



# Computer aided drug design- an overview

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**Abstract:** Being that Computer aided drug design (CADD) is the backbone of designer's way of communicating their design ideas, it is very crucial to examine the Attitude level of engineering students toward the usage of CADD application software. An instrument was developed and used in carrying out this work on engineering students of SRM University Chennai India, to find out the level of their attitude toward it. The students' attitudes were found high in nature, also no significant difference with students' mode of stay, and branches was observed. But significant difference and association were observed in students' interest and having personal computer. And also most of the students have difficulty in following online video tutorials, the research shows that there is need for video tutorials makers to make it in an episodic way so that the students would be able to comprehend what they watched and be able to practice it. Lastly it was concluded that more practical time was needed to the students to improve their competency in using the CADD application software.

**Key words:** computer aided drug design (CADD), virtual screening (VS), Quantitative structure activity relationship (QSAR), molecular modelling

## 1. INTRODUCTION

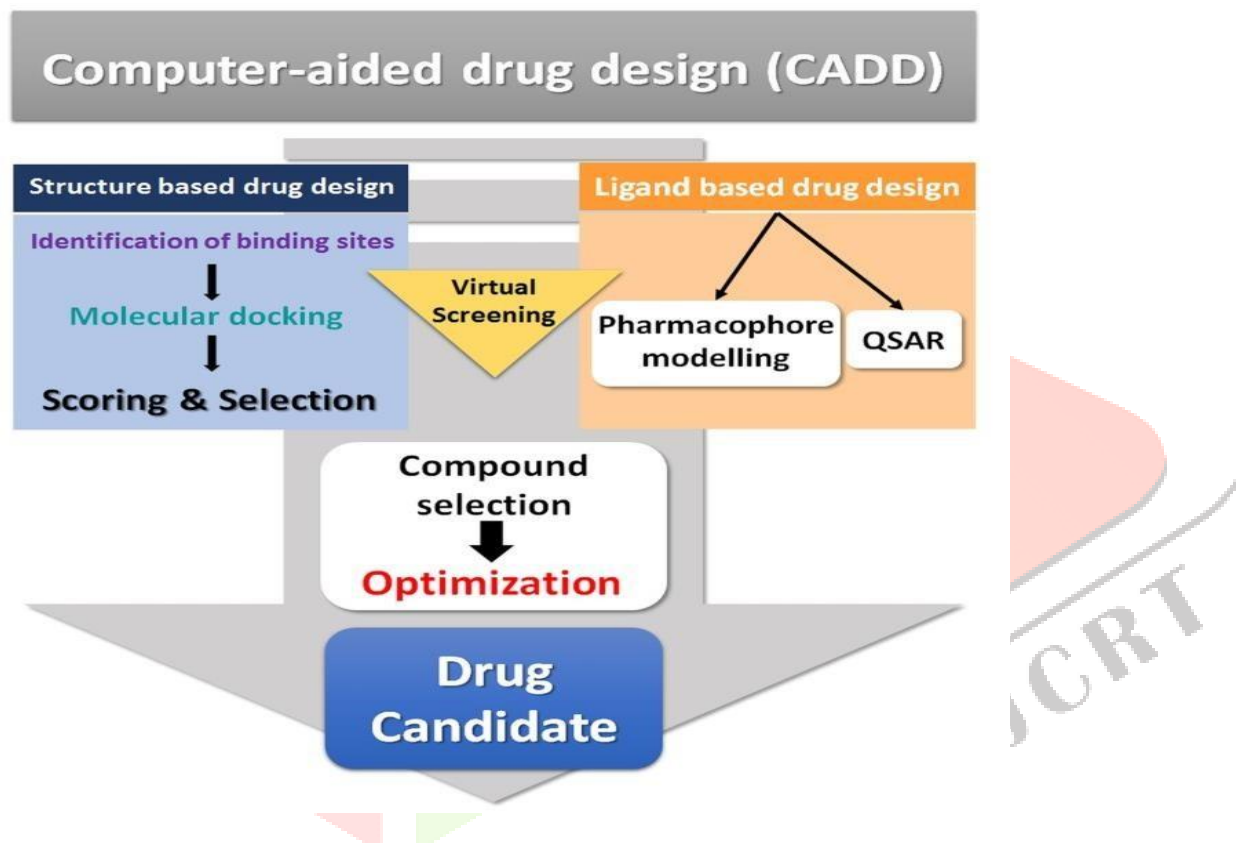
Throughout the history of human civilization many a times the whole human civilization or a large fraction of it came to the brink of eradication by epidemics such as plague, small pox, chicken pox, cholera etc. This threat to human civilization is a constant phenomenon governed by the process of evolution itself, which has given rise to diseases not known just a few years back like AIDS caused by HIV. Certain diseases like malaria, dengue etc. which were thought to have been brought under control, re-emerges from ashes and challenges human intellect to search for new weapons that can be effective against these demons.

Finding an effective drug molecule which is 100% target specific is the ultimate challenge in the modern drug design arena. Besides this, tackling the problem of side effect or drug toxicity is another burning issue. Again we are at the mercy of the natural evolution, a drug which is quite effective today may be just a dud in few years to come – the phenomena is known as drug resistance. So the challenge is at the fundamentals, it to understand how molecular evolution occurs. Only then, this seemingly invincible problem of drug resistance can hopefully be tackled.

In the days of competition and urgency one thus is in urgent need of some predictive model which can accelerate the process of finding the effective molecules with improved properties and diminished side-effects with the investment of minimum time and money. But now the reality is that the drug discovery and development is an intense, lengthy and an interdisciplinary endeavour. It is mostly portrayed as a linear, consecutive process that starts with target and lead discovery, followed by lead optimization and pre-clinical in vitro and in vivo studies to determine if such compounds satisfy a number of pre-set criteria for initiating clinical development. For the pharmaceutical industry, the number of years to bring a drug from discovery to market is approximately 12-15 years and the costing is about 500 – 2000 million dollars. Traditionally, drugs were discovered by synthesizing compounds in a time-consuming multi-step processes against a battery of in vivo biological screens and then investigating the promising candidates for their pharmacokinetic properties, metabolism and potential toxicity. In addition, the assessment of the risk of chemicals released to the environment is a

very crucial factor and development of environmentally benign synthetic methods is strongly desirable. Furthermore, there is also a demand on scientific methods that replace or at least reduce the use of laboratory animals. In particular, the U. S. Environmental Protection Agency (EPA), and the European Centre for the Validation of Alternative Methods (ECVAM) aims to develop and implement no animal alternative tests into regulatory and validation procedures. These methods should be used in the design, and evaluation of experimental tests, and in the selection of appropriate test chemicals for validation studies.

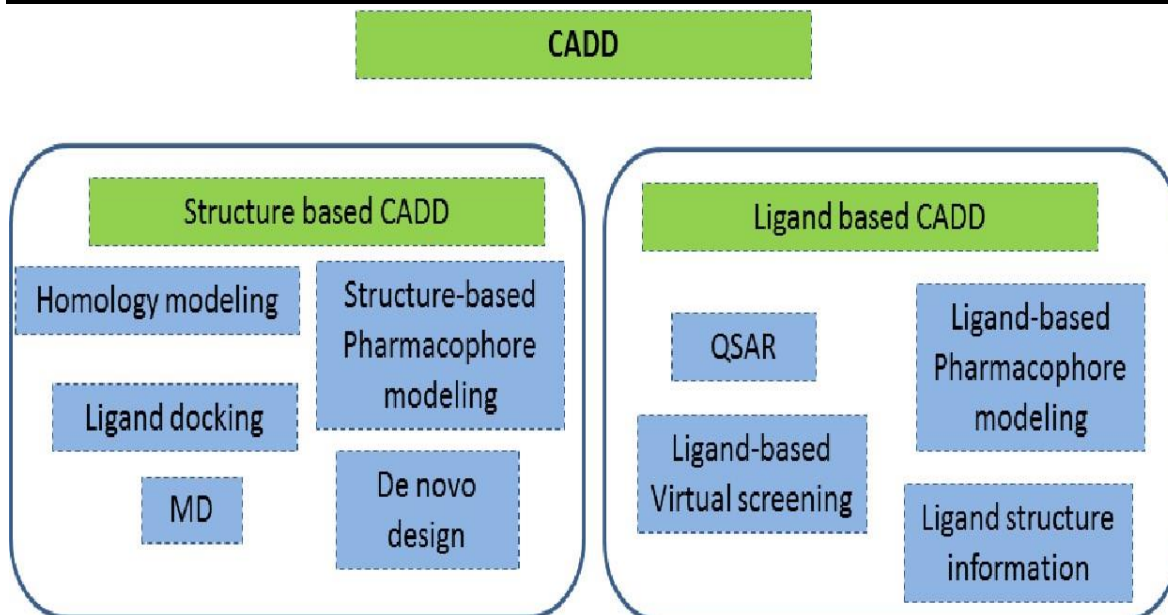
To introduce a new drug to the market is a costly affair that involves considerable time and money. The average time taken to discover/develop a drug is around 12-15 years and the cost stands at around US\$ 500 -2000million. Not surprisingly, pharmaceutical companies focus on reducing development times and budgets without adversely affecting quality. In the 1990's, a large number of developments were undertaken using combinatorial and high-throughput screening technologies, which accelerated drug discovery. These technologies were widely adopted because they enabled the rapid synthesis and screening of large libraries, but unfortunately, no significant success was achieved and little progress toward the development of new molecular entities was made.



**Figure 1: Overview of CADD process**

A combination of advanced computational techniques, biological science, and chemical synthesis was introduced to facilitate the discovery process, and this combinational approach enhanced the scale of discovery. Eventually, the term computer-aided drug design (CADD) was adopted for the use of computers in drug discovery. An overview of CADD is provided in Fig. (1).

Advanced computational applications have been shown to be effective tools and notable successes have been achieved using these techniques. CADD is a specialized discipline, whereby different computational methods are used to simulate interactions between receptors and drugs in order to determine binding affinities. However, the technique is not limited to studies of chemical interactions and binding affinity predictions, as it has many more applications ranging from the design of compounds with desired physiochemical properties to the management of digital repositories of compounds. CADD may be broadly categorized embracing both structure- and ligand-based drug design. Fig. (2) illustrates various approaches applied in CADD.



**Figure 2: Various approaches applied in CADD**

### 1.1 Background

Drugs are essential for the prevention and treatment of disease. Thus, ideal drugs are in great demand. But the process of Drug design is a tedious, time-consuming and cost intensive process. Thus several approaches are required which collectively would form the basis of Computer Aided or In Silico Drug Designing. [1] Use of computational methods in drug discovery and development process are nowadays gaining popularity, implementation and appreciation. Different terms are being applied to this area, including computer-aided drug design (CADD), computational drug design, computer-aided molecular design (CAMD), computer-aided molecular modeling (Camm), rational drug design, In Silico drug design, computer-aided rational drug design. [2] All the world's major pharmaceutical and biotechnology companies use computational design tools. At their lowest level the contributions represent the replacement of crude mechanical models by displays of structure which are a much more accurate reflection of molecular reality capable of demonstrating motion and solvent effects. Beyond this, theoretical calculations permit the computation of binding free energies and other relevant molecular properties. [3] Extensive genome decoding of various organisms, including man, proteomic investigations, discoveries of molecular mechanisms of many diseases, advances of protein chemistry lead to dramatic increase of number of new potential targets. [4] During the last decades the field of drug discovery process that direct to new ligands finding turns into the modern science employing of computer, bioinformatics and experimental approaches, which are denominated as rational drugs design which consist of computational drug designing. [4] Computer Aided Drug Design (CADD) and Delivery Systems offers an in-depth discussion of the computer-assisted techniques used to discover, design, and optimise new, effective, and safe drugs. [5] The objective of drug design is to find a chemical compound that can fit to a specific cavity on a protein target both geometrically and chemically. [5] The use of computers and computational methods permeates all aspects of drug discovery today and forms the core of structure-based drug design. [6] The day is not far away when Computer Aided Drug Designing will be dominant in modern medical services, thus the purpose is to bring forward, the significant advancements, which Computer Aided Drug Designing has made to serve mankind in producing newer drugs with improved effects.

#### 1.1.1 A Brief History of CADD

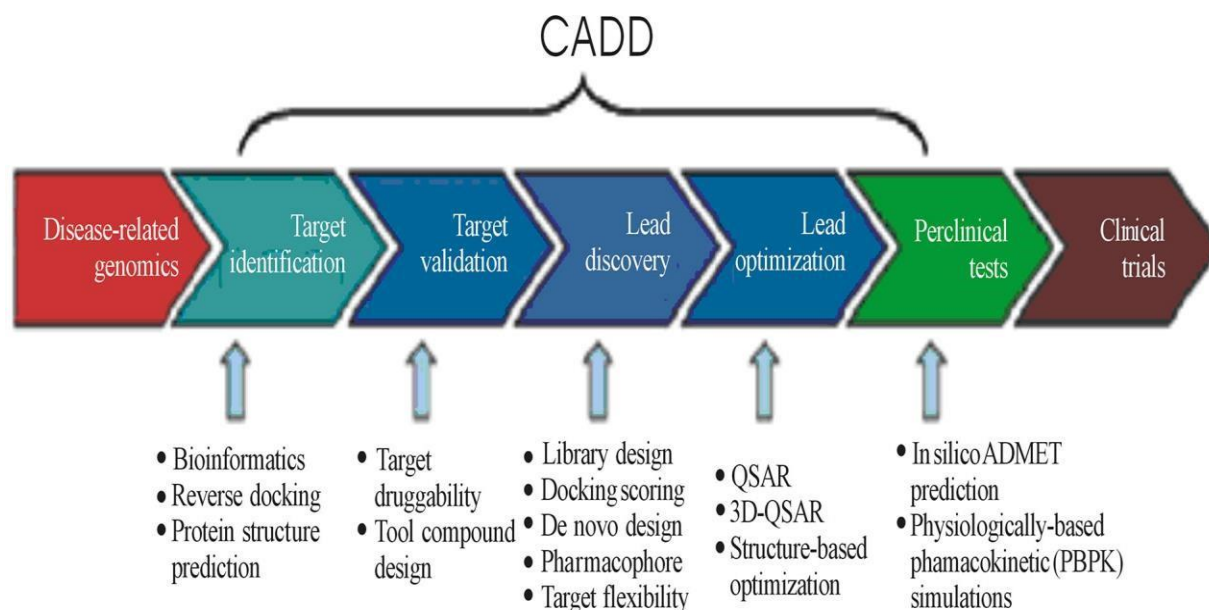
In 1900, the concept of receptor and lock-and-key was given by P.Ehrlich (1909) and E. Fisher. In 1970s, the concept of Quantitative structure activity relationships (QS-AR) was established, it had Limitations: 2- Dimensional, retrospective analysis; in 1980s there was Beginning of an era of CADD Molecular Biology, X-ray crystallography, multidimensional NMR Molecular modeling along with computer graphics. In 1990s more modern techniques like Human genome Bioinformatics along with Combinatorial chemistry and High-throughput screening were introduced in the world of innovative medical science. [3]

#### 1.1.2 How Does CADD Work?

Computer aided drug designing process consists of 3 stages (Fig. 3):

- **Stage 1:** Involves identification of therapeutic target and building a heterogeneous small molecule library to be tested against it. There is development of virtual screening protocol initialised by docking of small molecules.
- **Stage 2:** The selected hits are checked for specificity by docking at binding sites of other known drug targets.

- **Stage 3:** The selected hits are subjected to computational ADMET profiling studies and those who pass these studies are called leads.[6]



**Figure 3: Computer aided drug designing process**

#### 1.1.2.1 Target Identification

It is the first key stage in the drug discovery pipeline. Identification of correct targets from thousands of candidate macromolecules is a tedious process, which can be achieved by literature referring, Genomic analysis, pathway analysis.[6]

#### 1.2.2.2 Target Validation

After target identification, a rigorous evaluation is needed to demonstrate that modulation of target will have desired therapeutic effect. Target validation process determines whether modulation of target will have desired therapeutic effect.[1]

#### 1.2.2.3 Lead

Leads can be identified with the help of techniques like Structure based design. At this point, the structure of the target protein in complex with the lead molecule can be extremely useful in suggesting ways to improve the affinity of the lead for the target. Leads which are used in this case may be far from perfect, thus they should be optimised in order to increase their affinity for the target sites. Optimisation may be obtained by altering their structural features.

#### 1.2.2.4 IN SILICO ADMET (Absorption, Distribution, Metabolism, Excretion, Toxicity)

Prediction Techniques like molecular modelling, data modelling are used to study the interaction of proteins involved in ADMET process.[8]

Rational drug design is the inventive process of finding new medications based on the knowledge of a biological target. The drug is most commonly an organic small molecule that activates or inhibits the function of a biomolecule such as a protein, which in turn results in a therapeutic benefit to the patient. In the most basic sense, drug design involves the design of small molecules that are complementary in shape and charge to the biomolecular target with which they interact and therefore will bind to it. Drug design frequently but not necessarily relies on computer modeling techniques.

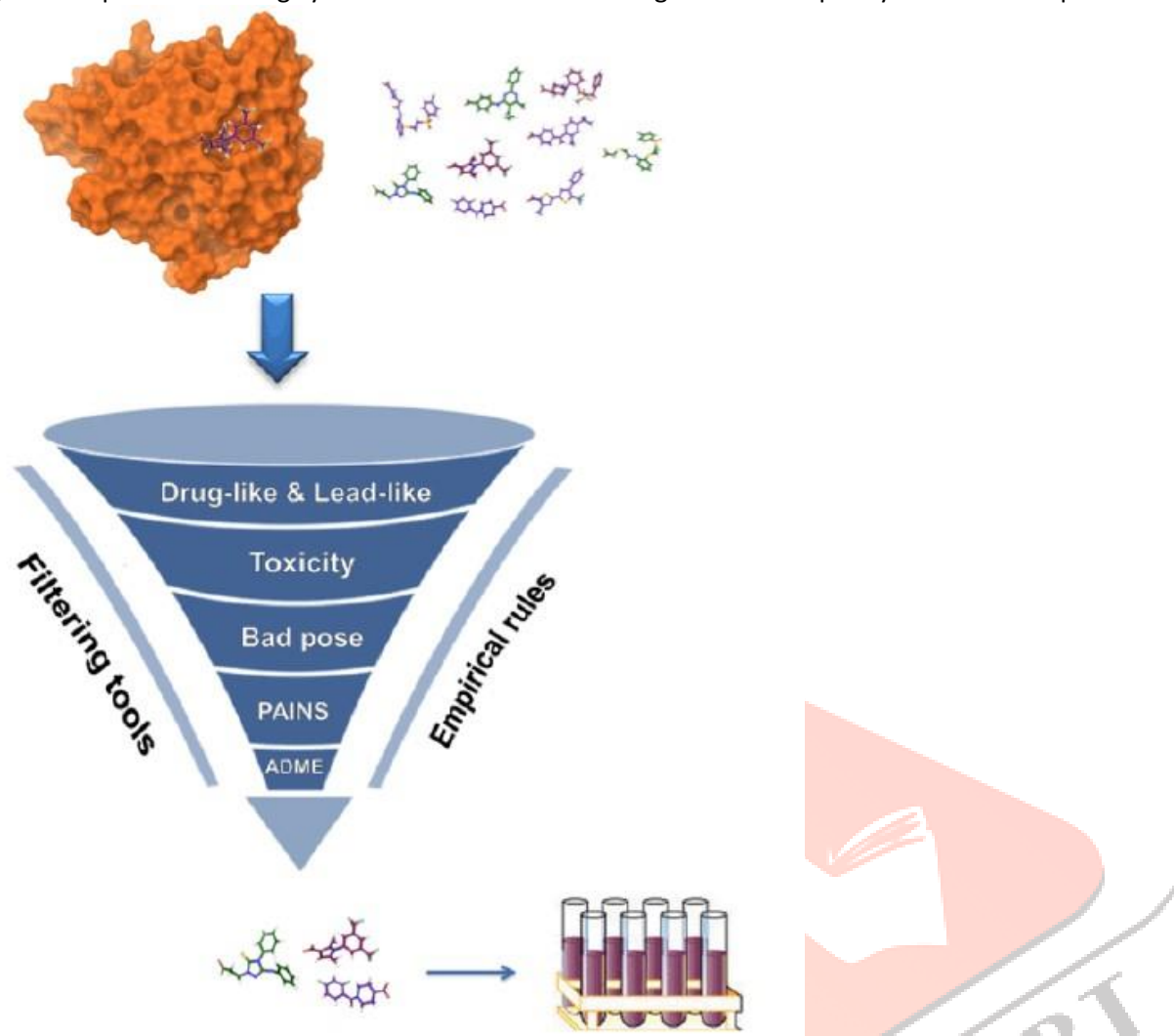
However, in relation to the application of computers as a tool in the drug design process, it is important to emphasize that computers can no way be a substitute for a clear understanding of the system under study. Computers only act as additional tools to have a better insight into the chemistry and biology of the problem. Researchers have devoted many years in the process of developing drugs based on computer aided rational drug design methods. Easy access to computational resources was not possible when these efforts began.

### 3.METHODS

There are different methods or approaches in computer aided drug designing

Virtual screening (VS) is a computational technique used for screening large datasets of molecules, and has been successfully used to complement High Throughput Screening (HTS) for drug discovery (Fig. 4). The major aim of VS is to enable the rapid, cost-effective evaluation of huge virtual compound databases to screen for effective leads for synthesis and further study. Virtual database screening can be applied to screen large libraries of compounds using various

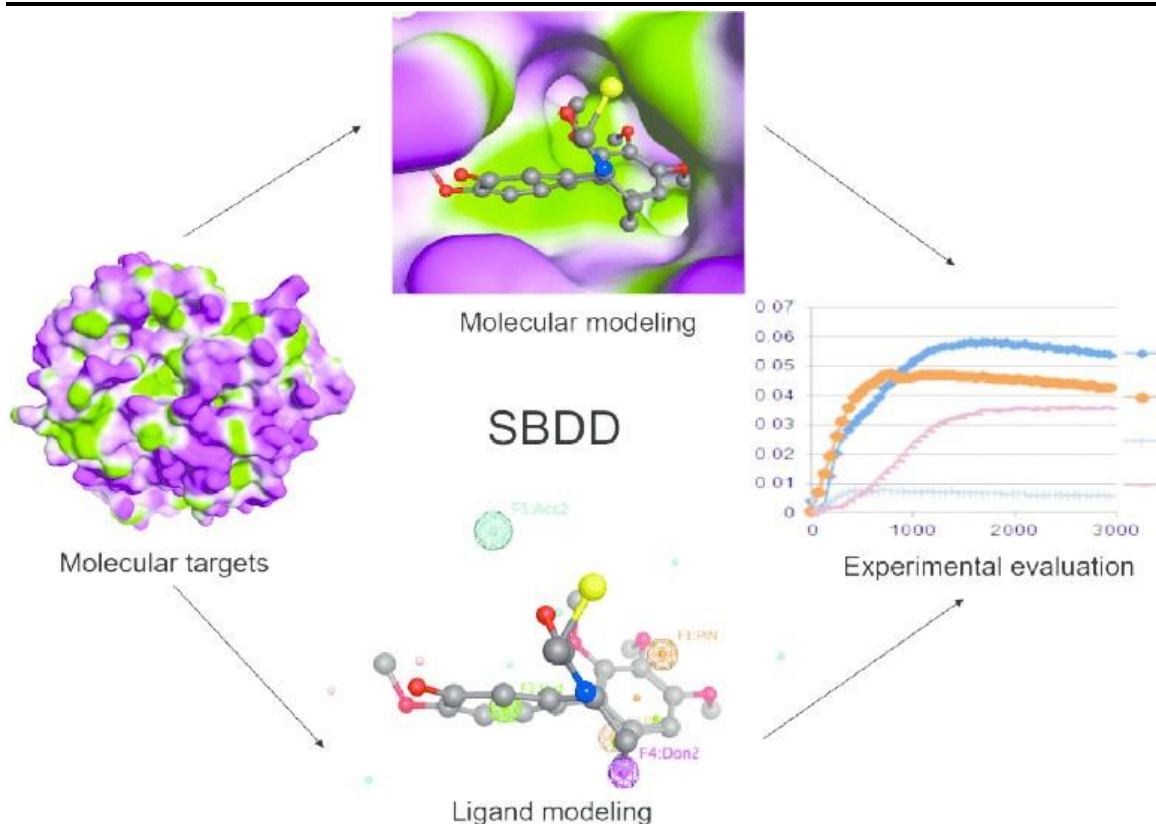
computational approaches to identify those entities likely to bind to a molecular target of interest. To a large extent, VS mitigates the problem of drug synthesis because it utilizes large libraries of pre-synthesized compounds.



**Figure 4: Process of Virtual screening**

### 3.1. Structure-based Drug Design (SBDD)

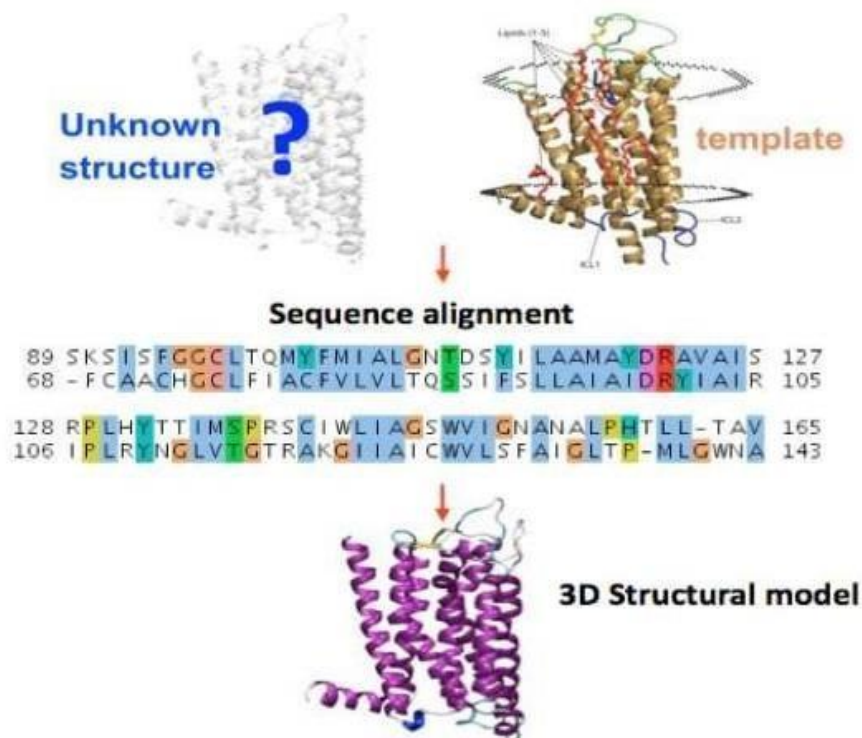
Structure-based drug design utilizes protein three-dimensional (3D) structural information to design new biologically active molecules (Fig. 5). Thus, the identification of a target molecule and the determination of its structure is the main, initial step of SBDD. The identified target may be an enzyme associated with a disease of interest. Based on binding affinity determinations, potential compounds are determined which attenuates the activity of target by its inhibition. Thus, SBDD utilizes information about a biological target and identifies potentially new medications. As such SBDD constitutes a marked advancement in the computational techniques used in the biophysics, medicinal chemistry, statistics, biochemistry, and other fields. Scientific advancements have resulted in a large number of techniques for predicting protein structures. These state-of-the-art technologies enable the determination of the structures of large numbers of proteins by using cryo-electron microscopy (EM), nuclear magnetic resonance (NMR), X-ray crystallography and computational methods like homology modeling and molecular dynamic (MD) simulation.



**Figure 5: Process of Structure-based Drug Design**

### 3.1.1. Homology Modeling

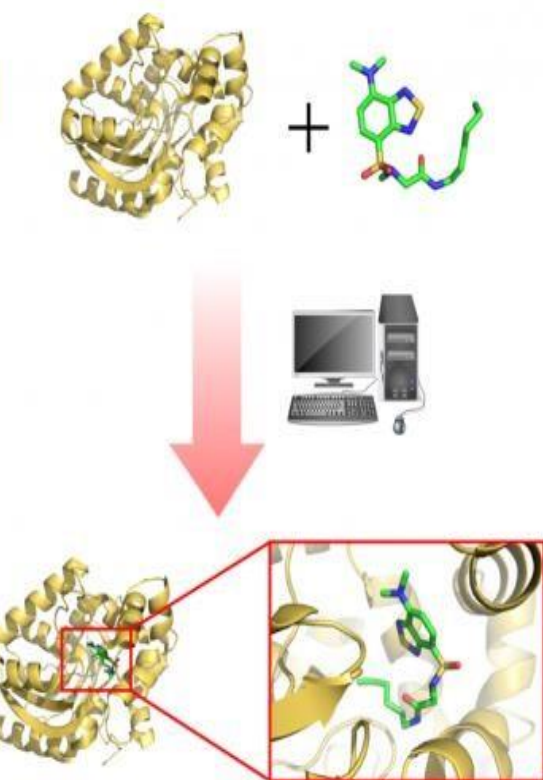
Determining the structure of a target molecule follows the identification of a specific drug target. Despite the availability of advanced techniques, the structures of a large number of proteins have not been identified. Homology modelling helps in this situation because it can be used to generate the structures of proteins on information available for similar proteins. Structural information about an identified target is a prerequisite for SBDD, but the structures of several identified neurodegenerative drug targets have yet not been determined. A large number of studies have been conducted using the homology modelling approach to generate structures of identified target molecules. Structural information is also required to gain insights of protein activities. Dhanavade et al. generated the structure of cysteine protease, which degrades amyloid beta peptide, an important causative agent of Alzheimer's disease. Several in Silico experiments have been conducted using the modeled structure of cysteine protease to investigate the nature of its binding site. The concept of homology modelling is shown in fig 6.



**Figure 6: Concept of Homology Modelling**

### 3.1.2. Molecular Docking

Molecular docking is a computational process widely used for rapidly predicting the binding modes and affinities of small molecules against their target molecules (usually proteins). This in silico process has achieved a position of great importance in the drug discovery field. Molecular docking has emerged over the last two decades and is now considered an indispensable tool for CADD and in the structural biology field, and has been shown to be more efficient than traditional drug discovery methods. Molecular docking has been greatly facilitated by dramatic growth in computer power and the increasing availability of small molecule and protein databases. Fig. (7) Illustrates the basic principle of molecular docking.



**Figure 7: Basic principle of molecular docking**

Recent advancements in computer methods and access to 3D structural information of biological targets are set to increase the effectiveness of this technique and facilitate its large-scale application to studies of molecular interactions

involved in ligand-protein binding. Generally, small molecules can be docked in three different ways, that is; (a) by rigid docking, where both target and ligands are treated as rigid entities; (b) by flexible docking, where both ligand and target are considered to be flexible; and (c) by flexible ligand docking, where the ligand is considered to be flexible and the target is considered rigid. Many molecular docking programs have been developed during recent years, such as, AutoDock, Dock , FlexX , Glide , Gold , Surflex , ICM, and LigandFit ,and been used successfully in many computer based drug discovery projects. Table 1 provides a list of major molecular docking tools in practice.





Sr. No.	Program	Availability	Search Method
1	AutoDock	Freely available	Genetic Algorithm/Monte Carlo
2	Gold	Paid	Genetic Algorithm
3	Glide	Paid	Monte Carlo
4	FlexX	Paid	Incremental construction
5	Dock	Freely available	Shape fitting (sphere sets)
6	FRED	Freely available	Shape fitting (Gaussian)
7	EHITS	Paid	Incremental construction
8	Surflex-Dock	Paid	Incremental construction

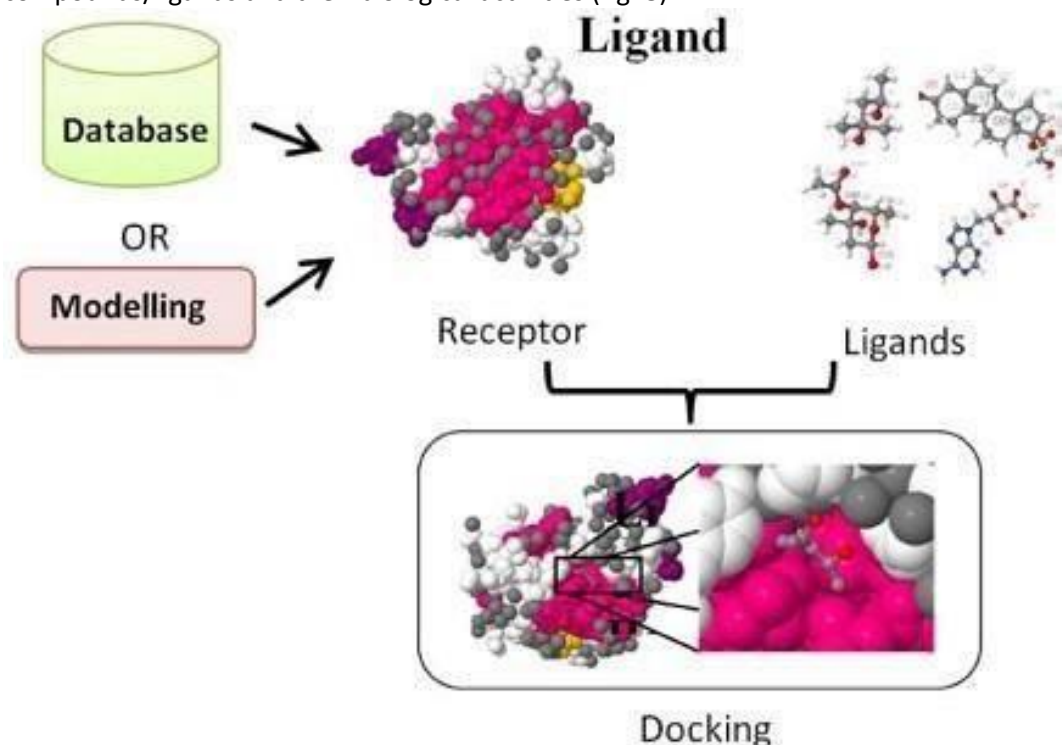
Table 1: List of major available molecular docking tools

Typically, the major goal of molecular docking is to identify ligands that bind most favorably within receptor binding sites and to determine its most energetically favored binding orientations (poses). The term “binding pose” is the orientation/confirmation of a ligand relative to its receptor. A binding pose either refers to a conformation of a ligand molecule within the binding site of its target protein which has been confirmed experimentally, or a computationally modelled hypothetical conformation. The search algorithm and the scoring function are two important components for determining proteinligand interactions. The search algorithm is responsible for searching different poses and conformations of a ligand within a given target protein and the scoring function estimates the binding affinities of generated poses, ranks them, and identifies the most favorable receptor/ligand binding modes. An ideal search algorithm should be fast and effective, and the scoring function must be capable of determining the physicochemical properties of molecules and the thermodynamics of interactions.

A large number of trials are being conducted to identify binding modes of ligands and selection of the most energetically favored poses. In order to achieve this, molecular docking tools are used to generate a set of different ligand binding poses and a scoring function is used to estimate the binding affinities of generated poses to identify the best binding mode. The energy change caused by ligand/receptor complex formation, is given by the Gibbs free energy ( $\Delta G$ ) and the binding constant ( $K_d$ ). The binding energy of a complex is predicted by evaluating physicochemical features involved in ligand-receptor binding, which include desolvation, intermolecular interactions, and entropic effects.

### 3.2. Ligand Based Drug Design (LBDD)

LBDD offers a general approach for elucidating relationships between the structural and physicochemical properties of compounds/ligands and their biological activities (fig. 8).



**Figure 8: Process of Ligand Based Drug Design**

This approach is applied when 3D structural information of a target protein is unavailable. In this process the available information of ligands and their biological activity is used for the development of new potential drug candidates. LBDD is widely used in pharmaceutical research, as more than 50% of approved drugs targeting membrane proteins (for which 3D structures are often not available, such as, GPCR). It is based on the assumption that compounds with similar structural features share common biological activities and interact/inhibit common target molecules.

The representation of molecules is the basis of LBDD approach. Molecular descriptors are numerical values used to represent the structural and physicochemical properties of molecules. The molecular descriptor field is strikingly interdisciplinary and includes a number of different theories. Active molecules are represented by the 0D-4D class of molecular descriptors. Constitutional and count descriptors are 0D molecular descriptors, chemical fingerprints or lists of structural fragments, such as, SMILES and SLN, are 1D descriptors, graph invariants in which atoms are denoted as nodes and bonds as edges are 2D-descriptors, geometrical, WHIM and others are 3D descriptors, and those derived from CoMFA or DRID methods are classified as 4D descriptors. Similarity searching is a key aspect of the LBDD method. This technique uses a known active compound as a query compound to find similar compounds and then rank compounds identified in a database. Based on this belief, structurally similar molecules exhibit similar biological activities and physicochemical properties. Numerical descriptors are applied and similarity coefficient is defined to quantify the degree of similarity (similarity/ dissimilarity). Fingerprint-based similarity or 2D similarity measures are widely used for similarity searching. LBDD is generally categorized as Quantitative Structure Activity Relationship (QSAR) or pharmacophore modeling.

#### 3.2.1. QSAR and its Role in Drug Discovery

The QSAR method and pharmacophore modeling are the most popular approaches to ligand-based drug design. QSAR methods are based on the belief that molecular structures are directly associated with biological activities, and thus, that molecular or structural variations alter biological activities. QSAR is defined as a process involving the construction of computational or mathematical models using chemometric techniques to identify significant correlations between a series of structures and functions. For QSAR, the primary hypothesis is that "compounds with similar structural or physicochemical properties show similar activities". To identify potential leads, a library of lead compounds with the desired biological activities is produced. A model is then developed to predict the quantitative relation between the structural and physicochemical features of these compounds and their biological activities. A statistical model generated using such relations is then used to mathematically optimize the biological properties of sets of compounds and maximize relevant biological activities. QSAR is used to modify existing compounds and improve their activities, and has been widely used in drug discovery. (fig. 9)

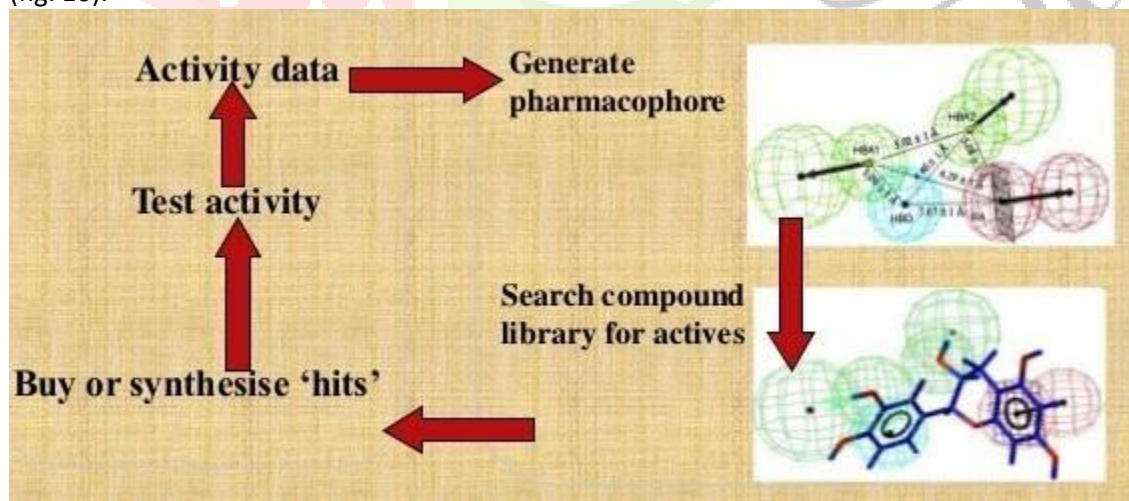


**Figure 9: QSAR based drug design**

### 3.3. Pharmacophore Modelling

A pharmacophore is an assembly (3D arrangement) of 'steric' and 'electronic' features required for optimal supramolecular interaction with a specific biological target structure and to prompt/block its biological response. Ligand-based pharmacophore model generation is based on available information on the biological activities of compounds/ligands. A pharmacophore does not symbolize an actual molecule/ligand or real connection between functional groups, but rather provides an abstract description of molecular features that are vital for molecular interactions between molecules and macromolecular ligands.

Pharmacophore modeling is widely used to identify potential lead molecules quickly. During the recent era of drug design, many therapeutically potent and well accepted drug targets with unknown active site geometries have been identified (fig. 10).



**Figure 10: Pharmacophore modelling based drug design**

Pharmacophore modeling provides an efficient means of rapidly screening huge databases of compounds. The elucidation of common pharmacophore features is conducted by aligning conformational models and active compounds three dimensionally. A superimposition algorithm assembles training set compounds (3D structure) in the same position/arrangement of their respective chemical properties/features. Pharmacophoric features are positioned such that all/maximum compounds share a common chemical functionality. To refine a shared pharmacophore feature, information

regarding inactive compounds can be included in the model generation process. A number of tools and software have been developed for pharmacophore development, such as, Phase, Catalyst/Discovery Studio, MOE, and LigandScout.

### **BENEFITS OF CADD**

- Cost savings: Many biopharmaceutical companies use CADD in order to reduce cost burden.[9]
- Traditional experimentation requiring animal and human models are now replaced by CADD, which saves both time and cost.[14]
- It is hoped that in case of certain diseases like Influenza, Computational Drug Designing will play an important role in reducing the chances of drug resistance and thus would lead to production of lead compounds which would target the causative factor.[14]
- Taking advantage of computational methods, potent hits can be obtained in a Matter of weeks. CADD has also led to construction of high quality datasets and libraries that can be optimised for high molecular diversity or similarity.[15]

### **LIMITATIONS**

Despite a number of successful applications of CADD to modern drug design, it has its limitations. In particular, like any computer assisted hypothetical system results must be validated in actual systems, and many lead molecules identified using CADD have failed to exhibit desired activities in biological systems. Several parameters must be met before potential compound to be approved as potent lead/drug, as it has to pass several pharmacological criteria. In fact, an average of only 40% of lead/drug candidates passes the different phases of clinical trials and obtains approval for clinical use.

Any computational tool based on pre-defined algorithms and scripts has its limitations, and the computational tools/methods used in CADD, such as, molecular docking, virtual screening, QSAR, pharmacophore modeling, and molecular dynamics, have their own limitations. Furthermore, ADME and many toxicity prediction tools are not supported by solid experimental data, and many examples of the failure of these computational approaches can be found in the literature.

To overcome limitations and improve accuracy in terms of predicting potent leads, regular updates of tools and algorithms are needed. Database reliability and high quality validated experimental molecules is to be developed and updated because many pharmacophores do not pass biological activity process due to non-availability of good quality data sets. Databases should contain detail data on genomics and proteomics, high quality sequence information, physicochemical properties, and structures.

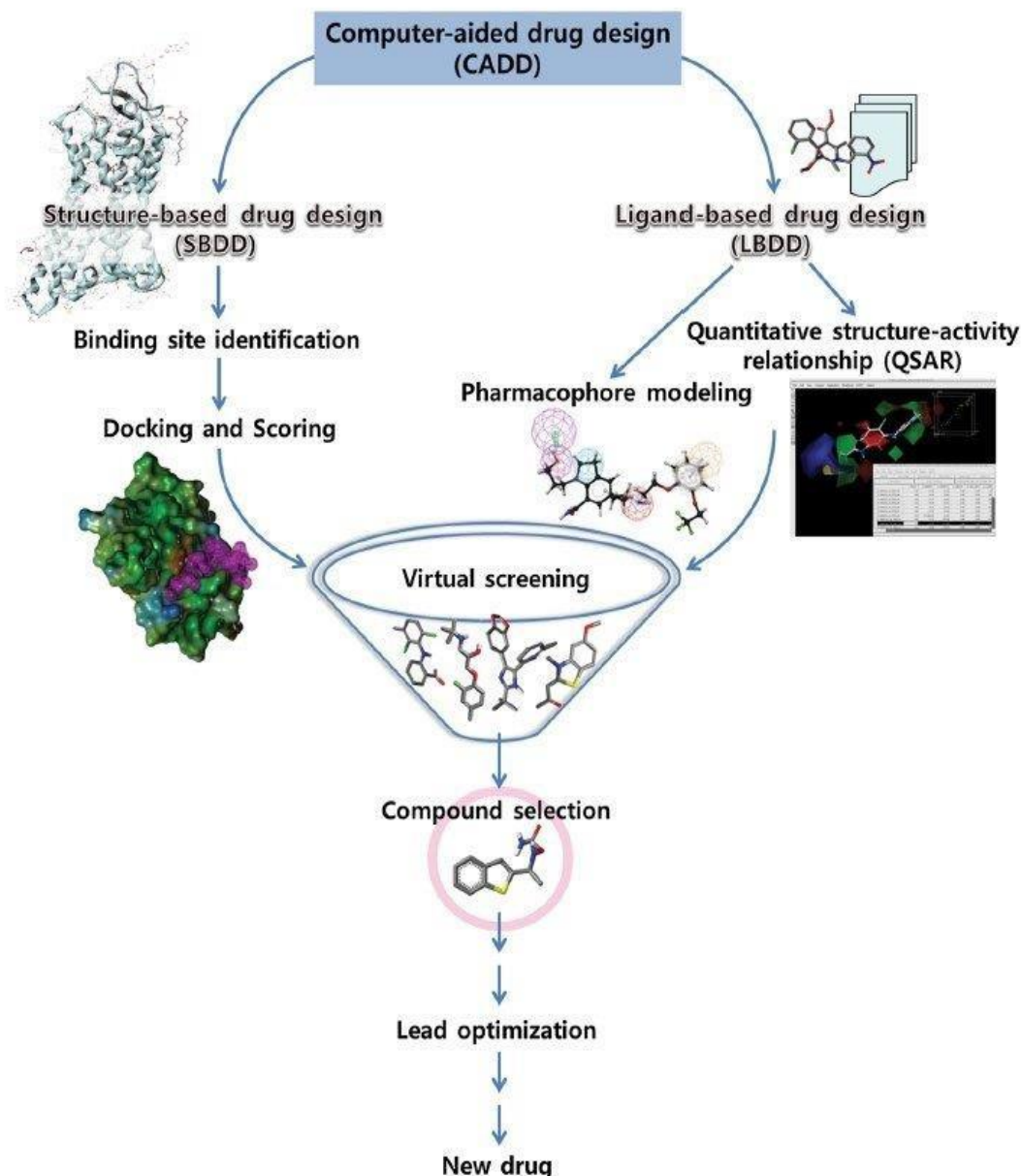
### **FUTURE PROSPECTS**

- Computer Aided Drug Designing will be beneficial for pharmaceutical development, but the extent of that role needs to be seen.
- According to experts, the companies which can successfully implement CADD will probably beat those in competition which still use old fashioned ways. □ This technique is hoped to be more pocket friendly.[6]

#### **4.Points observed**

- Designing of drugs and their development are a time and resource consuming process. There is an increasing effort to introduce the role of computational approach to chemical and biological space in order to organise the design and development of drugs and their optimisation. The role of Computer Aided Drug Designing (CADD) are nowadays expressed in Nanotechnology, Molecular biology, Biochemistry etc.
- Computer-aided drug design (CADD) techniques are used for the rapid assessment of chemical libraries in order to guide and speed up the early-stage development of new active compounds. CADD entails a vast number of computational methodologies like virtual screening, virtual library design, lead optimization, de novo design, and so forth. Because of the proven ability of computational techniques to guide the selection of new hit compounds, computational chemistry and chemoinformatics are still scientific disciplines in full bloom.
- It is a diverse discipline where various forms of applied and basic researches are interlinked with each other. Computer aided or in Silico drug designing is required to detect hits and leads. Optimise/ alter the absorption, distribution, metabolism, excretion and toxicity profile and prevent safety issues.
- Some commonly used computational approaches include ligand-based drug design, structure-based drug design, and quantitative structure-activity and quantitative structure-property relationships. In today's world, due to an avid interest of regulatory agencies and, even pharmaceutical companies in advancing drug discovery and development process by computational means, it is expected that its power will grow as technology continues to evolve.
- In the present era of drug discovery, the application of CADD counts up the most important accountability, and provides computational tools and algorithms that save time, costs, and reduce the risk of detecting non-viable developmental leads. The discovery of a new lead/drug using recent CADD paradigms requires a systematic understanding of the molecular and pathological conditions induced by diseases.

- However, CADD can assist researchers studying interactions between drugs and receptors. The pharmacoinformatic approach is being applied to modern drug discovery and is providing much basic knowledge regarding drug-receptor interactions. Novel technologies and computational algorithms are required to move the CADD approach forward, as new developments are likely to lead to tools for disease identification and the screening of potential lead compounds.
- CADD has become an indispensable tool to accelerate the development of epigenetic inhibitors helping in the selection, design, and lead identification of novel compounds. LBDD approaches employ the chemical structures of experimentally established epigenetic inhibitors to conduct SAR studies. From this, chemoinformatics and similarity tools have been used to identify new epigenetic inhibitors by searching in commercial and focused databases.



**Figure 11: Summary of computer aided drug design**

- Pharmacophore and QSAR models have been employed to find statistical models to correlate the biological property to the chemical structure and screen millions of chemical compounds to match these models. On the other hand, SBDD approaches use 3D structures of the current epigenetic target to carry out docking and MD studies (Fig. 11).
- Docking has been used to propose the possible binding mode of the compounds that were found with LBDD techniques, to explain the activity of compounds evaluated experimentally, and to screen a large number of compounds obtained from chemical databases.
- Additionally, filtering methods and protein flexibility considerations have been employed to select more potential epigenetic inhibitors. Finally, MD has been used to simulate the conformational changes that take place within different epigenetic targets with and without the inhibitor, which allows evaluating the stability of it in the binding site of the target.

- These developments are closely related to calculation power, macromolecules structural information, and the biochemical knowledge of concern to epigenetic regulation mechanisms.

## 5. CONCLUSION

In today's world, Computer Aided Drug Design, its application and development has made great progress in order to make a significant impact in both industry and academics. CADD approach provides valuable information for target identification and validation, lead selection, small-molecular screening and optimization, but still, it needs to be kept in mind that experimental tests have a role to play in this field. Due to large scale usage of CADD in industrial field, propelled by increasingly powerful technology and distributed computing for large-scale screening initiatives, the effective cost for making new drug molecules has reduced. cases of drug resistance against some diseases can also be dealt nowadays. Due to this gift of Computer Aided Drug Designing, new drug molecules can still be designed by altering the structure of molecules of conventional drugs, which can play a beneficial role in counteracting drug resistance and improving patient compliance. In the future, it is expected that Computer Aided Drug Designing will comprise of integration of computer aided chemistry and biology, along with chemoinformatics, bioinformatics, thus leading to creation of a new field pharmacoinformatics. Nowadays, Computational approach for Drug designing is grabbing more attention as everyone is keen on saving time and money and aiming for more profit at lesser time, especially in case of industries. There was a time where design of newer drug molecules was tedious process, which would consume time and money, but due to advent of this technique and especially numerous researches on this topic we can say that the impossible has been made possible. Also, the new molecules designed by it may be used as a probe for further research thus ensuring CADD a bright future in coming years.

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