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Computer Aided Drug Design: An Overview

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ABSTRACT

A new drug's discovery and development is often regarded as a lengthy, expensive process that requires a lot of resources. Therefore, to improve the effectiveness of the drug discovery and development process, computer-aided drug design methodologies are currently used extensively. Structure-based drug design and ligand-based drug design approaches are known as particularly effective and powerful techniques in the field of drug discovery and development, among other CADD approaches that are considered as promising techniques based on their necessity. Both of these approaches can be used in conjunction with molecular docking for virtual lead optimisation and identification. In recent years, the pharmaceutical industry and research fields have made extensive use of computational technologies to increase the efficiency and effectiveness of the drug discovery and development process. In this article, we provide an overview of computational techniques, a creative method for identifying new leads that supports the investigation of drug discovery and development.**(1)**

INTRODUCTION:

Computer-aided drug design (CADD) offers a number of tools and approaches to help with the various stages of drug design, lowering the price of drug research and shortening the time it takes to produce new drugs. Drug research and development is a protracted, expensive, risky, and expensive process that has no equivalent in the business sector. In order to expedite the process, computer-aided drug design (CADD) techniques are frequently used in the pharmaceutical business. Using computational techniques during the lead optimisation stage of drug development has a major financial advantage. Pharmacological research laboratories spend a lot of money and time at different stages of the drug discovery process, from selecting therapeutic targets to candidate drug discovery, to assessing the efficacy and safety of recently developed drugs, to optimising drugs through preclinical and extensive clinical trials. Significant investments have been made by major pharmaceutical corporations in routine ultra high throughput screening (uHTS) of several drug-like compounds. Parallel to this, computerised virtual screening is being used more and more in medication formulation and optimisation. Numerous genes that are involved in a disease can be used to gather detailed information on disease targets, metabolic pathways, and drug toxicity, according to recent developments in DNA microarray research. Empirical molecular mechanics, quantum mechanics, and more recently statistical mechanics are examples of theoretical techniques. The most recent development made it possible to include overt solvent effects. All of this is largely due to the availability of workstations that handle high-quality computer graphics.**(2)**

CADD in the Drug Discovery Process:

CADD can be used in conjunction with wet laboratory methods to clarify and speed up the drug discovery process and create new medications (such as antibiotics) for both established and undiscovered targets. CADD streamlines the drug design procedure by cutting down on time and expense.**(3)**

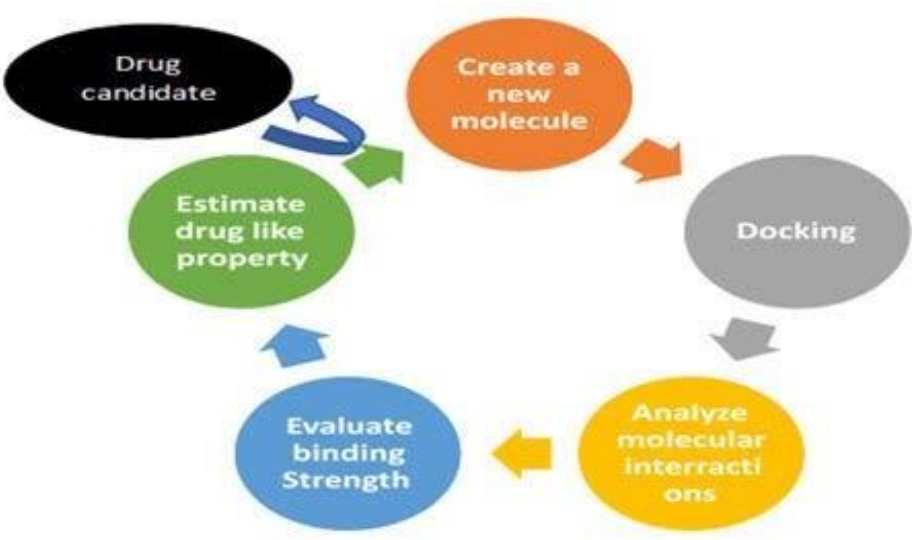


Fig 1: Computer Aided Drug Design

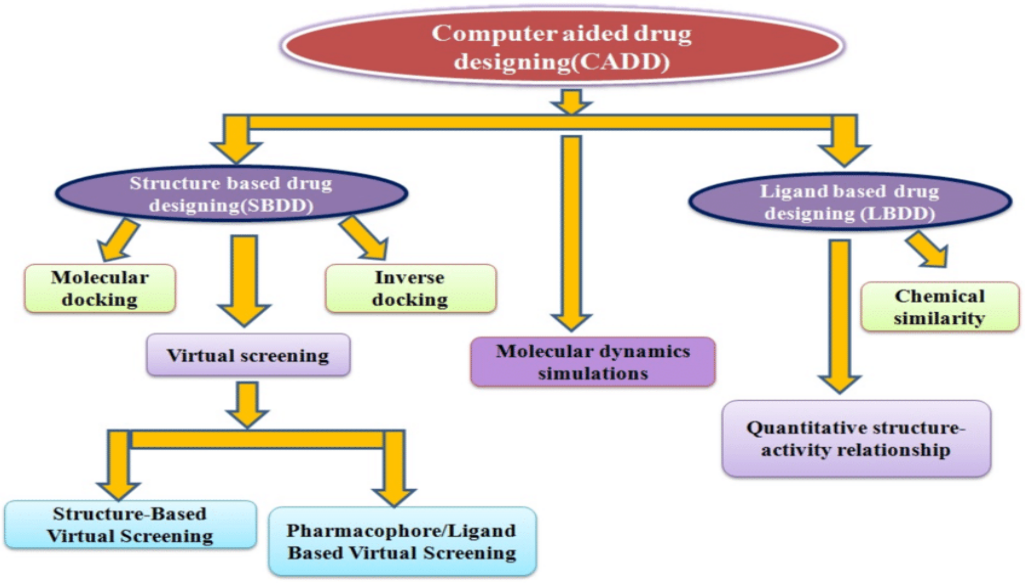
Definition:

The term "computer-aided drug design" (CADD) refers to a variety of theoretical and computational methods used in contemporary drug development. CADD techniques have played a significant role in the creation of some medications that are currently being tested in clinical settings. **(4)**

OR

The process of locating, creating, and assessing drugs and associated biological active substances using computer approaches is known as computer-aided drug design (CADD). The application of CADD techniques facilitates and expedites drug discovery while accelerating the early stages of chemical research. **(5)**

Types Of CADD:



1) Structure-based drug design or direct drug design:

The goal of structure-based drug design (SBDD), also known as direct drug design, is to create new therapeutic molecules that interact with the target protein more effectively. In SBDD, the structure of the target protein is known, and interaction or bio-affinity for all tested compounds iscalculated following the docking procedure.[1]

De novo drug design and virtual screening are both steps in the process known as "structure- based drug design" (SBDD). These techniques offer a highly effective alternate strategy for discovering and creating new medication designs. Drug chemical compounds are computationally screened against known target structures during virtual scanning. Rational drug design is very expensive and effective in traditional, advanced, or legacy drug design anddevelopment. Finding intriguing target proteins for small compound library screening is the first stage in the reverse pharmacology approach to rational drug creation. Because they are roughly related to the 3D structure of a Target protein, technologies including structure-based virtual scanning (SBVS), molecular docking, and molecular dynamics (MD) are utilised in SBDD, a more focused, effective, and quick procedure for lead discovery and optimisation. Analysis of disease and molecular binding energies, ligand protein interaction induction process. With the aid of some methodologies, SBDD has identified numerous medications, including thymidylate synthase inhibitors, raltitrexed, and possible HIV protease inhibitors. These were found using MD simulation and the drug

norfloxacin. More than 100,000 proteins' three-dimensional (3D) structures are presented in SBDD.[7]

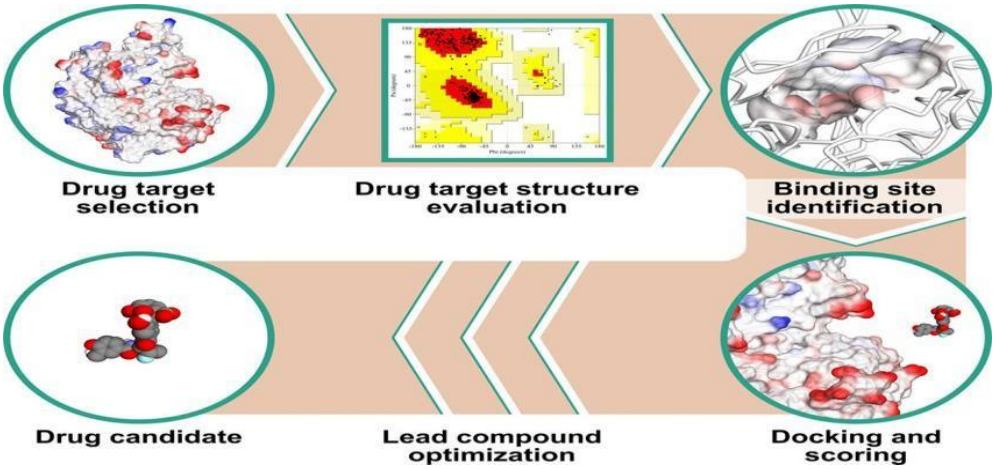


Fig 2: Workflow of Structure-based drug design (SBDD)

2) Ligand Based Drug Design:

Target is a ligand in this approach. A relationship between a molecule's structural and electrical features and its biological activity is known as a structure-activity relationship (SAR).Compounds are designed using data from the CADD methodologies and then put through chemical synthesis and biological testing.

In LBDD, the target protein's 3D structure is unknown, but it is known which ligands bind to the intended target location. These ligands can be used to create molecules or pharmacophoremodels that have all the structural characteristics required to bind to a target active site. Pharmacophore-based approaches and quantitative-structure activity relationships (QSARs) are two common ligand-based methodologies. In LBDD, it is presummated that substances with structural similarities also share the same biological properties and interactions with the target protein.[7]

Indirect drug design, also known as ligand-based drug design, is dependent on understanding the other molecules that bind to the desired biological target. These additional molecules can be utilised to create a pharmacophore model that specifies the minimal structural requirements for a chemical to bind to the target.[8]

A strategy called ligand-based drug design, which focuses on understanding of compounds that bind to the desired biological target, is employed in the lack of 3D information about the receptor. The most significant and often used methods in ligand-based drug design are pharmacophore modelling and 3D quantitative structure activity relationships (3D QSAR). They can offer forecasting models appropriate for lead optimisation and lead identification. Othersections of the study provide more details on these techniques and how to use them to design andproduce 5-LOX inhibitors.[9]

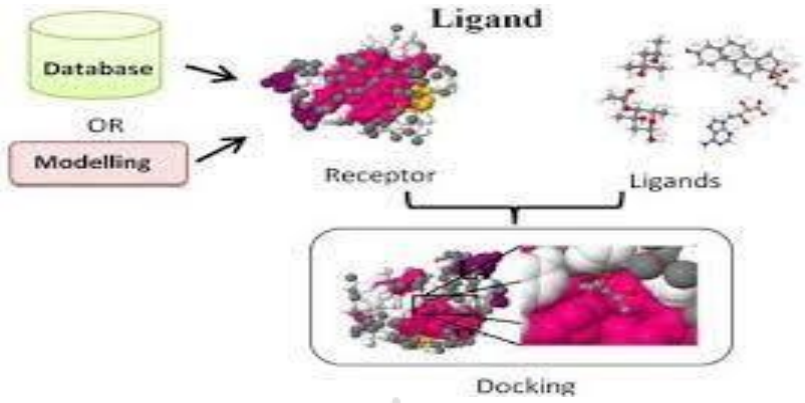


Fig 3: Process Involved In Ligand Based Drug Design

SOME PROMINENT EXAMPLES OF COMPUTER-AIDED DRUG DISCOVERY MECHANISM:

A number of effective treatments and medications have emerged as a result of computer-aided drug discovery processes. These medications have been used to treat conditions ranging from glaucoma to AIDS. Following are some examples of medications and the illnesses they are used to treat:

- Captopril: High blood pressure
- Dorzolamide: Ocular hypertension and glaucoma
- AIDS drug Saquinavir
- Leukaemia drug imatini
- Influenza drug Zanamivir
- Peptic ulcers: Cimetidine[11]

Recently used Example of CADD:

1) Covid 19:

We've briefly touched on the importance of computer-aided drug design in the context of COVID-19 and how researchers continue to rely on these computational techniques in the quick identification of promising drug candidate molecules against various drug targets implicated in the pathogenesis of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2).

The development of drugs to treat coronavirus disease-19 (COVID-19), an infectious viral disease brought on by SARSCoV-2, has made extensive use of both ligand-based and structure- based drug design methodologies.**(22)**

Epidemiology:

Transmission channels, infection sources, and susceptible hosts are the three main elements that influence the transmission of infectious diseases. The most current studies from China's National Health Commission state that SARS-CoV-2 is spread between persons through respiratory droplets, close contact, and surface contamination, with the possibility of aerosol transmission (Wu et al., 2020a).

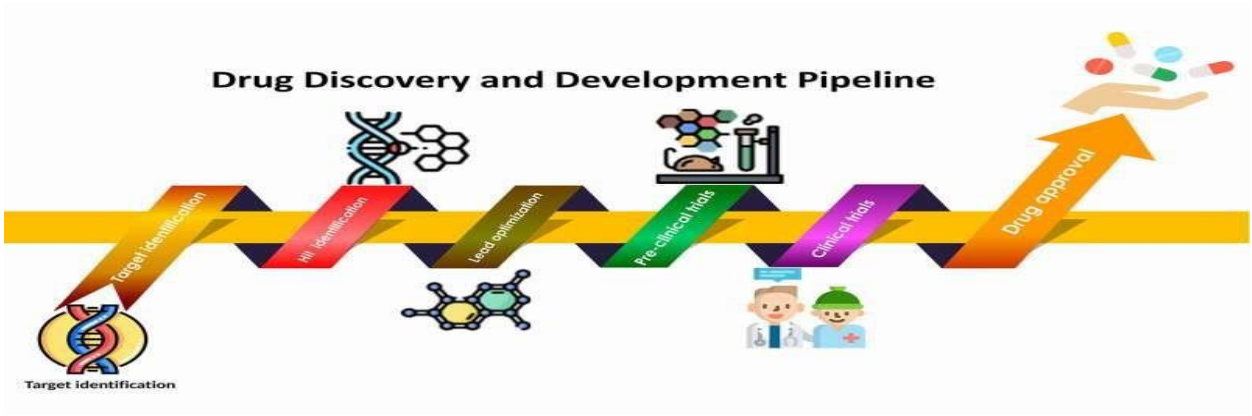
CADD's advantages and disadvantages in COVID-19:

Research Infectious disease transmission is governed by three important factors: transmission channels, infection sources, and the number of confirmed positive and fatal cases of SARS-CoV-2 infection.hosts that are weak. The most current studies from China's National Health Commission state that SARS-CoV-2 is spread between persons through respiratory droplets, close contact, and surface contamination, with the possibility of aerosol transmission (Wu et al., 2020a). Computer-aided drug design (CADD), which helps to reduce expenses associated with creating therapeutic agents, is emerging as a quick and dependable tool in pharmaceutical and medicinal research.

The CADD method makes it possible to find potent drugs in less time by facilitating the discovery of new drugs or the repurposing of FDA-approved drugs whose safety and adverse effects are already known. Additionally, realising the severity of COVID-19 and the lack of approved therapeutic agents justifies the need for finding potent drugs in less time. The SARS- CoV-2 genome's inherent mutability may make disease prevention and treatment more difficult, hence CADD can be effectively utilised to forecast how a mutation will affect drug binding to molecular receptors. As a result, CADD can significantly speed up the process of discovering and developing new drugs. However, there are several drawbacks to CADD approaches, including the necessity for preclinical and clinical testing to validate lead compounds obtained from the virtual screening process before a product can be approved for sale. The ongoing molecular mechanism investigations underlying the illness pathogenesis of COVID-19, as well as bias and imbalance in the little available data, might significantly affect how accurately CADD techniques like artificial intelligence forecast outcomes.**(23)**

2) Cancer:

Recently, the creation of anticancer drugs has been significantly impacted by the exponential expansion of computational techniques like computer-aided drug discovery (CADD). Faster, less expensive, and more effective medication creation is made possible by CADD, which also offers useful insights into the field of cancer therapy.**(24)**



Drug development is a difficult, drawn-out, expensive, and time-consuming process. It involves collaboration between various disciplines, such as medicinal chemistry, pharmacology, clinical research, drug metabolism, process chemistry, etc. Additionally, the modern drug development approach heavily relies on molecular modeling, high throughput

screening, and combinatorial chemistry. Bringing a novel lead from a drug discovery to market takes roughly 7–12 years and $800–$1.8 billion. To identify a single highlighted medicine, initially 1,00,000 candidate chemicals, hundreds of preclinical animal tests, and clinical trials on thousands of participants and patients are communicated. The pipeline, which includes the subsequent genuine advancements, refers to the process from the identification of new medications through their marketing.**(5)**

Disease choice Targets are identified Identification of lead Lead improvement Preliminary studies**(25)**

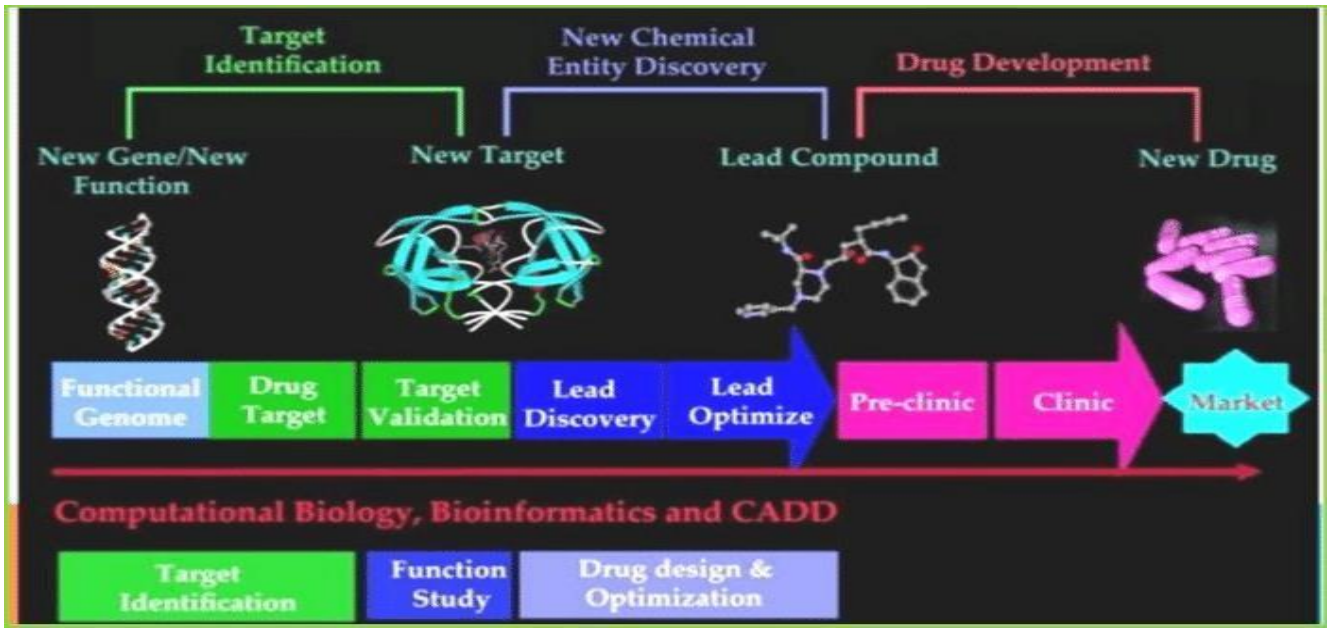


Fig 4: Overview of usual process of drug development

SOFTWARE USED IN COMPUTER AIDED DRUG DESIGN:

Software is necessary for a computer to perform tasks like run programmes. This programme streamlines and expedites our job. Numerous businesses, including Accelrys, Schrodinger, Auto Dock, and Argus Lab, provide software for creating drugs. **(12)**

The software is further divided into subcategories based on the tasks that they perform and how they operate, such as software that analyses pharmacokinetic parameters, ligand interactions, molecular dynamics, structural activity relationships, image analysis, and visualizers.

1) Accelrys:

A software company called Accelrys has offices in Europe and Japan in addition to its US headquarters. It offers software, particularly for materials science and drug discovery. The stagesof the drug discovery and development process are addressed by their products and technologies4. Accelrys produces the following software products:

a) Insight II

b) Pipeline Pilot c)Discovery Studio

d) Materials Studio

e) Accord.

a) Insight II:

Insight II is a programme for graphically modelling molecules. We can create and modify practically any type of molecules or chemical systems using this software. Some of these insight II computational engines can re-start calculations using data from saved files.

b) Pipeline Pilot:

Pilot pipeline: The foundation of the pilot data is a robust client-server platform that enables the creation of graphical workflows for data retrieval, filtering, analysis, and reporting. This software uses modelling tools, statistical filters, and clustering components that are designed for huge real-world data sets to model data. Using diverse technologies like Perl, Java, SOAP, and simple command line access, one can build extra components. This software is used in sequence analysis, gene expression, cheminformatics to examine the ADME characteristics of 20 medications and determine whether any harmful ingredients are present.

c) Discovery Studio:

Discovery Studio is a cutting-edge software solution for life science researchers that is simple touse, has a graphical user interface, and sophisticated tools for protein modelling, sequence analysis, pharmacophore analysis, and structure-based designing. Active X control, a visualising tool offered by Discovery Studio, offers 3D molecular structures and

the sharing of scientific findings. Tools like BLAST (Basic Local Alignment Search Tool) and DS Modeller's protein modelling are used for the sequence analysis. It can be used in environments with Linux and Windows operating systems, among others.

d) Materials Studio:

The most cutting-edge technology is employed to tackle issues in the R&D process through the usage of Materials Studio software. It is intended for computational and structural researchers working on chemicals and material R&D. Materials Studio offers tools for modelling crystal structure and crystallisation processes, as well as for predicting the properties of molecules, polymers, and catalysts and establishing the relationship between structure and activity. They offer a variety of density functional techniques, linear scaling, and semi-empirical tools for forecasting structures that are based on quantum mechanics. The Materials studio's QSAR integration offers a wide range of descriptors, including topological and electro-topological descriptors, which make the computation process simpler.

e) Accord:

Accord is specialised cheminformatics software. They are able to collect, organise, process, and mine chemical data. Software called Accord, which is based on Oracle, is used to save, retrieve, and analyse chemical structures as well as related biological, chemical, and inventory data.Accord has a user-friendly interface and a powerful, well-tested chemistry engine that can handle any form of chemistry. **(13)**

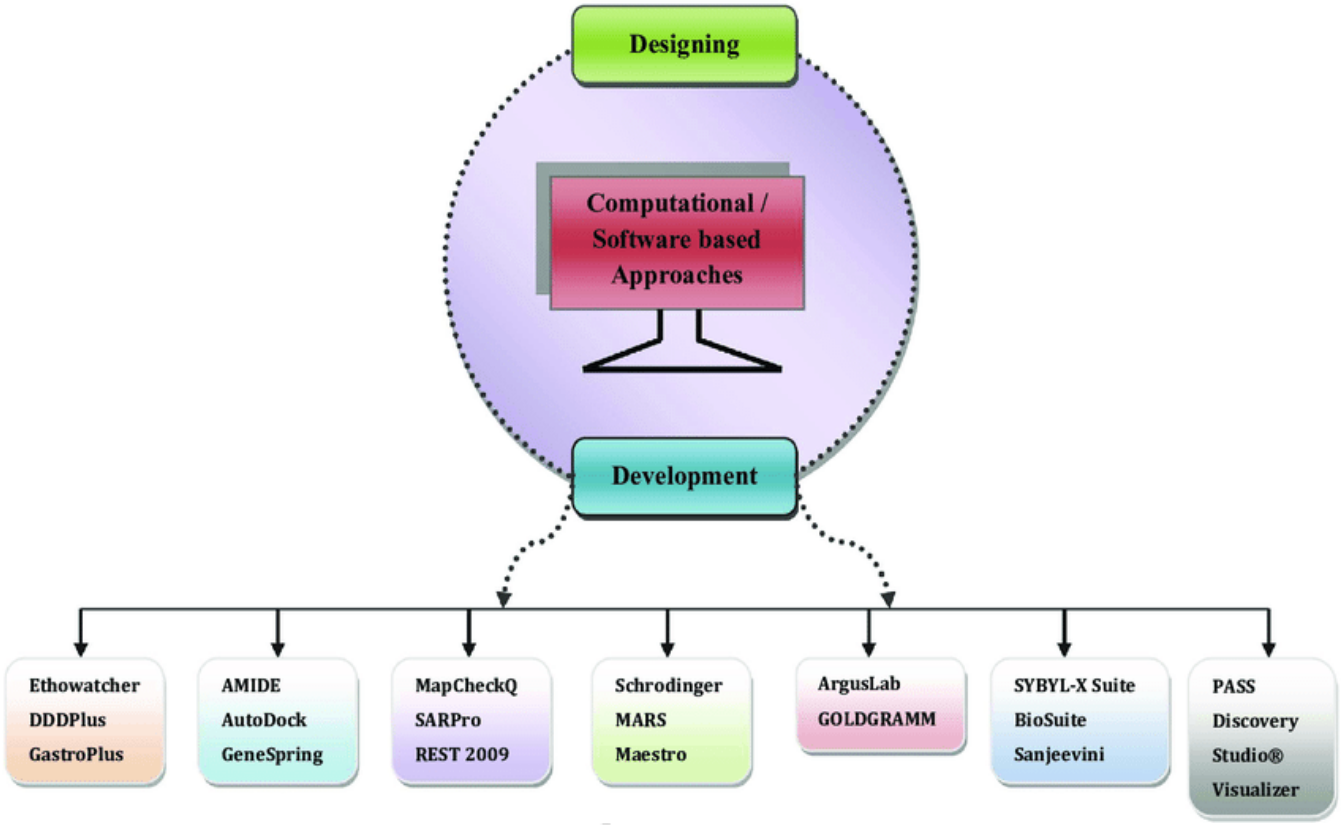


Fig. 5: Software based approaches for drug designing and development

TOOLS USED IN CADD:

1) Molecular Docking

2) Molecular Modelling

3) Rational Drug Design

4) Computational Chemistry

5) Molecular Design

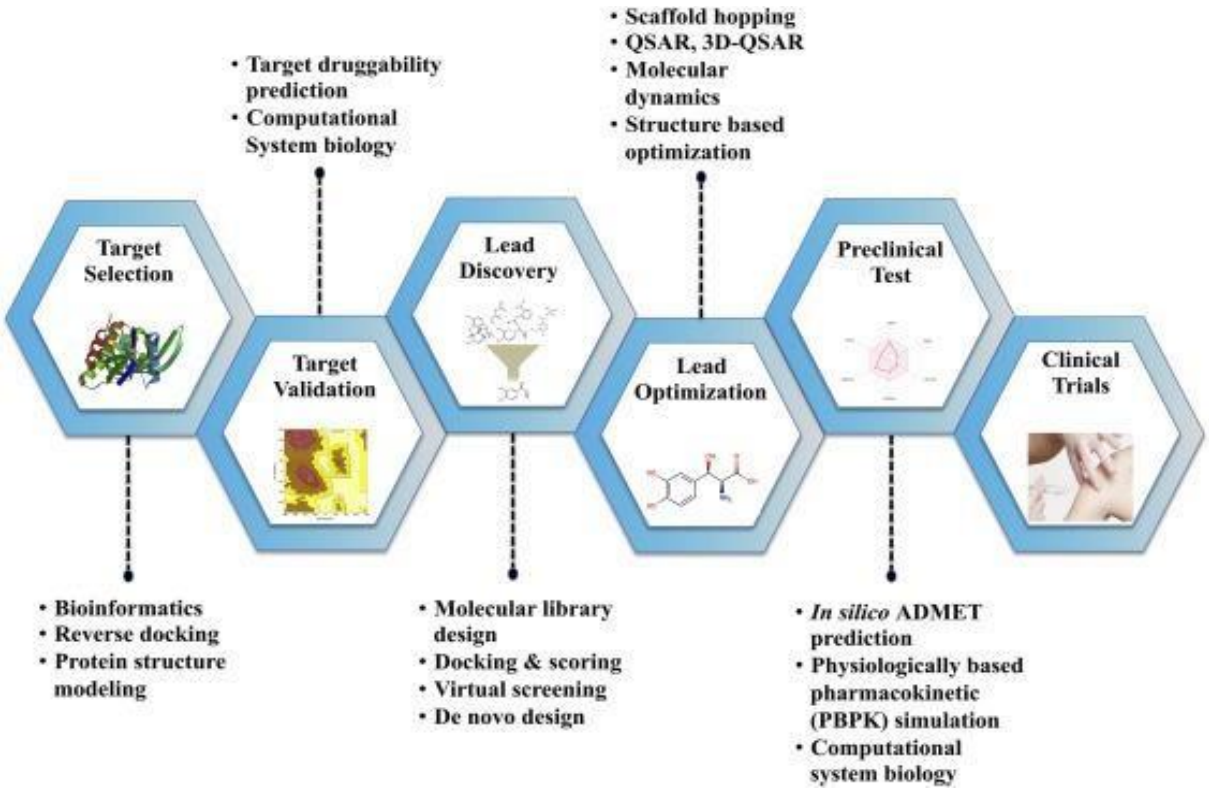


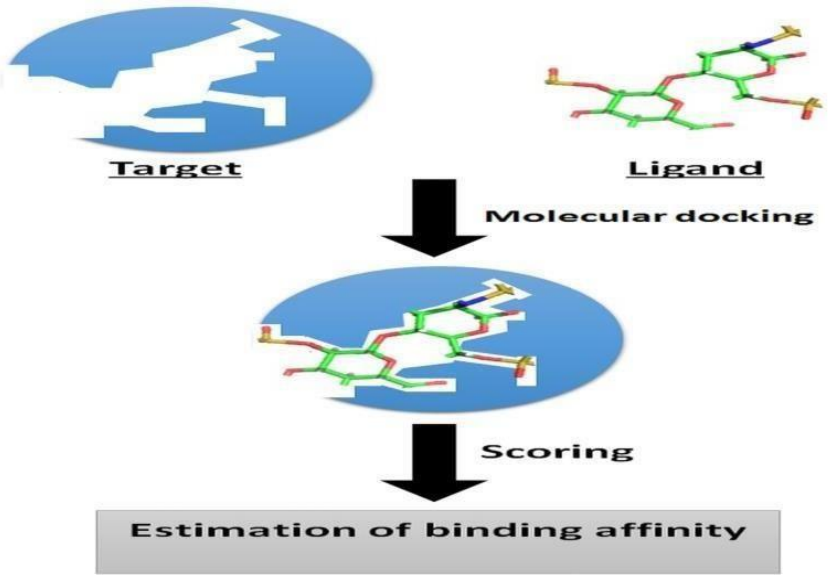
Fig. 6: Modern Tools and Techniques in Computer-Aided Drug Design

1) Molecular docking:

Molecular docking is a popular computational method for quickly predicting the binding affinities and modes of small molecules to their target molecules, which are typically proteins. This in silico method has become extremely significant in the realm of drug discovery. Molecular docking, which has been demonstrated to be more effective than conventional drug discovery techniques, has arisen during the last two decades and is now recognised as a crucial tool for CADD and in the field of structural biology. The enormous increase in computing power and the growing accessibility of small chemical and protein databases have greatly aided molecular docking.

The fundamental concept of molecular docking is shown in Fig. This technique is expected to become more effective as a result of recent developments in computer technologies and the availability of 3D structural data for biological targets, which will also make it easier to apply widely to investigations of the molecular interactions involved in ligand-protein binding. Small molecules can typically be docked in one of three ways: (a) rigid docking, where the target and ligands are both treated as rigid entities; (b) flexible docking, where

both the target and ligand are considered to be flexible; or (c) flexible ligand docking, where the ligand is treated as flexible and the target is treated as rigid.[17]



2) Molecular Modelling :

All computer techniques for predicting molecule structure and behaviour collectively are referred to as molecular modelling. Molecular modelling approaches are utilised in various domains,from structural biology to material science, to comprehend systems made up of a wide spectrum of complexity, from tiny molecules to biological macromolecules including proteins, receptors, and nucleotide chains. These systems can be represented by using wave functions at the atomic and subatomic scales (quantum mechanics) or by considering atoms as particles with charges and potential energy using forcefields (molecular mechanics).

Molecular modelling has advanced significantly over time, moving from hand-drawn illustrations of chemical structures to millisecond-long simulations of biological systems.[18]

3) Rational Drug Design:

Designing therapeutic compounds that bind to a target (such as a protein or nucleic acid) is referred to as rational drug design. It avoids testing thousands of molecules at random by relying on prior knowledge of the structure, function, and mechanism of the target. To assist medicinal chemists in the target-to-hit, hit-to-lead, and lead optimisation stages of

developing a therapeutic candidate, computer-aided drug design is essential. We concentrate on structure-based drug design and molecular dynamics-based strategies among these techniques in this article.**(19)**

4) Computational Chemistry:

To find and develop a promising lead in the drug development process, CADD is a contemporary computer technique. Computational chemistry, molecular modelling, molecular design, and rational drug design are all components of computer-aided drug design. The detected leads are being optimised using CADD. Diverse computational chemistry techniques are used in drug design and discovery to compute and anticipate events, such as the drug's binding to its target and the chemical characteristics for developing prospective new medications. CADD in the pipeline for medication development. There is a designated therapeutic target for which a medication must be created. A structure-based method or a ligand-based approach is used, depending on the availability of structure information. Multiple lead compounds will be able to be identified by a successful CADD campaign.

5) Molecular Design:

Software for molecular modelling known as molecular design software offers unique assistance for creating molecular models from scratch. As opposed to the typical molecular modelling programmes , such as those for quantum chemistry and molecular dynamics, such software directly supports the following features of building molecular models: **(20)**

Molecular graphics, interactive molecular drawing and conformational editing, the construction of polymeric molecules, crystals, and solvated systems, the production of partial charges, geometry optimization, and support for various force field development facets.

USE OF COMPUTER-AIDED DRUG DESIGN (CADD):

By concentrating primarily on the most effective chemicals, CADD assists scientists in minimising the synthetic and biological testing efforts. It not only explains the chemical underpinnings of therapeutic efficacy but also makes predictions about potential compounds that could enhance activity.

(1) The utilisation of computational power to speed up the drug research and development processes is what CADDD includes (Kapetanovic, 2008).

(2) Finding and improving novel medications by utilising chemical and biological data about targets and/or ligands.

(3) Designing filters for undesired chemicals with poor activity and/or poor absorption, distribution, metabolism, excretion, and toxicity in silico, which makes it easier to choose the candidates with the best chances of success.**(30)**

LIMITATIONS OF COMPUTER AIDED DRUG DESIGN :

- expensive
- lengthy
- Demands technical knowledge.

FUTURE PROSPECTS:

- Pharmaceutical development will benefit from computer assisted drug design, however it is still unclear to what extent.
- Experts predict that businesses who successfully utilise CADD will likely outperform their rivals who continue to rely on antiquated practices . It is envisaged that this method will be more cost-effective.**(16)**
- The creation and use of computational methods for predicting the free energy of drug binding.
- Creation and use of fresh approaches to computational chemistry of carbohydrates.
- Research on proteins, carbohydrates, and DNA using biomolecular simulation.
- Studies of the condensed phase using QM/MM
- Molecular modelling is used to create mutations, examine potential interactions with other proteins or nucleic acids, and provide 3-dimensional structures for proteins that are interesting to us as drug design targets.

 Creating lead drug structures and compounds that bind to DNA, tRNA, ribozymes, or enzyme active sites.

 Modifying proteins for molecular engineering, such as creating GFP versions that can be selectively chemically tagged to register enzyme activity, such as the activity of caspase 3inside cells going through apoptosis.

 Creating compounds having unusual chemical functions, including DNA breakage.

- Recognising the energetics and structural characteristics of tiny molecules.
- Recognising how various ligand families dock into the binding regions ofmacromolecules.**(16)**

DISCUSSION:

CADD's main goal is to screen, improve, and assess the compound's activity against the target. For both academic institutions and significant pharmaceutical firms, it creates a multidisciplinary strategy for higher efficacy with no/fewer side effects.The process of locating, creating, and assessing drugs and associated biological active substances using computer approaches is known as computer-aided drug design (CADD). The application of CADD techniques facilitates and expedites drug discovery while accelerating the early stages of chemical research. CADD is a crucial element of the interdisciplinary methodologies being used for the drug's development. Since its introduction in 1981, computer-aided drug design (CADD) has been attributed with influencing contemporary patterns in chemical characterization in drug discovery. Modern drug development uses CADD as a potent method to find possible medicinal molecules. It is now the best substitute for high-throughput screening, which is frequently utilised in the research and development of new drugs. As it can expedite the hit identification, hit to lead, and lead optimisation processes (binding affinity, ADME and toxicity, etc.), CADD techniques and tools are employed in nearly all stages of the drug discovery pipeline. We'll talk about the various CADDs. The two main categories of computer-aided drug design (CADD) methods currently in use are structure-based drug design (SBDD) and ligand-based drug design (LBDD). Global health issues have been raised by the recent outbreak of the devastating coronavirus disease 19 (COVID-19) pandemic. It is still difficult to have

medicines or vaccines licensed, which makes it even more important to find novel therapeutic compounds.

CONCLUSION:

High throughput screening is increasingly being replaced and complemented by CADD. The development of top-notch datasets and design libraries that can be optimised for molecular diversity or similarity has resulted from the search for novel molecular entities. On the other hand, breakthroughs in computational infrastructure and molecular docking methods are allowing screening throughput to increase quickly. Distributed computing is becoming more and more common for large-scale screening initiatives, driven by ever-more-powerful technology. These developments will, for the first time, enable the realisation of the full potential of lead discovery by design when combined with coordinated work towards the design of more precise physical models, such as solubility and protein solvation.**(21)**

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