecular interaction between the small molecule and to its biological target.

Molecular modeling has become essential and valuable tool in medicinal chemists in the process of drug designing. Drug design is often stated as simply rational design or rational drug design. It is the new inventive process in finding new medications based on biological target and its knowledge.

Drug design frequently relies on computer modelling techniques but not necessarily rely on computer modelling techniques. This type of modelling is referred as computer-aided drug design.

The drug is commonly an organic small molecule which inhibits the function of biomolecule like protein, which in turn results in therapeutic benefit to the patient.

In the basic sense, drug design involves the design of molecules which are complementary in shape and charge to the biomolecular target which will bind to it. In addition to the small molecules, biopharmaceuticals including peptides and therapeutic antibodies which increase importantance of drugs and computational methods for improving the affinity, selectivity, and stability of these protein-based therapeutics have developed.

Although the techniques for designing and prediction of binding affinity which are reasonably successful, having other properties like metabolic half-life, bioavailability, side effects, etc., which were first optimized before a ligand and become a safe and efficacious drug.

Due to high attrition rates during clinical phases of drug development, more attention is focused in the drug design process on selecting drugs whose physicochemical properties are predicted to result in complications during the development and more likely to lead to an approved, marketed drug.

In, in vitro experiments with computation methods are increased in early drug discovery to select compounds with more favorable ADME (absorption, distribution, metabolism, excretion) and toxicological profiles.

Finally, the drug design rely on the knowledge of the 3 dimensional structure of the biomolecular target is known as structure-based drug design.

In the basic sense of drug design it involves in the design of molecules which are complementary in shape and charge to the molecular target with which they interact and bind.

The main process in a successful discovery of drug pipeline is the identification of small potent compounds that selectively bind to the target of interest with high affinity.

Knowledge of protein-protein interactions and binding sites of indispensable in-depth understanding the networks of living cells.