New drug discovery by computational-drug design method.

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Abstract

Computational drug design has emerged as a powerful technique that plays an important role in the development of new drug molecules. Structure-based drug design and ligand-based drug design are two commonly used methods in computational drug design. This article describes the theory behind the methods and their successful applications and limitations. To accomplish this, we reviewed structure-based and ligand-based virtual screening methods. Molecular dynamics simulations, which have become one of the most influential tools for predicting small molecule conformation and conformational changes within biological targets, are also being explored. Finally, we discuss the principles and concepts of molecular docking, pharmacophore, and other methods used in computational drug design.

Keywords: Computer-aided drug design, Virtual screening, Molecular docking, Chemical-biological interactions.

Introduction

Drug discovery research uses chemical biology and computer-assisted drug discovery approaches for efficient lead identification and optimization. Chemical biology is primarily concerned with elucidating the biological function of targets and the mechanisms of action of chemical modifiers. Computational drug design, on the other hand, uses structural knowledge of target molecules or known biologically active ligands (ligand-based) to facilitate the identification of promising drug candidates. Various virtual screening techniques are currently being used by both pharmaceutical companies and academic research groups to reduce the cost and time required to discover effective drugs. Although these techniques are advancing rapidly, continuous improvement is essential for future drug discovery tools. The advantages of structure- and ligand-based drug design suggest that their complementary use and integration into experimental routines will have a strong impact on rational drug design. This article provides an overview of its application to rational drug development integrated with current computational drug design to support advances in drug discovery [1].

Computational approaches are useful tools for interpreting and directing experiments to speed up the antibiotic design process. Structure-based drug discovery (SBDD) and ligand-based drug discovery (LBDD) are her two general types of computational drug discovery (CADD) approaches that exist. SBDD methods analyze the 3D structural information of macromolecules of targets to identify critical sites and interactions that are important for their respective biological functions. This information can then be used to design antibiotic drugs that can compete with the essential interactions involving the target, disrupting biological pathways essential for microbial survival [2]. The LBDD method focuses on known antibiotic ligands for targets and establishes relationships between their physiochemical properties and antibiotic activity, called Structure-activity relationships (SAR). This information can be used to optimize known drugs or to design new drugs with improved activity. This chapter introduces standard CADD protocols for both SBDD and LBDD. In particular, we focus on methods and targets that are routinely studied in our antibiotic discovery lab [3].

Modern drug discovery is characterized by the need to generate large numbers of compounds and screen these vast libraries in a short period of time. The need to store, manage, and analyse these rapidly increasing resources has spawned a field known as Computer-Aided Drug Design (CADD). CADD stands for computational methods and resources used to facilitate the design and discovery of new therapeutic solutions [4]. A digital repository of detailed information about pharmaceuticals and other useful compounds is a gold mine for exploring chemical reaction possibilities. Design libraries with the potential to generate entire molecular variants enable selection and sampling of compounds with diverse properties. Fold detection, which examines sequence-structural homology between protein sequences and structures, helps infer binding sites and molecular function. Virtual screening, an in silico analogue of high-throughput screening, has shown promise for the systematic evaluation of large chemical libraries to identify potential lead candidates to be synthesized and screened. . This article provides an overview of the most important data sources and computational methods for discovering new molecular entities. We describe the workflow

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for the entire virtual screening campaign, from data collection to post-screening analysis [5].

Conclusion

To facilitate the drug discovery process, computational approaches have set milestones throughout the drug discovery pipeline, from target identification and mechanism of action to lead lanes and drug candidate identification. In addition to this, there is a resolute effort to explain the importance of in silico studies in predicting absorption, distribution, metabolism, excretion, and toxicity profiles. CADD is therefore accepted worldwide with various tools for studying, virtual screening, protein structure prediction, quantum chemistry, material design, and physical and biological property prediction. Computational tools are used as drug discovery tools in various disease areas. Here, bearing in mind the increasing importance of diabetes treatment, we have reviewed aspects of collaboration between information technology and chemoinformatics tools in antidiabetic drug discovery.

References

1. Taft CA, Da Silva VB. Current topics in computer-aided drug design. J Pharm Sci. 2008;97(3):1089-98.
2. Yu W, MacKerell AD. Computer-aided drug design methods. Antibio method proto. 2017:85-106.
3. Song CM, Lim SJ, Tong JC. Recent advances in computer-aided drug design. Brief Bioinform. 2009;10(5):579-91.
4. Van Drie JH. Computer-aided drug design: the next 20 years. J Comput Aided Mol Des. 2007;21(10):591-601.
5. Poonan P, Agoni C, Ibrahim MA, et al. Glioma-targeted therapeutics: computer-aided drug design prospective. Protein J. 2021:1-55.

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