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Digital Transformation in Pharma: A Comprehensive Review of Software Tools in Drug Discovery and Development.

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Abstract: *Drug discovery and development is a resource-intensive process that benefits significantly from computer-aided drug design (CADD), which integrates computational methods to provide mechanistic insights, propose novel molecular structures, and guide cost-effective decisions before expensive synthesis. Numerous CADD-derived compounds have advanced to clinical trials or gained FDA approval, highlighting its practical impact across various project stages. This review aims to deliver a comprehensive overview of essential software and resources in CADD, emphasizing structure-based drug design (SBDD), ligand-based drug design, chemical databases, and cheminformatics tools. While not exhaustive in technical details, it directs readers to cited literature for in-depth exploration. CADD complements traditional high-throughput screening (HTS) by offering faster, more economical alternatives for ligand identification and optimization, enhancing binding affinity, selectivity, and pharmacokinetic properties. Virtual screening (VS)—encompassing structure-based (SBVS) and ligand-based (LBVS) approaches—enables efficient evaluation of vast compound libraries, including virtual ones, accelerated by advances in computing. The growing availability of protein structures has blurred distinctions between these methodologies, supported by diverse commercial and open-source molecular modeling programs widely adopted in pharmaceutical, academic, and governmental settings. In conclusion, proficiency in a broad spectrum of CADD tools is vital for computational medicinal chemists, positioning CADD as an indispensable pillar in modern drug discovery pipelines*

Keywords: drug discovery, computer-aided drug design (cadd), structure-based drug design (sbdd), virtual screening (vs), cheminformatics, AutoDock Vina, Schrodinger, SwissADME, Molinspiration, QSARINS, BIOVIA Discovery Studio, SYBYL – X, MOE

I. INTRODUCTION

The process of drug discovery and development is both expensive and time-intensive, requiring the integration of every available discipline, including computer-aided drug design (CADD), to achieve the desired outcomes. CADD offers critical insights into experimental results and mechanisms of action, proposes new molecular structures for synthesis, and aids in making cost-effective decisions prior to initiating costly synthesis. Numerous compounds identified and/or refined through CADD methods have progressed to clinical study phases or have even received approval from the US FDA [1, 2]. Various CADD techniques are employed at different stages of a drug discovery project, and it is not possible to identify a single 'best' computational drug design technique universally. Therefore, computational medicinal chemists should be knowledgeable about and ready to utilize a wide range of software and resources associated with CADD in their daily work, even though they may choose to specialize and become proficient in just one or a few specific techniques.

Ligands, whether they are inhibitors, activators, agonists, antagonists, or substrate analogs, can be identified through traditional hit-identifying techniques such as high-throughput screening (HTS) assays or by utilizing various computer-

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aided drug design (CADD) methods. Due to their individual advantages and disadvantages in drug discovery, HTS and CADD techniques are frequently regarded as complementary to one another [3]. HTS has been employed alongside, or replaced by, CADD methods, which are typically faster, more cost-effective, and simpler to implement than HTS. Furthermore, by applying CADD techniques, it is possible to optimize ligands to enhance their binding affinity and selectivity, as well as to achieve acceptable pharmacokinetic properties, which are generally not addressed by HTS.

Many techniques employed in CADD tend to be more cost-effective and quicker than most experimental assaying methods. As a result, extensive databases of compounds are frequently evaluated in silico prior to their submission for in vitro testing, or ideally, subsets of these compounds. Today, drug design initiatives often commence with hundreds of thousands or even millions of compounds, which may include large corporate repositories, catalogs of commercially available screening samples, or extensive virtual libraries. In this context, one of the most valuable resources is known as virtual screening (VS), also referred to as in silico screening. This involves the computational search for molecules exhibiting desired biological activities within vast computer databases of small molecules that may not even physically exist [4]. When initiating a screening campaign, the virtual screening (VS) approach can be divided into two main categories: structure-based virtual screening (SBVS) and ligand-based virtual screening (LBVS) [5]. SBVS utilizes the three-dimensional structure of the target protein, whereas LBVS concentrates on existing ligands linked to a known target. Recent progress in parallel computing hardware and algorithms has enabled the execution of large-scale VS campaigns within a practical timeframe [6]. With the significant rise in the number of protein structures pertinent to drug discovery, the distinction between structure-based and ligand-based methodologies in drug design has become increasingly unclear [7]. Over the past thirty years, a multitude of molecular modeling programs have been developed, integrating these techniques into both commercial and free software applications. Many of these programs are widely used in the pharmaceutical and biological fields, as well as in academic institutions and government research organizations. The extensive range of applications for these software tools, coupled with additional resources such as chemical databases, has solidified CADD as a crucial element in the drug discovery process.

The purpose of this review is to offer readers a comprehensive overview of the software and resources typically utilized in CADD [8]. Since it is unfeasible to include all technical specifics regarding the background and applications of these software tools and resources,readers are urged to refer to the cited literature for further details. Due to their significance in CADD, this review specifically emphasizes SBDD, ligand-based drug design, chemical databases, and cheminformatics tools [9].

Software for identifying drugs:

AutoDock Vina:

Among the docking programs in the AutoDock Suite [11] are AutoDock Vina (Vina) [10], AutoDock4 (AD4) [12], AutoDock-GPU [13], AutoDockFR [14], and AutoDockCrankPep [15]. In addition to being free source, Vina is regarded as one of the most popular applications, perhaps because it is quick and easy to use when compared to other docking solutions in the suite and beyond [16]. Research groups throughout the world have modified and improved the Vina source code, improving the search algorithm (QuickVina2 [17]), developing an interface that is easier to use, and allowing modifications to score words through the user interface (Smina). They have also improved ranking and scoring (Vinardo), as well as the scoring function for halogen bonding (VinaXB) and carbohydrate docking (Vina-Carb).

Apart from these noteworthy developments, there are still several methods in the AutoDock Suite that are absent from the Vina program since they were created especially for the AD4 scoring feature or the AD4 program itself. These methods include explicit water modeling, coarse-grained ligand models, irreversible ligand binding, docking with macrocyclic flexibility [18], and specialized models for metal coordination. Even though AD4 is regarded as a less effective application, it is especially useful for creating novel docking techniques since it gives users direct access to several internal engine components and allows them to modify a broad variety of docking settings. The Vina interface,

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on the other hand, requires very little user input to perform a docking because it is extremely specialized and tuned. As a result, this restriction makes it hard to introduce new features without significantly altering the source code.

The AD4 program's poor search efficiency limits the efficacy of these specific techniques. In fact, depending on how complicated the search is, AD4 may be up to 100 times slower than Vina (1). Vina's better search method, which combines a Monte-Carlo (MC) iterated search with the BFGS [19] gradient-based optimizer, is the cause of this notable performance disparity. Vina's improved search efficiency leads to better docking results with fewer evaluations of the scoring function when compared to the Lamarckian Genetic Algorithm (LGA) and the Solis-Wets local search used by AD4 (3).

Here, we implemented the AD4 scoring system using the Vina program. In order to utilize Vina's powerful MC/BFGS search algorithm, a number of the unique features discovered in AD4 were also moved to the Vina source code [20]. The Vina program may now dock several ligands at once, and Python bindings have been added to allow programmatic access to the docking engine's functionality.

Versions of AutoDock Vina:

List of AutoDock Vina Versions:

Versions:	Release Date:	Key Feature:
V1.2.6#1	Mar 3, 2025	focus on expanded force fields, new sampling methods, and better Python integration
V1.2.6#0	Jan 14, 2025	focus on enhancing stability, compatibility, and performance.
V1.2.5#3	May 30, 2024	focus on enhanced flexibility, speed, and usability for molecular docking.
V1.2.5#2	May 9, 2024	focus on increased flexibility, enhanced usability for high-throughput virtual screening, and integration with modern computational pipelines.
V1.2.5#1	Sep 13, 2023	focus on improved efficiency, expanded force fields, and better Python integration.
V1.2.5#0	Aug 2, 2023	focus on improved usability, expanded docking capabilities, and integration with modern bioinformatics workflows.
V1.2.3#0	Nov 15, 2021	focus on enhanced functionality, improved performance, and expanded flexibility for protein-ligand docking.
V1.2.2#0	Sep 2, 2021	focus on enabling advanced virtual screening, and improving usability.

Schrodinger:

Schrodinger software offers a broad spectrum of applications capable of addressing most challenges posed by bio-molecules. It emphasizes significant advancements in molecular modeling, molecular dynamics, ligand-receptor docking, and biologics specifically designed to tackle these issues. The software can analyze structure-based properties of molecules, such as the understanding of conformational changes and the hydrophobicity of structures.

The confirmation of macrocycles is achieved through a high-performance molecular dynamics simulation engine tailored for bimolecular systems, which merges speed with accuracy [21]. This, in turn, provides insights into the atomic movements of macrocycles, which are further utilized to comprehend shape, stability, and energetics. Schrodinger also offers robust and user-friendly graphical interfaces for system setup, simulation execution, and trajectory analysis.

The molecular dynamics simulation software is utilized to investigate a series of stabilized stapled α-helical peptides at various temperatures. The predicted α-helical propensities obtained from the simulations align well with the experimentally observed circular dichroism melting curves [22]. The local flexibility of critical residues can be correlated with variations in the affinity of the stapled peptides for MDM2 [23]. These simulations pave the way for

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innovative strategies in the design of α-helical stapled peptides and the development of effective inhibitors targeting α-helical protein–protein interfaces.

Schrodinger software packages:

CombiGlide	Lead compound design and optimization.
Desmond	High-performance molecular dynamics simulations.
Glide	Ligand–receptor docking and scoring.
Induced-Fit Docking	Modelling conformational changes induced by ligand binding.
Liason	Ligand–receptor binding free-energy prediction.
MacroModel	Full-featured program for molecular modelling.
Prime	Protein structure prediction and refinemen.
QSite	Quantum mechanics/molecular mechanics calculations on biological systems.
SiteMap	Binding-site identification and analysis.

Software utilized for assessing the physical characteristics of drugs:

SwissADME:

The Swiss Institute of Bioinformatics (SIB) made SwissADME, a web-based tool that can help you figure out how drug-like, pharmacokinetics, and medicinal chemistry suitable small molecules are [24,25].

Researchers use it a lot to look at different properties that are important for drug discovery, such as absorption, distribution, metabolism, and excretion (ADME) characteristics, as well as possible toxicity and how much the drug looks like a drug. The tool figures out a number of physicochemical properties, including topological polar surface area (TPSA), molecular weight, lipophilicity (LogP), and water solubility. It also checks to see if a compound follows Lipinski's rule of five, which says that it will be easy to absorb by mouth.

SwissADME offers a bioavailability radar, which is a visual tool that illustrates six essential physicochemical properties, enabling rapid assessment of a molecule's drug-likeness. Furthermore, SwissADME forecasts pharmacokinetic attributes including gastrointestinal absorption, penetration of the blood-brain barrier, interactions with cytochrome P450, as well as other metabolic and excretion features. It also assesses the synthetic accessibility of compounds and their likelihood of promiscuous binding to different biological targets.

This comprehensive collection of computational forecasts, derived from the chemical structure of compounds, renders SwissADME an essential resource for medicinal chemists, pharmacologists, and researchers engaged in the initial phases of drug discovery and development, facilitating the identification of potential drug candidates. SwissADME is available at no cost with the hope that it will prove beneficial. While this in silico platform is frequently utilized for assessing medicinal chemistry initiatives, the Swiss Institute of Bioinformatics (SIB) does not provide any guarantees or warranties regarding the outcomes obtained from using any information accessed through their server. The SIB is not responsible for any incidental, consequential, direct, or indirect damages resulting from the use of results, data, or information obtained through their server.

SwissADME provides results based on the following specific versions of various algorithms:

Lipophilicity Models:	Hydrophilicity Models:	Pharmacokinetics Models:
ilogpA	ESOL	BOILED- Egg Model
XLOGP3	ALI	Lipinski Filter
WLOGP	SILICOS-IT	Veber Filter
SILICOS-IT	FILTER-IT	Muegge Filter

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Molinspiration:

Molinspiration is a molecular properties computation toolkit that is written in Java. It is used to process a large number of molecules in batch mode and can process data of roughly 10,000 molecules per 60 seconds. It is accessed directly through a web interface on the internet [26].

In Molinspiration, Log p calculates the sum of correction factors and fragment-based assistance. All organic and organometallic compounds are processed using this technique. TPSA, or topological polar surface area, is the total of segment contributions, polar pieces centered on O and N are taken into account [27]. It is a useful descriptor that includes intestinal absorption, bioavailability, blood-brain barrier penetration, and medication absorption. Group contributions are the basis for molecular volume. mainly compounds that resemble drugs. The ability to rotate several bonds is a gauge of molecular flexibility.

It is a useful indicator of a drug's oral bioavailability. Only a non-terminal heavy atom may have a rotatable bond, which is unique for any single non-ring bond. The reign of Lipinski of five confirms that the majority of drug-like compounds have molecular weight < than or equal to 500, number of hydrogen bond acceptors ⩽ than or equal to 10, number of hydrogen bond donors less than or equal to 5, and log P ⩽ than or equal to 5 [28]. Molecules that violate more than one of these guidelines may have had bioavailability issues. The Lipinski Rule of Five is the name of the regulation.

Core Molinspiration Tools:

Tools:	Key feature:
mib	focus on the high-speed, batch processing of chemical structures (SMILES or SDF formats) to calculate molecular properties, normalize structures, and perform fragmentation, enabling efficient virtual screening and QSAR studies.
mipc	focus on the rapid calculation of molecular properties and descriptors essential for drug discovery, virtual screening, and assessing drug-likeness.
mimv	focus on the visualization of molecules encoded as SMILES or SDfiles.
midv	focuses on the visualization of molecular structures and their associated numerical data, enabling easy data mining, analysis, and interpretation of chemical datasets.
galaxy	focus on generating 3D molecular structures from SMILES strings, enabling in-silico 3D modeling and visualization in drug discovery.
miscreen	focus on virtual screening, specifically the development and application of pharmacophore models to predict the bioactivity of small molecules.

Software utilized for drug 2D QSAR research:

QSARINS:

In accordance with OECD guidelines, QSARINS is suggested as a new program for the computation, analysis, validation, and use of QSAR MLR-OLS models. It enables automated processes to import, reduce, and display incoming data. The outcomes in both graphical and tabular form. Before the models are calculated, a customizable data preparation system is suggested, which includes several methods for separating the dataset into training and prediction sets as well as an exploratory analysis of the chemicals space using PCA (based on molecular descriptors) [29]. The selection of descriptors is then carried out using a variety of strategies, such as GA and all subsets. After the models are acquired, several techniques may be used to list and filter them. For a more thorough investigation, models can be assessed singly or as a comparison list. Distinct validation methods for assessing their performances as well. A lot of focus has been placed on external validation through the comparison of different criteria, their combination utilizing the MCDM technique, and the model's visual examination. Data using educational plots Consensus modeling based on the best models may be carried out after model review to produce forecasts that are typically more trustworthy [30]. The

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top models can be kept for further use. Single MLR models that were previously created using other tools may be redeveloped, verified, validated, and applied to any new compounds using QSARINS.

In order to offer a database for storing models and a tool to make their application easier, QSARINS-Chem was presented in 2014 as an extra module integrated into the program QSARINS. In addition to multiple linear regression (MLR) models based on descriptors determined by the free program PaDEL-Descriptor, the QSARINS-Chem module contained a database of chemical structures (with 3D representation) and experimental data for various end-points (physico-chemical properties and biological activities) [31]. The QSARINS-Chem module also contained the QSAR model reporting format (QMRF) papers, which demonstrate the models' adherence to the "OECD principles for the validation, for regulatory purposes, of (Q)SARs" .

List of the datasets included in the structural database of QSARINS-Chem standalone version:

General class:

End point type:	Dataset type:
1. Physico-Chemical properties.	1. Soil organic carbon-water partition coefficient.
2. Environmental Persistence.	1. Sediment half-lives.
	2. Soil half-lives.
	3. Water half-lives.
	4. Air half-live.
	5. NO3 reactivity.
	6. O3 reactivity.
	7. OH reactivity.
	8. Global half-life index (GHLI).
2. Bioconcentration Factor (BCF)	1. BCF-Fernandez.
	2. BCF-Lu.
3. Metabolic Transformation	1. Fish biotransformation.
	2. Human biotransformation Model 1.
	3. Human biotransformation Model 2.
	4. Human biotransformation Model 3.
	5. Human biotransformation Model 4.
	6. Human total elimination.
4. Aquatic Toxicity	1. Fish acute toxicity (P. promelas).

BIOVIA Discovery Studio:

Molecular docking findings may be shown and analyzed using the software program BIOVIA Discovery Studio. Furthermore, BIOVIA Discovery Studio offers a number of analytic tools to assess the binding affinity, binding free energy, and other characteristics of the ligand-target complex.

Additionally, the program's user-friendly interface lets users alter how the animations and graphics look, making it simple to build superior numbers for publishing.

The term "Biovia Discovery Studio" (BDS) refers to the process of creating graphical representations of molecular structures and simulation results utilizing the software's features. The BDS visualization tools are intended to assist researchers in comprehending and sharing the outcomes of docking experiments, molecular simulations, and other molecular investigations [32]. This procedure can provide instructions for displaying chemical structures in three dimensions and highlighting certain interactions, such as hydrophobic and hydrogen bonding, between proteins and ligands.

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The stability of the complex and the protein-ligand binding affinity are determined by these interactions. Electrostatic potential mapping is one of the additional BDS visualization features. Depiction of surfaces and volumes, as well as intricate visualization [33]. By changing parameters like color, transparency, and labels, the visuals produced by BDS may be personalized. For usage in publications, presentations, and other applications, they can be exported or saved.

BDS offers a comprehensive drug discovery and molecular biology research platform that integrates a variety of molecular modeling and simulation techniques solution. Because of its user-friendly interface and sophisticated visualization features, BDS is accessible to researchers of all skill levels [34]. Additionally, BDS may offer customisable output, enabling users to add labels and comments as well as create unique perspectives for their visualization output. strong data administration.

Software utilized for drug 3D QSAR research:

SYBYL – X:

Docking investigations have been conducted using SYBYL-X software. This docking computer software illustrates how structural alterations affect the selected protein in the direction of their inhibitory effects and aids in gaining a thorough grasp of the targeted compounds' binding method [35]. The hydrogen bond interaction of amino acid residues allowed for the description and acceptance of the X-ray crystal structure in the case of proteins and enzymes. The protein was created using SYBYL-X as the foundation for the software's preparation module. In this way, a protein model was charged with AMBER7

FF99, the bond ordering were assigned, water and other residues were eliminated, and H atoms were inserted [36]. In silico screening has led to the development of coumarin-based molecules that are easily synthesized. A series of graded analyses for locations of attainable ligand affinity inside a receptor's binding region are performed using the SYBYL docking procedures. Following torsional energy optimization on optimal potentials for liquid simulation-AA non-bonded potential energy grid to generate potential candidate poses, a crude arrangement and counting procedure is used during the early evaluation stage. A total score, a model energy function that combines the empirical and force field-based factors, is used to choose the ultimate docked configuration.

MOE (MOLECULAR OPERATING ENVIRONMENT):

A drug discovery software platform called Molecular Operating Environment (MOE) combines technique development, modeling, simulations, and visualization into a single package [37]. Biologists, medicinal chemists, and computational chemists employ MOE scientific applications in academic, pharmaceutical, and biotechnology research. MOE is compatible with Linux, macOS, Windows, and Unix. Structure-based design, fragment-based design, ligand-based design, pharmacophore discovery, medicinal chemistry applications, biologics applications, structural biology and bioinformatics, protein and antibody modeling, molecular modeling and simulations, virtual screening, cheminformatics, and QSAR are among the primary MOE application areas. MOE's built-in command, scripting, and application development language is called Scientific Vector Language (SVL) [38].

As previously mentioned, MOE is a flexible program with primary uses in 3D molecular visualization, structure-based protein-ligand design, antibody and biologics design, structure-based protein engineering, SAR and SPR visualization, ligand-based design, protein, DNA/RNA modeling, virtual screening, 3D pharmacophore screening, fragment-based discovery, structural bioinformatics, molecular mechanics and dynamics, peptide modeling, structural biology, cheminformatics, and QSAR [39].

Although molecular models and simulations are frequently employed in computational chemistry, researchers from a wide range of disciplines can utilize them. Scientists may thoroughly examine the characteristics of molecules thanks to this theoretical technique, and by employing the data, they can get insight into how these molecules might behave in chemical and/or biological systems. The creation of novel materials and compounds depends on this knowledge [40].

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