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Review

Various Softwares Programs Available for Computer Aided Drug Discovery – An Updated Review

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Abstract

The methods and uses of computer-aided drug design (CADD) to speed up drug development procedures are examined in this research. The paper highlights crucial techniques that use structure-based and ligand-based methodologies and are supported by specialized software tools, such as molecular docking, pharmacophore modeling and virtual screening. The results demonstrate that CADD significantly accelerates lead selection and optimization by enabling precise target interaction analysis and efficient chemical screening. Computational techniques combined with biological data increase prediction accuracy, reduce costs and expedite research. These advancements facilitate the creation of novel therapies with improved efficacy and safety records. The implications underscore the pivotal function of CADD in modern pharmacology, promoting more efficient, ethical and easily accessible drug development projects worldwide. This illustrates how future pharmaceutical innovation will be transformed by computational methods.

Keywords: Computer aided drug design, Virtual Screening, Molecular Docking.

1.INTRODUCTION

In the rapidly evolving area of drug research, computer-aided drug design, or CADD, is a disruptive force that unites biology and technology. This paper covers the historical evolution of CADD, its categorization into structure-based and ligand-based approaches and its crucial role in expediting and simplifying drug discovery. Integrating a range of biological data and safeguarding data privacy become crucial as CADD advances. Strong ethical frameworks and algorithmic advancements are still needed for some problems. Combining artificial intelligence and machine learning boosts CADD's predictive abilities, but there are still scalability and ethical

concerns. Open-Source Malaria is one example of how multinational initiatives and collaborative efforts have democratized medication research.

The development of CADD was influenced by two major developments: the exponential growth in computing power, which made it possible to execute complex simulations in relatively shorter amounts of time, and the emerging field of structural biology, which demonstrated the three-dimensional structures of biomolecules. The creation of the anti-influenza medication Zanamivir was one of the earliest and most well-known uses of CADD. This process illustrated how this approach may significantly reduce the amount of time required for drug discovery. The two primary types of CADD are ligand-based drug design (LBDD) and structure-based drug design (SBDD).

SBDD uses information about the biological target's three-dimensional structure to understand how potential drugs could fit and interact with it. Instead of requiring knowledge of the target structure, LBDD creates innovative drug candidates by using existing drug molecules and their pharmacological features.

Finding and developing a novel therapeutic agent may be a time-consuming and expensive process in the broad field of drug discovery, which is where biology and chemistry collide. This procedure has historically relied on random discoveries or traditional trial-and-error methods, which can take decades and substantial resources with no guarantee of success. The late 20th century saw the introduction of Computer-Aided Drug Design (CADD), which, by combining the intricacy of biological systems with the predictive capacity of computer algorithms and creating databases that are carefully curated with both biological and chemical data, brought in a new age in this subject. [(1)]

There is a significant cost benefit to using computational methods during the lead optimization phase of drug development. From choosing therapeutic targets to finding candidates for new drugs, to evaluating the safety and effectiveness of newly created medications, to optimizing medications through preclinical and comprehensive clinical trials, pharmaceutical research labs invest a significant amount of time and resources in each step of the drug discovery process. [(2)]

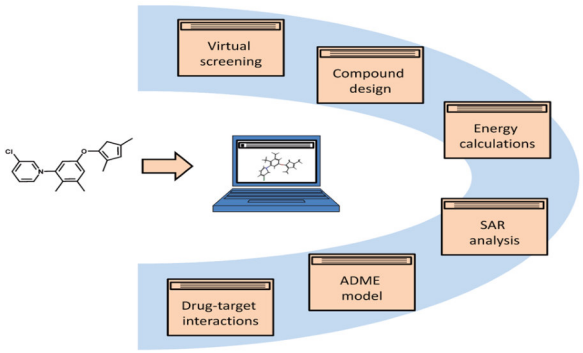

Fig 1: Areas of Computer Drug Discovery [(3)]

2.APPROACHES OF COMPUTER AIDED DRUG DICOVERY

When it comes to drug design using CADD, there are primarily two kinds of approaches:

- Direct method and structure-based drug design
- Drug design based on ligands or indirect methods

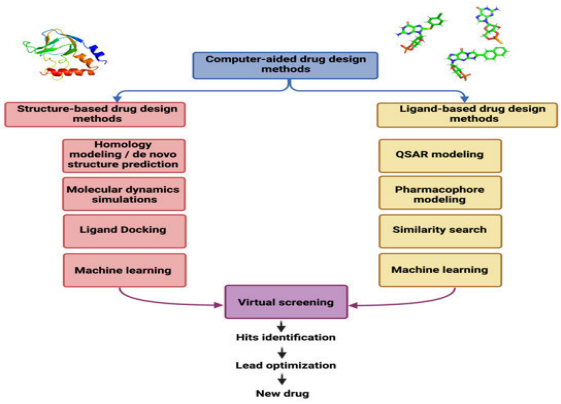

Fig 2: Overview of computer-aided drug design methods and their role in drug discovery [(4)]

2.1. STRUCTURE BASED DRUG DESIGN

In structure-based drug design (SBDD), the target protein's structure is known. A novel medicinal molecule with an improved contact with the target protein may be designed thanks to the docking process, which determines the interaction or bio-affinity for each examined chemical. These methods are quite successful and offer an alternative viewpoint on medication design course research and development. SBDD contains the three-dimensional (3D) structures of over 100,000 proteins.

STEPS INVOLVED

STEP 1: SBDD goes through several rounds before the best lead is used in clinical trials. One of three crucial methods nuclear magnetic resonance (NMR), homology modeling, or X-ray crystallography is used to identify, purify and determine the structure of the target protein in the first cycle. Before being incorporated into the protein's active site, compounds are discovered by a virtual search of several databases. The grade and rating of these compounds are determined by their steric, hydrophobic and electrostatic interactions with the active region of the target protein. Biochemical techniques are used to test the substances with the highest scores

STEP 2: The second cycle involves determining the structure of the protein and identifying regions of the drug that might be reinforced for even higher potency, in addition to the most promising lead the one with the lowest in vitro micro molar inhibition from the first cycle. After countless more cycles, such as lead manufacturing and further lead optimization via a complex protein structure with lead molecule, the enhanced compounds often exhibit a significant improvement in target selectivity binding affinity. [5]

2.2 LIGAND BASED DRUG DESIGN

The idea behind LBDD is that molecules with similar structures are probably going to have similar characteristics. LBDD requires the retrieval and preparation of small molecule libraries. Typically, molecular graphs are used to construct, process, and use chemical structures. A molecular graph is made up of nodes and edges, where bonds and atoms are shown as nodes and edges, respectively. Molecular graphs are commonly communicated with using connection tables and linear notations. Atom kinds, connection types and coordinates are all covered in parts of a connection table. [6]

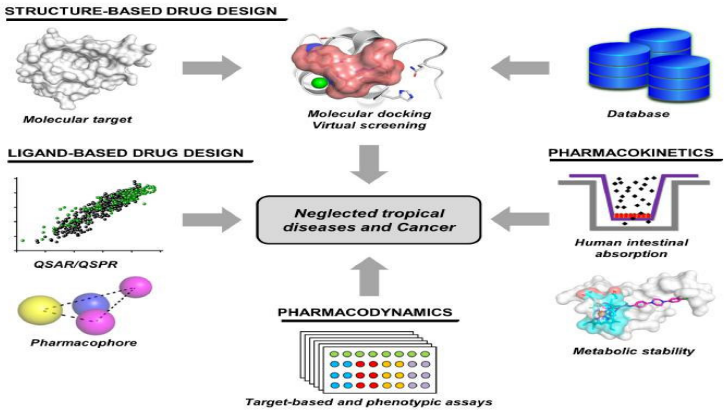

Fig 3: Approaches of Computer Aided Drug Discovery [7]

3.KEY STEPS IN COMPUTER AIDED DRUG DESIGN

3.1 TARGET IDENTIFICATION AND VALIDATION-

- Identification of biological targets associated with diseases.
- Validation of target relevance and feasibility.

3.2 LEAD DISCOVERY-

- The discovery of early lead chemicals that may have medicinal value.
- `• Utilization of virtual screening methods.

3.3 LEAD OPTIMIZATION-

- Lead compounds undergo modifying the structure to enhance their medicinal properties
- . • Predictive modeling for optimization strategies.

3.4 PRECLINICAL AND CLINICAL TRIALS-

- In silico prediction of Absorption, Distribution, Metabolism, Excretion and Toxicity properties.
- Risk assessment and optimization for clinical trials. [8]

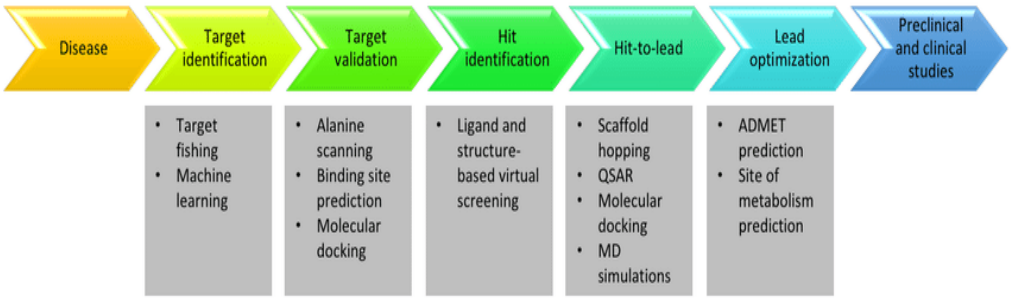

Fig 4: Steps Involved in Computer Aided Drug Discovery [9]

4.SOFTWARES USED

Some of the frequently used software for drug design and their salient features are as follows:

4.1. Affinity

• Automated, flexible docking automatically picks the optimal ligand-receptor binding modes by using the energy of the ligand/receptor complex (energy-driven technique).

4.2. AutoDock (Automated Docking of Flexible Ligands to Receptors)

• It consists of three separate programs: AutoDock performs the docking of the ligand to a set of grids describing the target protein AutoGrid precalculates these grids AutoTors sets up which of the ligand's bonds will be considered rotatable

• Provide an automated procedure for predicting the interaction of ligands with biomolecular targets and help to narrow the conformational possibilities and in identification of the most suitable structure

• Uses a Monte Carlo (MC) simulated annealing (SA) technique for configurational exploration with a rapid energy evaluation using grid-based molecular affinity potentials

• An effective method for resolving the issue of docking a flexible substrate into a static protein's binding location

• It has application in X-ray crystallography, SBDD, lead optimization, virtual screening, combinatorial library design, protein-protein docking and chemical mechanism studies

4.3. Combibuild

• The development of a structure-based drug design software to facilitate combinatorial library design

• Uses a computer to screen a library of potential reactants and determine which will be the strongest.

• effectively used to identify nanomolar Cathepsin D inhibitors

4.4. Dock Vision

• Monte Carlo, genetic algorithms and database screening docking techniques are all included in this docking suite that was developed by scientists for scientists.

4.5. FRED

• The multi-conformer docking algorithm is remarkably quick and accurate.

• Before scoring with more traditional functions, it looks at every conceivable position inside a protein active site, screening for form similarity and optional pharmacophoric characteristics.

4.6. FlexiDock

• The straightforward and adaptable docking of ligands into protein binding sites

• Fast genetic algorithm for generation of configurations

• The best control over ligand binding properties is offered by rigid, moderately flexible, or fully flexible receptor side chains.

• Conformationally flexible ligands

• Tunable energy evaluation function with special H-bond treatment

• Very fast run times

4.7. FlexX

• Fast computer program for predicting protein-ligand interactions

• Two main applications: Complex prediction (create and rank a series of possible protein ligand complexes) Virtual screening (selecting a set of compounds for experimental testing)

• Conformational flexibility of the ligand; rigid protein

• The interaction geometry database is used to precisely characterize patterns of intermolecular interactions, while the MIMUMBA torsion angle database is utilized to create conformers.

• Boehm function (with minor adaptations necessary for docking) applied for scoring.

4.8. Glide

- High-throughput ligand-receptor docking for fast library screening.
- Fast and accurate docking program.
- Identifies the best binding mode through Monte Carlo sampling.
- Provides an accurate scoring function for ranking of binding affinities.
- A drug development program's chances of success will be significantly increased if it can quickly and accurately forecast binding affinity, which will enrich the proportion of viable lead candidates in a chemical database.

4.9. Gold

- The docking mechanisms of small compounds into protein binding sites are calculated.
- Based on genetic algorithm for protein-ligand docking
- Studies full ligand and partial protein flexibility
- Predicts energy functions partly based on conformational and non-bonded contact information from the CSD
- Choice of scoring functions: GoldScore, ChemScore and User defined score
- Has virtual library screening

4.10. Hint

- Hydropathic Interactions
- Empirical molecular modeling system with new methods for de novo drug design and protein or nucleic acid structural analysis
- Translates the well-developed Medicinal Chemistry and QSAR formalism of Log P and hydrophobicity into a free energy interaction model for all biomolecular systems based on the experimental data from solvent partitioning
- Determines 3D hydropathic interaction maps and 3D hydropathy fields.
- Estimates Log P for modeled molecules or data files [10]

Table 1: List of major available molecular docking tools [11]

S.No	PROGRAM	AVAILABILITY	SEARCH METHOD
1.	AutoDock	Freely available	GeneticAlgorithm /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.	LigandFit	Paid	Monte Carlo
7.	FRED	Freely available	Shape fitting (spheres sets)
8.	ICM	Paid	Monte Carlo
9.	eHiTS	Paid	Incremental construction
10.	Surflex-Dock	Paid	Incremental construction

5.PHARMACOPHORE MODELLING

The foundation of pharmacophoric modeling is the idea that biological activity on the same target results from shared chemical functions and a comparable spatial arrangement. The pharmacophoric model uses geometric concepts like spheres, planes and vectors to depict the chemical properties of a molecule that can interact with its ligand.

Hydrogen bond acceptors (HBAs), hydrogen bond donors (HBDs), hydrophobic regions (H), positively and negatively ionizable groups (PI/NI), aromatic regions (AR) and metal coordinating regions are the most significant pharmacophoric feature types (Figure 1). The size and shape of the binding pocket can be represented by additional size limitations in the form of exclusion volumes (XVOL), or banned zones. [12]

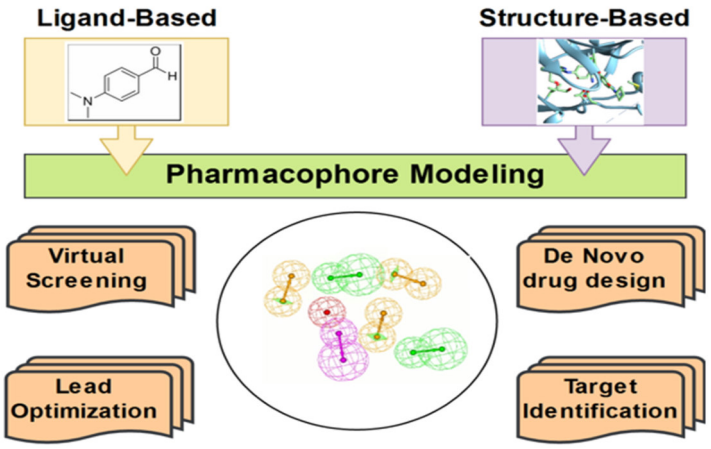

Fig 5: Pharmacophore Modelling [13]

6.VIRTUAL SCREENING

Virtual Screening (VS) is an insilico method used in the process of finding new drugs. VS uses computational techniques to automatically examine vast databases of molecular structures. It should be possible to find compounds that are more likely to attach to the molecular target usually a protein or enzyme receptor by using VS.

In order to reduce the number of final candidate molecules that may constitute a medicine, VS functions as a filter, removing more molecules than it started with. The first selection of compounds that have the potential to be useful medications is based on their similarity to known-functioning pharmaceuticals or on their favorable features.

The compounds that have pharmacophoric groups that suggest the possibility of toxicity are then removed from consideration of the candidate ligands. The next stage involves determining the ideal positions for potential ligands. To improve the qualities of the candidate ligands, particularly their pharmacokinetic properties (absorption, distribution, metabolism, excretion and toxicity, or ADMET), their compositions and structures can be changed throughout this VS process. It could need additional optimization cycles for the structure and makeup of potential ligands. In this manner, following this procedure, the ligands are ready for biological tests. [14]

Fig 6: An Overview of Virtual Screening Process [15]

7.RECENT SOFTWARES IN CADD

7.1. UNIPROT

UniProt is the most extensive database of protein sequence and functional annotation and the primary resource for storing and linking data from several, unrelated sources. It consists of four parts that are tailored for various applications.

An skillfully managed database, the UniProt Knowledgebase (UniProtKB) serves as a central repository for integrated protein knowledge that includes cross-references to other sources. The history of every protein sequence is reflected in the UniProt Archive (UniParc), a comprehensive sequence archive.

To expedite searches, UniProt Reference Clusters (UniRef) combine closely similar sequences according to sequence identity. The UniProt Metagenomic and Environmental Sequences (UniMES) database was created especially for the recently growing field of environmental and metagenomic data.

The vast bioinformatics infrastructure and scientific know-how of the Swiss Institute of Bioinformatics (SIB), Protein Information Resource (PIR) and European Bioinformatics Institute (EBI) serve as the foundation for UniProt. Researchers can readily and freely access it. [16]

Fig 7: Uniprot [16]

7.2. GENECARDS

GeneCards has been providing gene-centric information for more than 20 years. It does this by automatically mining and integrating data from a variety of sources, creating a web-based card for every one of the tens of thousands of human gene entries.

The Weizmann Institute of Science in Israel's Department of Molecular Genetics is responsible for creating and maintaining the GeneCards database.

The GeneCards project was established in 1997 with the intention of combining the disparate pieces of data from many specialist databases into a cohesive whole.

In partnership with LifeMap Sciences, Inc., the GeneCards relational database is available to commercial customers.

GeneCards offers two robust tools for working with gene sets, GeneAlaCart and GeneAnalytics, in addition to the comprehensive "card" view of individual genes: eneALaCart generates a tabular file with annotations for the gene set after receiving a batch (list) of gene symbols or IDs and the user-selected data fields of interest (such as aliases, descriptions, proteins, diseases, publications, etc.).

In order to give considerably enriched gene correlations to diseases, pathways, GO keywords, expression and chemicals from GeneCards and MalaCards, GeneAnalytics employs innovative algorithms. GeneAnalytics displays the data in an engaging and dynamic manner. [17]

Fig 8: Genecards[18]

7.3. METASCAPE

For experimental biologists, Metascape is a web-based portal that offers a comprehensive gene list annotation and analysis resource. Metascape leverages more than 40 separate knowledgebases in a single integrated gateway by integrating functional enrichment, interactome analysis, gene annotation and membership search as design elements.

Comparative studies of datasets from several different, orthogonal experiments are also made easier. In order to provide interpretable outputs, Metascape offers a one-click Express Analysis interface, which greatly simplifies the user experience. When combined, Metascape is a powerful and fast tool that allows experimental biologists to thoroughly examine and understand research based on OMICs in the big data age. [19]

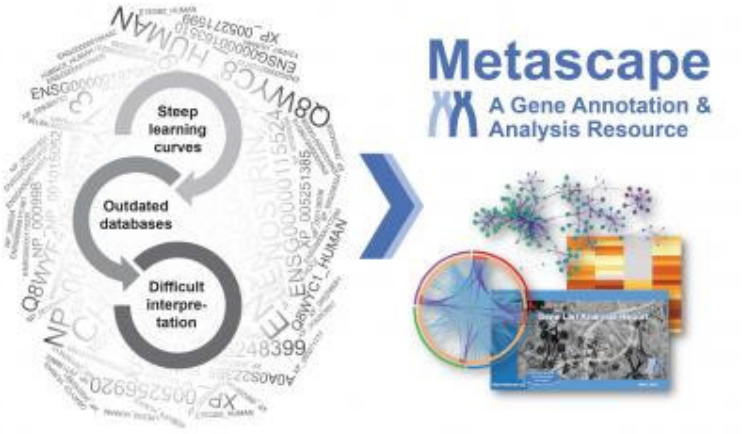

Fig 9: Metascape [20]

7.4. CYTOSCAPE

An open source software project called Cytoscape combines high-throughput expression data, various molecular states and biomolecular interaction networks into a single conceptual framework.

Cytoscape is most effective when used in conjunction with the extensive databases of protein-protein, protein-DNA and genetic connections that are becoming more and more accessible for humans and model organisms, even though it may be used to any system of molecular components and interactions.

Basic features for network layout and querying, visual network integration with expression profiles, phenotypes and other molecular states and network connectivity to functional annotation databases are offered by Cytoscape's Core program. [21]

Fig 10: Cytoscape [22]

7.5. PYMOL

Warren Lyford DeLano developed the source-available molecular visualization system PyMOL. DeLano Scientific LLC, a private software firm committed to developing practical tools that are widely available to the scientific and educational communities, was the first to market it. Schrödinger, Inc. is now in charge of its commercialization.

They were able to remove the original software license because it was permissive; new versions are now released under a custom license that grants broad use, redistribution and modification rights, but assigns copyright to Schrödinger, LLC. for any version and some of the source code is no longer available.

PyMOL is capable of generating high-quality three-dimensional pictures of biological macromolecules like proteins as well as tiny compounds. PyMOL is used extensively.

One of the few mostly open-source model visualization programs for structural biology is PyMOL.

PyMOL can solve Poisson-Boltzmann equations with the Adaptive Poisson Boltzmann Solver and utilizes FreeGLUT and the OpenGL Extension Wrangler Library (GLEW).With version 2.0, PyMOL's native Aqua binaries for macOS via Schrödinger and its usage of Tk for GUI widgets were swapped out for a PyQt user interface across all platforms. [23]

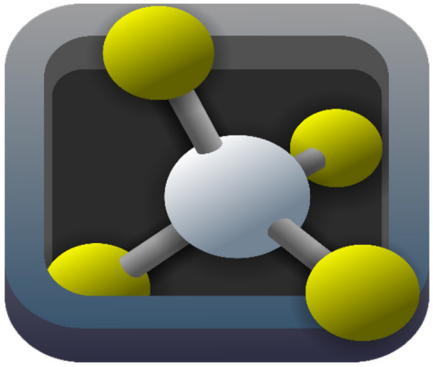

Fig 11: PyMoL [24]

8.APPLICATIONS OF COMPUTER AIDED DRUG DESIGN

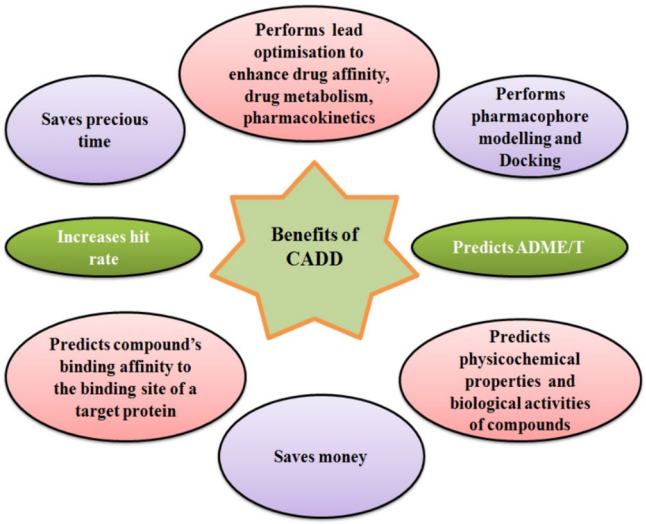

Fig 12: Benefits of Computer Aided Drug Design [25]

The entire history of CADD garners a lot of interest based on three main elements.

1) screening a huge number of compounds based on the desired structure, which is assessed both experimentally and computationally,
2) directing lead chemical optimization based on toxicity, pharmacokinetic characteristics and affinity
3) developing new compounds based on their structure to enhance their medicinal properties.

The use of CADD for drug modeling takes into account combinatorial chemistry and bioinformatics, which tackle the main problems of cost and time. [26]

9. LIMITATIONS

Despite being a pioneer in drug design, the SBDD method must overcome the obstacles that the community must consider. This improvement comprises chemogenomic chemicals, screening techniques, data improvement, quantity and quality of different tools and databases, toxicity prediction algorithms, multitarget drug structure modifications and integrating the strategy for improved compatibility and efficacy. Electrostatic interactions are the other most plausible parameter; entropy estimates were entirely disregarded. Above all, no one piece of software or package is effective for all specific targets and ligands, including the water molecule and other improvements, such as likely target confirmation, still need to be addressed. [26]

10.CONCLUSION

To sum up, by fusing biology and technology, Computer-Aided Drug Design (CADD) has transformed drug discovery by providing ligand-based (LBDD) and structure-based (SBDD) methods for identifying and refining drug candidates. Using programs like AutoDock, Glide, and Gold, CADD entails target selection, lead finding, lead optimization, and preclinical/clinical trials. CADD has drawbacks, including the requirement for better tools, databases, and toxicity prediction algorithms, despite its advantages in screening compounds and guiding lead modification. This highlights the significance of taking target confirmation and electrostatic interactions into account.

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