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Design and application of molecular modeling to drug discovery.

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Abstract

Large-scale molecular modeling-simulation of biomolecules and bio macromolecules is an interesting and rapidly developing field that is increasingly contributing to our fundamental understanding of living organisms. In today's era of petascale computing, large-scale modelling simulations are powering a wide variety of scientific endeavors, from biotechnology applications such as manufacturing new smart biomaterials to DNA sequencing, disease treatments and drug development. It has a big impact. Several challenges lie ahead when it comes to improving molecular and conformational space sensing, but given the success of these applications so far, large-scale molecular dynamics simulations will be of further interest in future research in this area. There is little doubt that it will play an important and growing role.

Keywords: Biomaterial, Drug discovery, Molecular modelling, Molecular mechanics.

Introduction

Molecular modeling techniques have made great strides in recent years and are becoming an integral part of many chemical, physical, and biological studies. Here we present three of his techniques that are widely used in the simulation of bimolecular systems. Structural and homology modeling, molecular dynamics, molecular docking [1].

The advent of high-performance computing has strengthened the role of computing as a tool for in-computer experimentation in all areas of research, including drug discovery. Describes the current state of computer applications in pharmaceutical research using molecular modeling as a tool. Molecular modeling is an essential tool for drug discovery and has evolved significantly as the computational power and biological information of drugs has increased. Current modeling techniques accelerate drug discovery and design strategies. The most extensive applications of molecular modeling include disease-related target structure prediction, identification of new drug molecules for disease treatment, and development/proposal of new chemical entities [2].

As structural genomics projects progress, comparative modeling becomes increasingly important as the method of choice for obtaining his 3D structures of proteins. Providing reliable and accurate protein models helps fill the gaps in available sequence and structural information. Comparative modeling based on sequence identities greater than 30% is currently approaching the natural template-based limit, and further improvement requires the development of effective refinement techniques that can bring models closer to native structures [3]. For difficult targets, for which the most significant advances have been observed in recent years, optimal template selection and alignment accuracy remain major issues. The last year has seen the maturation of molecular modeling, with an increasing number of comparative studies between established methods and an explosion of new research, especially in the areas of combinatorial chemistry and molecular diversity. To achieve this, knowledge of the three-dimensional structure of proteins is essential for understanding their mechanisms of function and rational drug design [4].

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 targets or known biologically active ligands to facilitate the determination of promising drug candidates. Various virtual screening techniques are currently 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 [5].

Conclusion

Drug development is one of the most important processes in the pharmaceutical industry. Various calculation methods have

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greatly reduced the time and cost of drug discovery. In this review, we first described the role of multiscale biomolecular simulations in identifying drug binding sites on target macromolecules and elucidating drug mechanisms of action. Subsequently, virtual screening methods (molecular docking, pharmacophore modeling, QSAR, etc.) and structure- and ligand-based classical/de novo drug design were presented and discussed. Finally, we investigated the development of machine learning methods and their application to the above computational methods to speed up the drug discovery process. In addition, some application examples for combining different methods have been described. Combining different methods to jointly solve difficult problems at different scales and dimensions will become an inevitable trend in drug discovery screening and design.

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