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Editorial

Computer Aided in Drug Design

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INTRODUCTION

Discovery and development of a new drug is generally known as a very complex process which takes a lot of time and resources. Computational approaches in drug design, discovery and development process gaining very rapid exploration, implementation and admiration. Introducing a new drug in a market is a very complex, risky and costly process in terms of time, money and manpower. Nowadays, in silico methodologies became a vital a part of the drug discovery process; principally as a result of they'll boost the complete drug development mechanical phenomenon, distinctive and discovering new potential medicine with a major reduction of the prices and time. what is more, computer-aided drug style (CADD) approaches are necessary for reducing the experimental use of animals for in vivo testing, for serving to the look of safer medicine and for emplacement famous medicine, helping healthful chemists in every step (design, discovery, development, and hit-optimization) throughout the drug discovery method. The traditional strategies for drug discovery imply the pricey random screening of synthesized compounds or natural merchandise. On the opposite hand, the machine procedures will be terribly multifaceted, requiring knowledge base studies and application of technology to rationally style effective and commercially possible medicine. Exceptional progresses are created each in technology field, which have sped up the drug discovery analysis, and within the development of latest experimental procedures for the characterization of biological targets. Among the strategies in drug discovery, pharmacophore modelling, three-dimensional quantitative structure activity relationships (3D-QSAR), Comparative Molecular Field Analysis (CoMFA) and Comparative Molecular Similarity Indices Analysis (CoMSIA) stay the well-liked ligand-based (LB) strategies for quick virtual screening (VS) procedures and for rationalizing the activities of a group of ligands. During a recent breakthrough, a unique approach in QSAR field is diagrammatical by the mixture of the Molecular Dynamics (MD), and therefore the relative computed descriptors, with the generation of QSAR models.

This approach provides machine tools, the supposed MD-QSAR models, with associate degree increased prophetic power. once the data of the 3D structure of the targets in advanced with ligands ar famous, structure-based (SB) drug style approaches like SB pharmacophore models as well as excluded volumes or high outturn dockings ar the elective strategies for distinctive novel chemical entities for a specific target. If we wish to research ligand–receptor complexes and normally the dynamics and physics of biological systems, MD simulations represent one amongst the most important machine resources and still stay the foremost representative technique for this type of investigation. Additionally, for higher characterizing biological systems, understanding the mechanism of action of enzymes conjointly in advanced with ligands, quantum mechanics/molecular mechanics (QM/MM) calculations will be useful in drug discovery and style. Currently, QM/MM will be combined with MD (QM/MM-MD) to utterly characterize accelerator mechanisms.

ADVANTAGES

1. Through it we can reduce the synthetic and biological testing efforts.

2. It gives the most promising drug candidate by eliminate the compounds with undesirable properties (poor efficacy, poor ADMET etc.) through in silico filters.

3. It is a Cost-effective, time saving, Rapid and automatic process.

4. Through it we can know about the drug-receptor interaction pattern.

5. It gives compounds with high hit rates through searching huge libraries of compounds in silico in comparison to traditional high throughput screening.

6. These approaches minimize chances of failures in the final phase.

Computer power-assisted drug style is an economical tool within the space of drug discovery and development; through it we are able to realize the foremost promising drug candidate in a very cost-efficient means. It continually provides a hope for betterment in drug discovery space. Within the past years through laptop power-assisted drug style several spectacular researches area unit achieved thus it'll play an awfully abundant vital role within the close to future. With this achievement's, there's a promising way forward for laptop power-assisted drug style to assist drug discovery of the many additional curatives in future.

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