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Commentary Article

Drug Design

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ABSTRACT

Drug design is also known as rational drug design, in which new drugs are found based on the biological target knowledge. The drug is a small molecule that inhibits or activates the function of biomolecule such as protein, which benefits the patient.

Keywords: Drug design; biomolecules

INTRODUCTION

Drug design involves the designing the shape and charge of the drug same as that of biomolecular target with which it interacts and binds. Drug design might or might not depend on the computer modelling techniques .If it is based on the computer modelling then it is known as computer-aided drug design. Drug design that relies on the knowledge of the three-dimensional structure of the biomolecular target is known as structure-based drug design.

A more accurate term for drug design is ligand design. Design techniques for prediction of binding affinity are reasonably successful, there are many other properties, such as bioavailability, metabolic half-life, side effects, etc., that first must be optimized before a ligand can become a secure and efficacious drug. More attention is being focused early within the drug design process on selecting candidate drugs whose physicochemical properties are predicted to end in fewer complications during development and hence more likely to steer to an approved, marketed drug. In vitro experiments complemented with computation methods are increasingly utilized in early drug discovery to pick compounds with more favorable ADME (absorption, distribution, metabolism, and excretion) and toxicological profiles.

A biomolecular target may be a key molecule involved in signalling or metabolic pathway that's related to a selected disease condition or pathology or to the infectivity or survival of a microbial pathogen. In some cases, small molecules will be designed to enhance or inhibit the target function in the specific disease modifying pathway.

In contrast to traditional methods of drug discovery, which rely on trial-and-error testing of chemical substances on cultured cells or animals, and matching the apparent effects to treatments, rational drug design begins with a hypothesis that modulation of a selected biological target may have therapeutic value . Molecular mechanics or molecular dynamics is often used to estimate the strength of the intermolecular interaction between the small molecule and its biological target.

CONCLUSION

These methods are also used to predict the conformation of the small molecule and to model conformational changes in the target that may occur when the small molecule binds to it. CADD is an exciting and continually evolving area that leverages new data and methods to supply approaches that tackle the ever-changing needs of drug discovery. The scope continues to grow, and applications now span the entire drug discovery process. The availability of experimental data for model building for multiple endpoints or selectivity targets enables CADD to tackle the needed multidimensional optimization challenge, and a combination of models for the different endpoints are often used, alongside a spread of methods.

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