Global Science Research Journals

Available online at
www.globalscienceresearchjournals.org/

Perspective | Open Access

International Journal of Biosciences and Bioinformatics

ISSN: Vol. 9 (3), pp. 1-2, December, 2022

Techniques involved in computer aided drug design

J Andreas*

Department of Biochemistry, Ladoke Akintola University of Technology, Ogbomosho, Nigeria

*Corresponding author. E-mail: johnandrea@gmail.com

Received: 21-Nov-2022, Manuscript No: IJBB-22-84247; **Editorial assigned:** 23-Nov-2022, Pre QC No: IJBB-22-84247 (PQ); **Reviewed:** 07-Dec-2022, QC No: IJBB-22-84247; **Revised:** 16-Dec-2022, Manuscript No: IJBB-22-84247 (R); **Published:** 26-Dec-2022, DOI: 10.15651/IJBB.22.9.015

DECSRIPTION

Computer Aided Drug Design (CADD) employs a number of tools and techniques to aid in the various stages of drug design, lowering the cost of drug research and development. The discovery and development of a new drug is a lengthy, complex, expensive, and high-risk process that has no commercial counterpart. To speed up the process, Computer Aided Drug Design (CADD) approaches are widely used in the pharmaceutical industry. Using computational tools in the lead optimization phase of drug development has a significant cost advantage. Pharmacological research laboratories invest a lot of money and time in various stages of drug discovery, from therapeutic target setting to candidate drug discovery to evaluating the efficacy and safety of newly developed drugs to drug optimization through preclinical and extensive clinical trials. Major pharmaceutical companies have made significant investments in the routine Ultra High Throughput Screening (UHTS) of large numbers of drug-like molecules.

Simultaneously, computers are increasingly being used for virtual screening in drug design and optimization. Recent advances in DNA microarray experiments have revealed that thousands of genes involved in a disease can be used to learn more about disease targets, metabolic pathways, and drug toxicity. Empirical molecular mechanics, quantum mechanics, and, more recently, statistical mechanics are examples of theoretical tools. This most recent advancement enabled the inclusion of obvious solvent effects. The process of identifying chemical entities with the potential to be therapeutic agents is known as "drug discovery." The identification of new molecular entities that may be useful in the treatment of diseases with unmet medical needs is an important role of drug discovery campaigns, a new development concept, market demands, emerging diseases, academic and clinical research, the commercial sector, and so on.

It can originate from a number of sources, including Once a target has been identified for discovery, pharmaceutical companies or related academic institutions work on early processes to identify chemical molecules with suitable properties for making targeted drugs.

Ligand-based drug design is an approach that relies on knowledge of molecules that bind to the biological target of interest in the absence of receptor 3D information. The most important and widely used tools in ligand-based drug design are 3D Quantitative Structure-Activity Relationships (3D QSAR) and pharmacophore modeling. They can provide predictive models that are suitable for lead identification and optimization.

Ligand-based drug design is an approach that relies on knowledge of molecules that bind to the biological target of interest in the absence of receptor 3D information.

1 Ligand-based drug design entails identifying molecules that bind to the desired target site.
2 From these molecules, a pharmacophore model can be derived.
3 A pharmacophore model is a molecule that has the structural ability to bind to a specific target site.
4 Once the pharmacophore has been identified, it is determined whether it is compatible with the receptor; if not, the pharmacophore is further modified to create a potential drug.

Technological advancements promise to revisit and expand the medicinally relevant chemical space, guide the repurposing of approved drugs and existing chemical libraries, and rescue missing hits hidden as "treasures to be discovered" in existing SAR of corporate or public data. Drug design can be viewed as a cyclic multi objective optimization process. Indeed, it is critical to understand not only that a drug is generally an effective ligand for a therapeutically relevant protein but also that these molecules must have drug-like properties.