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MOLECULAR DOCKING: A COMPREHENSIVE UNDERSTANDING OF TRENDS, AI INTEGRATION AND FUTURE PERSPECTIVES IN DRUG DISCOVERY

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ABSTRACT

Molecular docking has become an essential tool in modern drug discovery and structure-based drug design (SBDD) because it helps Predict how a small molecule interacts with target proteins quickly and cost effectively. Over time, docking method have advanced from simple rigid docking approaches to flexible and AI-assisted computational workflows. This review presents a comprehensive overview of molecular docking Including its principles, workflows, major software tools, databases, applications, challenges and future perspectives. Important docking tool Such as AutoDock Vina, GOLD, Glide, GNINA, PyRx and Discovery Studio are discussed along with major databases including PDB, ZINC, PubChem, DrugBank, ChEMBL and binding DB. The review also highlights the growing role of artificial intelligence, machine learning, deep learning and AlphaFold-based structure prediction in improving docking accuracy, Virtual screening, binding affinity prediction and De novo Drug design. Applications of molecular docking in cancer, infectious diseases, neurodegenerative disorders, Drug repurposing and natural product research are also summarised. Despite major advancements, challenges such as receptor flexibility, scoring inaccuracies, computational cost and limited interpretability of AI model still remain. Overall, the integration of molecular docking with AI and advanced computational technologies is expected to accelerate and improve future drug discovery workflows.

KEYWORDS: Molecular docking; virtual screening; drug discovery; artificial intelligence; protein-ligand interaction; computational chemistry.

INTRODUCTION

In molecular docking we see the interactions between small molecules and their target proteins, scientists can better predict the binding affinity and selectivity of potential drugs, leading to more efficient and targeted therapeutic strategies. This approach not only accelerates the discovery process but also enhances the precision of drug design, paving the way for innovative treatments.[1,2] This not only accelerates the drug discovery process but also reduces the costs associated with experimental screening, allowing scientists to focus their efforts on the most viable options. As a result, this innovative technique is poised to transform how new therapies are developed and brought to market.[3]

These innovations have significantly improved the accuracy and efficiency of predicting molecular interactions, making the way for more effective drug discovery processes. As researchers continue to refine these techniques, the potential for personalized medicine and tailored therapeutic strategies becomes increasingly promising.[4]

As researchers continue to refine these techniques, the integration of artificial intelligence and machine learning is expected to further enhances the accuracy and efficiency of molecular docking processes, making the way for more effective therapeutic solutions.[2]

To tackle challenges researchers are continuously developing the advance algorithms and techniques to enhance the precision of these processes, aiming to improve the predictive power of docking studies in drug discovery and design.

By integrating machine learning approaches, the field is progressing towards more efficient and effective identification of potential drug candidates.[5] These advancements not only enhance the accuracy of binding predictions but also allow for the exploration of novel binding sites and mechanisms, this led to ultimately making the way for breakthroughs in drug discovery and development. As these techniques evolve, researchers are better equipped to tackle the complex challenges posed by diverse molecular interactions (LMMC).[6] The increasing availability of free docking tools, better scoring methods, and faster computer systems has made molecular docking easier to use for researchers in many different fields.[7]

Our researchers use many types of methods and tools to improve the accuracy and efficiency of docking studies. These methods include energy landscapes, knowledge-based docking approaches, and advanced sampling techniques.[8,9]

The success of this algorithm is further supported by the availability of structural and binding affinity data from databases like Protein Data Bank,[10,11] ZINC,[12,13] PubChem,[14,15] DrugBank,[16,17] ChemDB,[18] ChEMBL,[19] along with modern resources such as AlphaFold,[20,21] and BindingDB.[22,23] These databases provide important information on protein structures, ligand properties, and binding affinities, which help improve docking algorithms and their prediction accuracy.[3,24]

These advanced approaches are now widely applied in disease such as Malaria,[25] Inflammation,[26,27] Tuberculosis,[28,29] Bacterial and Viral Infections,[30,31] Breast Cancer,[32] Ovarian Cancer,[33] Colon Cancer.[34,35].

Melanoma, Alzheimer's disease,[33,36,37] Diabetes,[38,39] and COVID-19,[13,40] along with emerging areas like Neurodegenerative and Cardiovascular disorders. Various biological targets have been explored, including enzymes and receptors such as Acetylcholinesterase,[41,42] Cyclooxygenase, p53 Protein,[34] Aromatase,[43] PD-1/PD-L1,[44]

SIRT2,[45,46,47] TNF-a,[48,49,50] BACE-1,[36,37] PDE inhibitors,[51,52] SARS-CoV-2,[53,54,55] Proteins, Tyrosinase,[56,57] Tubulin,[58,59] and Cell Cycle Regulatory Proteins.

In addition, Natural Products, Marine Drugs and Phytochemicals have been extensively studied using docking approaches, including compounds from Trigonella Foenum Graecum,[60] Hibiscus schizopetalus,[30,61] Eugenia punicifolia,[62,63] Pinus roxburghii,[64] Carica papaya,[65] Withania somnifera,[66,67,68] millets, marine sponges like Hyrtios species,[69,70] as well as other medicinal plant such as Curcuma longa,[35,71] Azadirachta indica,[72,73] and Camellia sinensis,[74,75,76] highlighting their importance in nutraceuticals and drug discovery research.

In spite of this advancement, some of the challenges still limit the effectiveness of molecular docking. These are such as inaccuracies in scoring functions, inadequate treatment of protein flexibility and difficulties in accurately predicting binding free energy. Sometime variability among different docking tool often leads to inconsistent results which show us we still need for improved methodologies and validation strategies.

Linus Pauling (1964), In the 1940s, early studies on intermolecular forces such as hydrogen bonding and van der Walls interactions laid the foundation for understanding molecular interactions. Building on this, in the 1950s, Linus Pauling (1964) introduced the concept of molecular recognition, explaining how molecules interact based on complementary shapes and chemical properties. This concept became essential for understanding drug-receptor interactions. In the following decades, advancements in structural biology, including X-ray crystallography and NMR spectroscopy, provide detailed insights into molecular structures.[77]

During the 1990s and early 2000s, docking algorithms were significantly improved with the development of programs such as AutoDock, FlexX, and GOLD, which introduced better handling of ligand and receptor flexibility along with improved scoring functions. At the same time, docking predictions were increasingly validated using experimental techniques like X-ray crystallography and NMR spectroscopy, enhancing their reliability. From 2000 onwards, increases computational power enabled large-scale virtual screening and more accurate structure-based drug design.

Between 2010 and 2015, molecular dynamics simultations became widely used to study the stability and flexibility of protein-ligand interactions.[78] Between 2015 and 2020, integration of high-throughput screening, cloud computing, and improved algorithms accelerated drug discovery processes. Around 2020, artificial intelligence and machine learning began transforming computational drug design by improving prediction accuracy and efficiency. In 2021, AlphaFold revolutionizes protein structure prediction, significantly enhancing docking studies.[79,80] From 2022 to 2025, the integration of AI, deep learning and hybrid computational approaches has further improved bioactive conformer identification, making drug discovery faster, more accurate, and cost-effective.[3]

This review aims to critically analyze current molecular docking strategies, comparing different tools and identifying the existing limitations to guide future research.

Classification Hierarchy of Molecular Docking

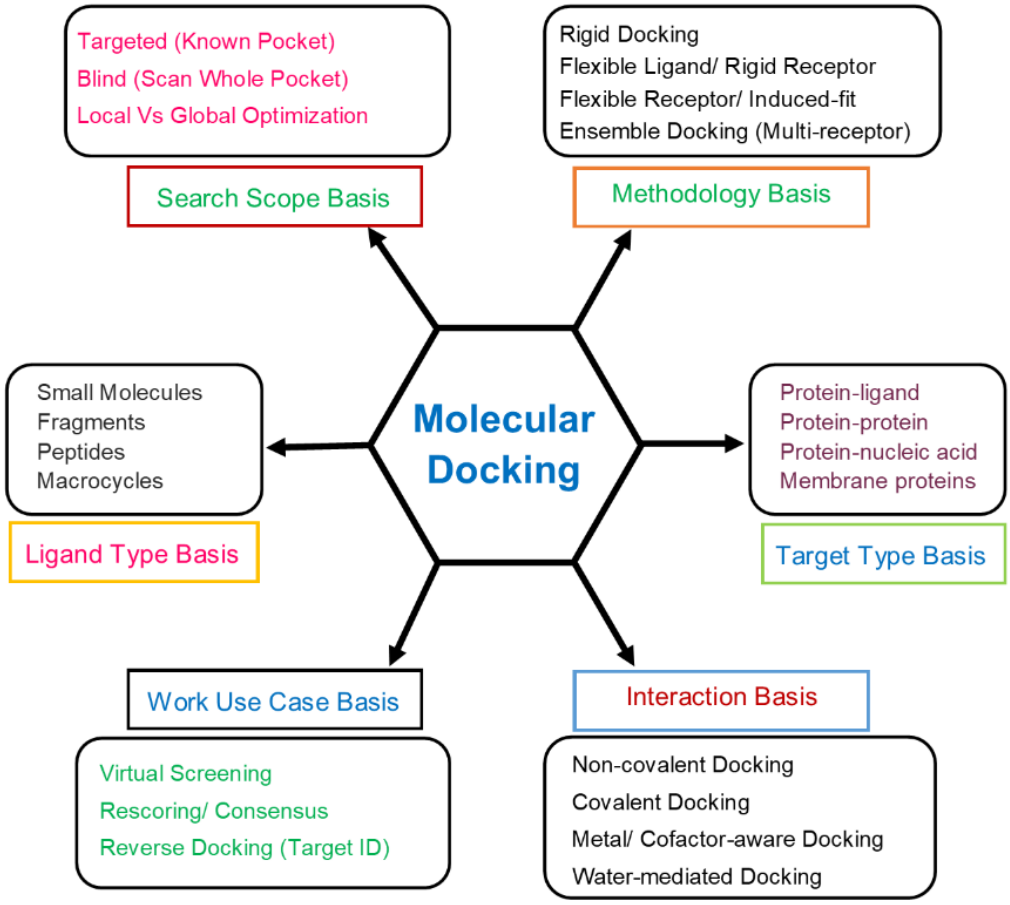

Figure 1: Different classification basis for molecular docking.

Docking Algorithms

The aim of molecular docking is to give a prediction of the ligand-receptor complex structure using computation methods. Docking is done in two basic simple steps in which the first one is different possible shapes and positions(conformations) of the ligand are generated inside the protein's active site and the second one is these conformations are ranked using a scoring function. However, the accuracy of docking predictions can be influenced by various factors, including these two the quality of protein structure and the choice of scoring function.

In docking when the computer generates different possible poses of a ligand (Sampling), one of these poses should best as real experiment and the scoring system (Scoring Function) should must have to identify this correct pose and rank it at top as the best result.[4],[6]

Steps Involved in Molecular Docking

So, the Docking process involves the following steps,[81,82,83]:

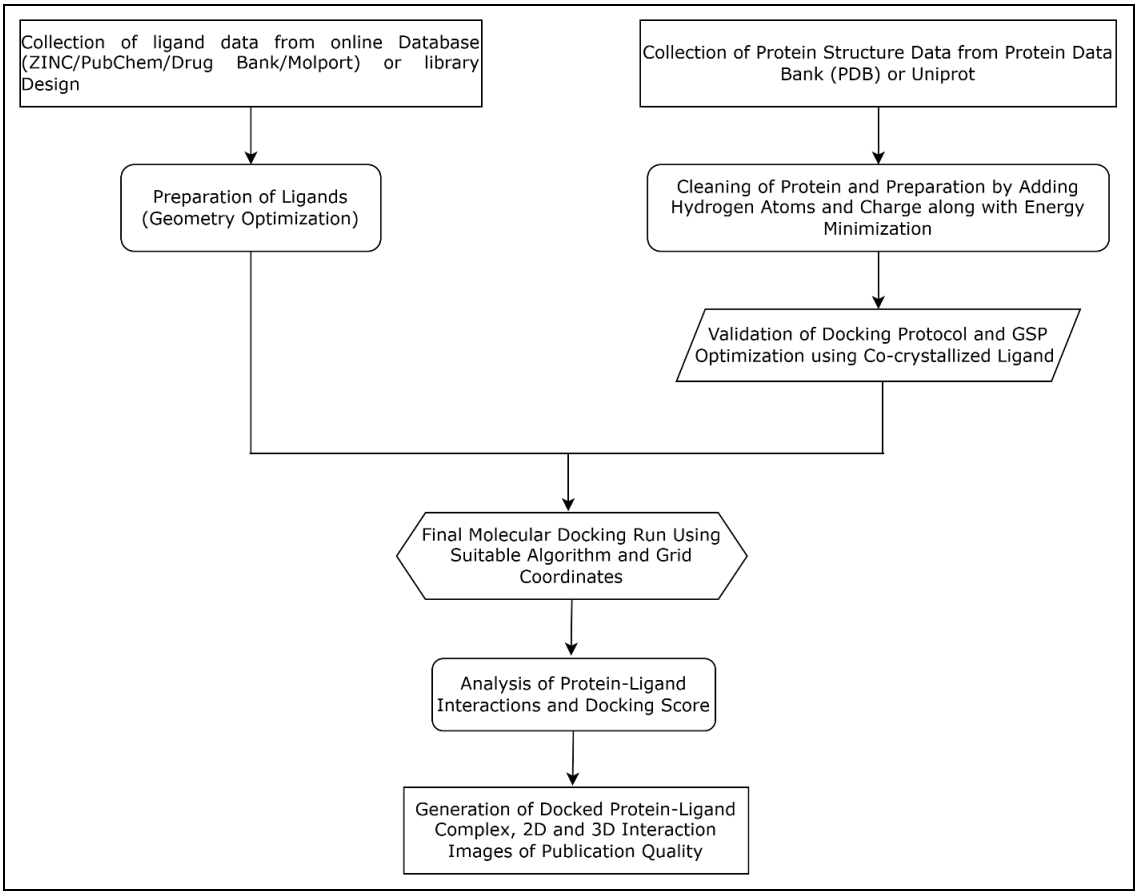

Figure 2: Flowchart representing steps involved in molecular docking, result analysis and publication quality image generation.

Step 1: Preparation of protein

The3D structure of the target protein is obtained from the Protein Data Bank and then pre-processed for docking studies. This process includes removing unnecessary water molecules from the active site, and then we do addition of hydrogen atom for adjusting protonation states, correcting missing residues or atoms, optimizing side chains, and performing energy minimization to achieve a stable structure. Proper protein preparation is essential for accurate docking results, as it ensure the structure represents its biologically active form.[84,85,86,87,88]

Step 2: Active site prediction

After protein preparation, the binding site of the protein must be identified. Although a protein has multiple potential binding pockets, only the relevant active site is selected for docking. During this process unnecessary water molecules and hetero atoms are usually ignored unless they play an important role in ligand binding.[84,85,87,88,89]

Step 3: Ligand preparation

Ligand can be retrieved from databases such as ZINC and PubChem or they can be drawn using tools like ChemSketch.

While selecting a ligand Lipinski's Rule of Five is commonly applied to evaluate its drug-likeness. This rule helps to distinguish between drug like and non-drug like molecules based on properties such as molecular weight, hydrogen bond donors and acceptors/ and lipophilicity. Ligands that satisfy most of these criteria are more likely to have good absorption and bioavailability making them suitable candidates for computer aided drug design (CADD) studies.

Lipinski's Rule of Five: It states that a compound is more likely to be orally active if it fulfils these criteria.[83,85,87,88,89]

a) It should have not more than 5 hydrogen bond donors (-OH and -NH groups)
b) It should have not more than 10 hydrogen bond acceptors (O and N atoms)
c) It should have molecular weight less than 500Da
d) It should have Log P (lipophilicity) not greater than 5
e) It should have molar refractivity between 40 – 130

Step 4: Molecular Docking

Step 4 is actual docking process where the prepared ligand is placed into the active site of the protein to predict its binding mode. This step mainly involves the two key process; sampling and scoring. In sampling different possible orientations and conformations (poses) of the ligand are generated within the binding site. In scoring each pose is evaluated using a scoring function to estimate its binding affinity and stability. The best pose is selected based on lowest binding energy or highest score which indicates a strong and stable interaction between the ligand and the protein.[85,87,88,89]

Step 5: Docking Assessment

Now we evaluate the reliability and performance of the docking results. The effectiveness of docking depends on both sampling and scoring functions, as they determine how accurately binding poses and affinities are predicted. Therefore, it is important to validate the docking protocol especially when experimental data is available to check its predictive accuracy.[84,90]

Docking performance can be assessed using several methods, including:

- Docking Accuracy (DA) which measures how closely the predicted binding pose matches the experimental structure.
- Correlation between docking score and experimental activity, evaluation using enrichment Factor (EF) which indicates how well active compound are identified.
- Measurement of distance between key functional groups (such as ion-bonding sites) and target residues in the active site.
- Consideration of induced-fit effects, where both ligand and protein flexibility are taken into account.

Step 6: Docking and scoring function validation

Docking validation and scoring function validation are important steps in molecular docking studies because it ensures that the predicted results are reliable and meaningful for drug discovery. Since molecular docking is widely used in structure-based drug design, it is essential to verify that the docking protocol can accurately predict how a ligand binds to a target protein and how strongly it interacts.

The overall performance of docking depends on two key components the sampling process which generates different ligand poses, and the scoring function, which rank these poses based on their binding affinity. Therefore, a proper validation of both aspects is necessary. In most of the cases, multiple validation techniques are used together to improve the confidence in docking results.[6,88,91,92,93,94]

1. Docking Validation

Docking validation focus on checking whether the docking method can correctly reproduce the binding mode of ligand with in the active site of protein.

- Redocking: In redocking where a ligand already present in the experimental structure is removed and then docked again into the same binding site. If the predicted pose closely matches the experimental one (usually measured by RMSD) the docking method is considered reliable.
- Cross-docking: In this a ligand is docked into different conformations of the same protein. This helps to evaluate in how well the docking method can handle the changes in protein structure and flexibility.
- Virtual Screening Studies: In this a set of known active compound and inactive molecules(decoys) is used. The ability of the docking method to correctly identify active compound indicates its effectiveness.

Several statistical measures are used in this context:

a) ROC-AUC
b) Enrichment Factor (EF)
c) BEDROC

2. Scoring Function Validation

Scorning function validation is an essential step in molecular docking, as it determines how accurately a scoring function can evaluate and rank protein-ligand interactions. A scoring functional model used to estimate the binding affinity and stability of a ligand-protein complex based on various molecular interactions such as hydrogen bonding, electrostatic forces, hydrophobic effects and steric compatibility. Different types of scoring functions are commonly used in docking studies, which are physics-based, empirical, knowledge-based approaches. The main goal of scoring function is correctly predicted and rank the binding strength of different ligand towards a protein, which helps in identifying a potential drug candidate and understanding biological interactions.

The reliability of virtual screening results largely depends on the accuracy of the scoring function. Therefore, proper validation is required to ensure that the scoring function can produce meaningful and reproducible results.

Evaluation criteria for scoring functions

a) Accuracy of Pose Prediction: This evaluates whether the scoring function can correctly identify and rank the near-native binding pose among multiple generated conformations. A reliable scoring function should assign the best (lowest energy) score to a pose that closely matches the experimentally determined structure, typically indicates by a low RMSD value.
b) Prediction of Binding Affinity: this aspect examines the correlation between docking scores and experimental binding data such as IC50, Kd, or Ki values. A good scoring function should show a strong correlation with experimental results, indicating its ability to accurately estimate binding strength.
c) Ranking Efficiency in Virtual Screening: This assesses the ability of the scoring function to rank true active compounds higher than inactive ones(decoys) during virtual screening. Metrics such as enrichment factor (EF), ROC-AUC, and BEDROC are commonly used to evaluate this performance.

Molecular Docking Tools and Software

AutoDock

AutoDock is a widely used freely available tool for studying protein-ligand interaction in molecular docking. It supports blind docking and flexible ligand docking, but has limited receptor flexibility. AutoDock is commonly applied in structure-based drug design, virtual screening and lead optimization studies,[3,24,95]

AutoDock Vina

AutoDock Vina is an advanced version of AutoDock that offers faster and more reliable docking performance. It provides improved accuracy in predicting protein-ligand interactions and widely used in structure-activity relationship (SAR) studies. AutoDock Vina simplifies the docking process by automatically handling atoms types and grid calculations and reduces the user input and setup time. Its efficient scoring function and optimization algorithms make it suitable for large scale virtual screening and modern drug discovery.[3,96,97,98,99,26]

Schrodinger Glide

Schrodinger Glide is a widely used commercial docking tool in the pharmaceutical and biotechnology industries especially for combinatorial chemistry and high-throughput virtual screening. Glide provide a good balance of speed and accuracy through different modes including High Throughput Virtual Screening (HTVS) for rapid evaluation of large compound libraries and Standard Precision (SP) and Extra Precision (XP) modes for more accurate docking results. It is known for reliably predicting correct binding poses with low root mean square deviation (RMSD) from experimental structures making it highly effective for large scale screening and lead optimization studies.[3,24,100]

Smina

Smina is an open-source docking tool derived from AutoDock Vina specially designed for improved scoring function development and enhanced energy minimization. It provides greater flexibility in customizing scoring functions and allows users to modify docking parameters for better accuracy. Smina supports efficient energy minimization and particularly useful for refining docking poses and improving binding predictions. The software is commonly used in Linux environments and works through command line execution making it suitable for automated workflows and scripting in large scale virtual screening studies. It is mainly preferred for research level customization rather than routine large-level drug discovery.[3,24,101]

PyRx

PyRx is an integrated virtual screening tool widely used for molecular docking and computational drug discovery. It provides a user-friendly graphical interface that simplifies the docking workflow for beginners and researchers. PyRx combines multiple tools such as AutoDock and AutoDock Vina allowing efficient ligand preparation, energy minimization and docking within a single platform. It is particularly useful for high-throughput virtual screening of large compound libraries. Modern uses of PyRx includes easy visualization of docking results, batch processing and integration into drug discovery workflows making it a convenient and accessible tool for academic research and initial screening studies.[102,103]

PyMOL

PyMOL is a widely used molecular visualization tool for structural biology and analysis of macromolecules, including proteins and protein-ligand complexes. It is mainly used to visualize, rotate and manipulate molecular structure making

it essential for analysing docking results and binding interactions. PyMOL also support basic task such as structure editing, image rendering and preparation of publication quality figures. Built on the python programming language, PyMOL allows scripting and automation of complex tasks. Modern versions include enhanced graphics, plugins and integration with computational workflows making it a valuable tool in drug discovery and molecular modeling studies.[104,105]

UCSF Chimera

UCSF Chimera is a widely used tool for interactive visualization and analysis of molecular structures, including protein, ligand, density maps, trajectories and sequence alignments. It is commonly used in docking studies for preparing and visualization protein-ligand complexes as well as performing basic energy minimization of ligand to improve their stability before docking. The software is freely available for academic and non-commercial use. In recent years, its advanced version UCSF ChimeraX has been introduced with improved graphics, better performance and enhanced support for large biomolecular systems making it more suitable for modern computational workflows.[106,107,108]

Discovery Studio

Discovery Studio is a comprehensive software suite for molecular modeling, simulation and computational chemistry widely used in life science research. It supports a wide range of applications including protein modeling, molecular docking, pharmacophore modeling and lead optimization. The platform provides an integrated and user-friendly environment that allows researchers to perform multiple drug discovery tasks within a single interface. Build on advanced workflows such as Pipeline Pilot Discovery Studio enables seamless integration of different computational tools and data analysis methods. Its modern version also supports enhanced visualization, simulation techniques and AI-assisted drug design making it suitable for end-to-end drug discovery processes.[3,109]

GOLD (Genetic Optimization for Ligand Docking)

GOLD is a widely used docking program that applies a genetic algorithm to predict the binding of flexible ligands within protein active sites. It is a commercial software known for accurately handling ligand flexibility and generating reliable binding poses. GOLD is commonly used for pose prediction, virtual screening and protein-ligand docking and it integrates well into automated workflow. The software also supports advanced features such as covalent docking and exploration of complex targets in areas like cancer, immunology and infectious diseases. Recent developments have improved its scoring functions and workflow integration making it suitable for modern structure-based drug design (SBDD).[3,110,111]

iGEMDOCK

Igemdock is an integrated molecular docking tool that provides both docking and post-docking analysis with a user-friendly graphical interface. It is designed to identify pharmacological interactions and support virtual screening by analysing protein-ligand binding mechanisms. The software combines docking with interaction profiling, helping to highlight key residues involved in binding. iGEMDOCK is widely used for lead identification and structure-activity relationship (SAR) studies particularly in targets such as enzymes, receptors and kinases. Its ability to integrate docking results with biological function analysis makes it useful in modern drug discovery workflows.[3,112]

Open Babel

Open Babel is an open source chemical informatics tool used for converting, analysing and managing molecular data across computational chemistry, bioinformatics and drug discovery applications. It supports interconversion between multiple chemical file formats such as SDF(Structure Data Format), SMILES(Simplified Molecular Input Line Entry System) and InChI(International Chemical Identifier). Open Babel is widely used for ligand preparation, format conversion and data preprocessing in molecular docking workflows.[3,113]

GNINA

GNINA is an advanced molecular docking program built on AutoDock Vina that utilizes deep learning techniques mainly convolutional neural networks(CNNs) to enhance the accuracy of binding pose prediction and scoring of protein-ligand interactions. GNINA combines traditional docking algorithms with AI-based scoring functions which allow it to more accurate evaluation of protein-ligand interactions compared to conventional methods. The software is widely used in modern drug discovery for virtual screening, binding affinity, prediction and lead optimization. Its integration of machine learning makes it particularly useful in large scale screening and next generation computational workflows.[114,115,116]

AlphaFold

AlphaFold is an advanced artificial intelligence system developed to predict highly accurate 3D structures of proteins from their amino acid sequences. It has transformed structural biology by providing near experimental level protein models which are highly useful for molecular docking and structure based drug design especially when experimental structures are not available. In modern drug discovery AlphaFold generated structures are widely used as reliable targets for docking, virtual screening and understanding protein-ligand interactions significantly accelerating research and reducing experimental time and cost.[20,21,117,118]

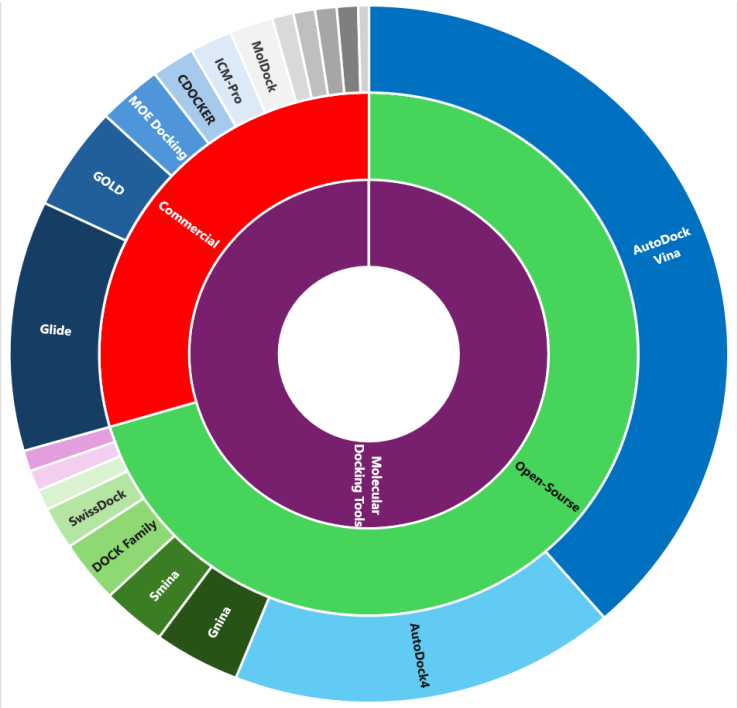

Figure 3: Sunburst chart summarizing representative open-source and commercial tools, Current usage trends are estimated from recent literature, benchmarking studies and community adoption patterns rather than exact market-share statistics.

Table 1: Advanced Molecular Docking Tools.

SN	Tools	Stage	Primary Function	Typical Applications	Ref.
1.	AutoDock Vina	Docking	General purpose small molecule docking engine using gradient based optimization with Vina/Vinardo scoring	Routine docking and large scale virtual screening	[96], [97], [98], [114], [119]
2.	AutoDock	Docking	Classical docking engine using Lamarckian Genetic Algorithm and empirical free energy scoring	Docking, redocking and benchmarking studies	[95], [120]
3.	AutoDockFR	Docking (Flexible)	Flexible receptor docking with genetic algorithm and explicit side chain flexibility	Flexible protein-ligand docking and induced fit studies	[121]
4.	AutoDock-GPU	Docking (Accelerated)	GPU-accelerated AutoDock4 implementation using CUDA/OpenCL/SYCL	High-throughput virtual screening on HPC systems	[122], [123], [124]
5.	DOCK6	Docking	Uses sphere matching, anchor and grow strategy and grid-based scoring	Docking, de novo drug design and rescoring	[3], [125]
6.	Schrodinger	Docking	High precision docking with HTSV, SP and XP modes and advanced scoring	Lead optimization and industrial drug discovery	[3], [24], [100]
7.	GOLD	Docking	Genetic algorithm based flexible docking with multiple scoring functions	Accurate pose prediction and binding analysis	[3], [110], [111]
8.	FlexX	Docking	Fragment based incremental construction algorithm for ligand placement	Fast docking and library screening	[3], [24]
9.	rDock	Docking	Open-source docking with stochastic search and scoring for proteins and nucleic acids	Virtual screening and nucleic acid targeting	[3]
10.	GNINA	Docking (AI-based)	Deep learning (CNN) based scoring integrated with AutoDock Vina framework	AI-driven docking, rescoring and lead optimization	[114], [115], [116]

Table 2: Support Tools (Visualization/Preparation/Utility).

SN	Tools	Stage	Primary Function	Typical Applications	Ref.
1.	PyMOL	Visualization	High quality 3D molecular visualization, rendering and structural analysis	Protein-ligand interaction analysis and publication quality figures	[104], [105]
2.	UCSF Chimera	Visualization/Preparation	Interactive visualization with structure editing, docking preparation and analysis tools	Structure inspection, energy minimization and docking setup	[99], [106], [107]
3.	UCSF ChimeraX	Visualization	Advanced GPU-accelerated visualization with improved performance and large structure handling	High resolution visualization and analysis of large biomolecular complexes	[126], [127]

4.	Discovery Studio Visualizer	Visualization/Modelling	Integrated platform for visualization, simulation, pharmacophore modelling and analysis	Drug design workflows and protein-ligand interaction studies	[119], [128]
5.	Open Babel	Preparation/Conversion	Molecular file conversion, structure cleanup, protonation and format compatibility	Ligand preparation and interconversion between docking file formats	[3], [24]
6.	PyRx	Preparation/Screening	GUI-based platform integrating AutoDock/Vina for ligand preparation and docking	Virtual screening and batch docking for small molecules	[102], [103]
7.	BIOVIA Pipeline Pilot	Workflow/Integration	Data pipeline automation, cheminformatics workflows and integration of multiple tools	Large scale data processing and automated drug discovery pipelines	[129], [130]

Table 3: AI/ Machine Learning Tools (Drug Discovery).

SN	Tools	Stage	Primary Function	Typical Applications	Ref.
1.	AlphaFold	Structure Prediction	Deep learning based protein structure prediction from amino acid sequence	Target structure generation for docking and drug design	[20], [117], [118]
2.	DeepChem	Modelling/Prediction	Machine learning framework for molecular property prediction and cheminformatics	QSAR modelling, toxicity prediction and virtual screening	[131], [132], [133], [134]
3.	GNINA	Docking (AI-based)	CNN-based scoring integrated with docking for improved pose prediction	AI-assisted docking and binding affinity prediction	[114], [115]
4.	DeepDock	Docking (AI-based)	Deep learning driven prediction of ligand binding conformations	Fast and accurate docking in virtual screening workflows	[2], [116]
5.	DeepPurpose	Interaction Prediction	Deep learning models for drug target binding affinity prediction	Drug repurposing and screening	[135], [136], [137], [138]
6.	REINVENT	De novo Design	Reinforcement learning based molecule generation and optimization	Novel drug design and lead optimization	[139], [140], [141]

Table 4: Databases (Drug Discovery/Docking).

SN	Tools	Stage	Primary Function	Typical Applications	Ref. Link
1.	Protein Data Bank(PDB)	Structure Retrieval	Repository of experimentally determined 3D protein and nucleic acid structures	Target structure retrieval for docking studies	https://www.rcsb.org
2.	PubChem	Compound Library	Large public database of chemical molecules and bioactivity data	Ligand retrieval and virtual screening	https://pubchem.ncbi.nim.nih.gov
3.	ZINC Database	Virtual Screening	Curated database of commercially available drug like compounds	Large scale virtual screening and lead identification	https://www.zinc.docking.org

4.	DrugBank	Drug Information	Contains detailed drug, target and pharmacological information	Drug repurposing and target analysis	https://go.drugbank.com
5.	ChEMBL	Bioactivity Data	Contains bioactive molecule structures and activity data	QSAR modelling and ligand-based drug design	https://www.ebi.ac.uk/chembl
6.	BindingDB	Binding Data	Experimental binding affinity data for protein-ligand complexes	Training ML models and scoring validation	https://www.bindingdb.org
7.	ChemSpider	Chemical Information	Aggregated chemical structure and property database	Structure search and ligand identification	https://www.chemspider.com
8.	SwissTargetPrediction	Target Prediction	Predicts probable protein targets of small molecules	Drug repurposing and target identification	https://www.swisstargetprediction.ch

Scope and Prospects of Molecular Docking Studies

1. Drug Discovery

Molecular docking is widely used in the discovery of new drug molecules. It helps identify compounds that can effectively bind with disease related targets. Docking reduces the time and cost required for experimental screening. It play a major role in modern computer-aided drug design.

2. Structure-Based Drug Design

Docking is used to design drug based on the three-dimensional structure of proteins. It helps researchers understand the active site architecture of Target molecules. Compounds can be optimised for better binding and activity. SBDD improves rational drug development strategies.

3. Virtual Screening

Virtual screening allows computational screening of thousands or millions of compounds in a short time. Docking identifies the most promising molecules for further testing. It is highly useful in pharmaceutical and biotechnology research. This approaches significantly reduces laboratory workload.

4. Lead Identification

Docking helps identify lead compounds showing favourable interactions with the target protein. These lead molecules serve as starting point for drug development. Binding affinity and interaction patterns are analysed during this process. It accelerates early-stage drug discovery.

5. Lead Optimization

Lead Optimization Improves the biological activity and selectivity of lead compounds. Docking predicts a structural modification that enhance binding efficacy. It also helps reduce toxicity and improve pharmacokinetic properties. Optimised leads have higher chances of becoming successful drugs.

6. Binding Mode Prediction

Docking predicts how a ligand fits into the active site of a receptor. It determines the orientation, position and confirmation of the ligand. This information helps understand molecular interactions at the atomic level. Binding mode prediction is essential for rational drug design.

7. Binding Affinity Prediction

Docking estimates the strength of interaction between ligand and protein using scoring functions. More negative docking response usually indicates a stronger binding affinity. This helps rank compound according to their potential biological activity. It assists researchers in selecting promising candidates.

8. Target Identification

Docking can identify possible biological targets for a compound. It is useful when the mechanism of action of a molecule is unknown. Researchers can predict interactions with multiple proteins. This application supports drug discovery and disease pathway studies.

9. Inverse Docking

Inverse docking involves docking a single ligand against multiple protein targets. It helps identify potential target proteins and off-target interactions. This technique is useful in drug repurposing and toxicity studies. It also supports systems pharmacology research.

10. Multi-Target Drug Design

Some diseases involves multiple biological pathways, requiring drugs that act on several targets simultaneously. Docking helps design such multi-target agents. This approach is important in treating complex disorders like cancer and neurodegenerative diseases. It improves therapeutic effectiveness.

11. Drug Repositioning\ Drug Repurposing

Docking helps discover new therapeutic uses four already approved drugs. Existing compounds are screened against new biological targets. Drug repurposing reduces development time and cost. It became highly important during the covid-19 pandemic.

12. Anticancer Drug Discovery

Docking is extensively used to identify inhibitors against cancer related proteins. It helps design molecules targeting kinases, growth factors and DNA-associated enzymes. Researchers can study molecular interaction involved in tumour progression. It supports the development of targeted cancer therapies.

13. Kinase Inhibitor Design

Protein kinase regulate many cellular activities and are major drug targets. Docking helps design inhibitors that point selectively to kinase active sites. Selective inhibition reduces unwanted side effects. Kinase inhibitors are important in cancer treatment.

14. Antimicrobial Drug Discovery

Docking is used in the discovery of antibacterial, antiviral and antifungal agents. Compounds are screened against microbial proteins essential force survival. This technique helps identify novel therapeutics against resistant pathogens. It supports infectious disease research.

15. Drug Resistance Studies

Mutations in target protein can cause drug resistance. Docking helps analyse how mutation affects ligand binding.

Researchers can design modified inhibitors to overcome resistance. This application is valuable in cancer and antimicrobial therapy.

16. Natural Product Research

Natural compounds from plants and herbs are screened using docking studies. Phytochemicals with a strong binding affinity can be identified as potential drug candidates. Docking supports herbal medicine research and nutraceutical development. It is widely used in ethnopharmacology.

17. Epigenetic Drug Discovery

Docking helps identify Inhibitors of epigenetic enzymes such as histone deacetylases and methyltransferases. These targets regulate gene expression without altering DNA sequences. Epigenetic drugs are important in cancer and neurological disorders. Docking Accelerates the discovery of such agents.

18. Enzyme Inhibitor Design

Many diseases are associated with abnormal enzyme activity. Docking helps design molecules that block enzyme active sites. It predicts enzyme-ligand interactions and inhibition mechanism. This application is important in metabolic and infectious diseases.

19. Vaccine Design

Docking is used in computational vaccine development. It studies interactions between epitopes and immune receptors.

This helps predict immune responses and vaccine effectiveness. Docking supports rapid vaccine design strategies.

20. Protein-protein Interaction Studies

Docking analyzes interactions between proteins involved in biological pathways. Understanding these interactions helps identify disease mechanisms. It is useful in singnaling pathway analysis and therapeutic target discovery. Protein-protein docking is an important area of structural biology.

21. Protein-Nucleic Acid Interaction Studies

Docking helps study interactions between proteins and DNA or RNA molecules. These interactions are important in gene regulation and viral infections. Researchers use docking to analyse transcription factors and nucleic acid-binding proteins. It contributes to molecular biological research.

22. Molecular Mechanism Understanding

Docking explains how drugs produce their biological effects at the molecular level. It identifies important amino acid residues involved in binding. Interactions maps help understand pharmacological mechanism. This applications improves rational drug development.

23. Toxicity Prediction

Docking can predict potentially harmful interactions of compounds with biological targets. Toxic compounds may bind to unintended proteins and produce side effects. Early toxicity prediction reduces failure during drug developments. It improves drug safety assessment.

24. ADMET-Oriented Drug Selection

Docking supports the selection of compounds with favourable ADMET properties. ADMET includes absorption, distribution, metabolism, excretion and toxicity. Compounds with poor pharmacokinetic behaviour can be eliminated early. This improves the efficiency of drug development.

25. Personalized Medicine

Docking can predict how drugs interact with patient-specific protein variants. Genetic mutations may alter drug binding and therapeutic response. Personalised docking studies support precision medicine approaches. It helps optimise individual treatment strategies.

26. Food Safety Applications

Docking is used to study interactions of food contaminants and additives with biological molecules. It helps predict toxicological effects of chemicals present in food products. Researchers can access food safety computationally. This application is important in public health research.

27. Computational Biology and Bioinformatics Research

Docking is an important tool in computational pharmacology and bioinformatics. It integrates structural biology, cheminformatics and molecular modelling. Researchers use docking for data analysis and biological prediction studies.

It supports interdisciplinary scientific research.

28. Fragment-Based Drug Design

Small molecular fragments are docked into target binding sites to identify favourable interactions. These fragments are later combined to create potent drug molecules. This method improves drugs optimization efficiency. Fragment-based design is widely used in pharmaceutical research.

29. Hit-to-Lead Development

Initial hit compounds identified during screening are improved through docking-guided modifications. Researchers optimise potency, selectivity and stability. Docking helps predict the effect of a structural changes. This step is essential in the drug development pipeline.

30. Pharmacophore Validation

Docking validates pharmacophore models by checking whether predicted features support target binding. It confirms the importance of hydrogen bond donors, acceptors and hydrophobic regions. This improves the reliability of pharmacophore-based screening. It supports rational drug discovery.

31. Clinical Candidate Prioritization

Docking helps prioritise compounds before expensive laboratory and clinical studies. Molecules with better docking scores and interaction profiles are selected. This reduces unnecessary experimental work. It improves resource management in pharmaceutical research.

32. Discovery of Selective Inhibitors

Docking helps identify compounds that selectively bind to a specific target. Selective inhibitors reduce interactions with non-target proteins. This minimises adverse effect and improves therapeutic efficacy. Selectivity is important in modern targeted therapy.

33. Allosteric Drug Discovery

Some drugs bind to sites other than the active site known as allosteric sites. Docking helps identify such alternative binding regions. Allosteric modulators can regulate protein function more precisely. This approach is increasingly important in drug development.

34. Molecular Interaction Visualization

Docking provides visual representations of protein-ligand interactions. Researchers can observe Hydrogen bonds, hydrophobic interactions and electrostatic contacts. Visualisation improves understanding of binding mechanisms. It is useful for analysis and scientific presentation.

35. Computer-Aided Optimization of Existing Drugs

Existing drugs can be a structurally modified using talking analysis. Researchers predict how modifications influence binding affinity and activity. This helps improve therapeutic performance and reduce side effects. It supports the development of better drug analogs.

36. Disease-Specific Drug Design

Docking is used to design drugs for a specific disease such as cancer, tuberculosis, diabetes and COVID-19. Disease-related proteins are selected as targets for screening. Compounds with high binding affinity are identified as potential therapeutics. This approach supports targeted medicine.

37. Docking-Based Decision Making in Drug Discovery

Docking results guide important decisions during drug development. Researchers use docking score and interaction profile to prioritise compounds. It helps design experimental studies more effectively. This improves efficiency in pharmaceutical research.

38. Predicting Selectivity and Off-Target Effects

Docking predicts whether a drug may interact with unintended proteins. Such off-target interactions can cause adverse effects on toxicity. Early prediction helps improve drug safety. This application is important in risk assessment and optimization.

39. Academic and Industrial Research

Docking is widely used in universities, research institutes and pharmaceutical companies. It supports teaching, research projects and industrial drug discovery programme. Scientists use docking for hypothesis generation and compound analysis. It has become an essential computational tool.

40. AI-Augmented Drud Design

Artificial intelligence and machine learning are increasingly integrated with molecular docking. AI helps predict active compounds, optimise screening and improved docking accuracy. This combination accelerates modern drug discovery workflows. AI-augmented docking represents the future of computational drug design.

The following diagram illustrate the major areas where molecular docking plays a crucial role.

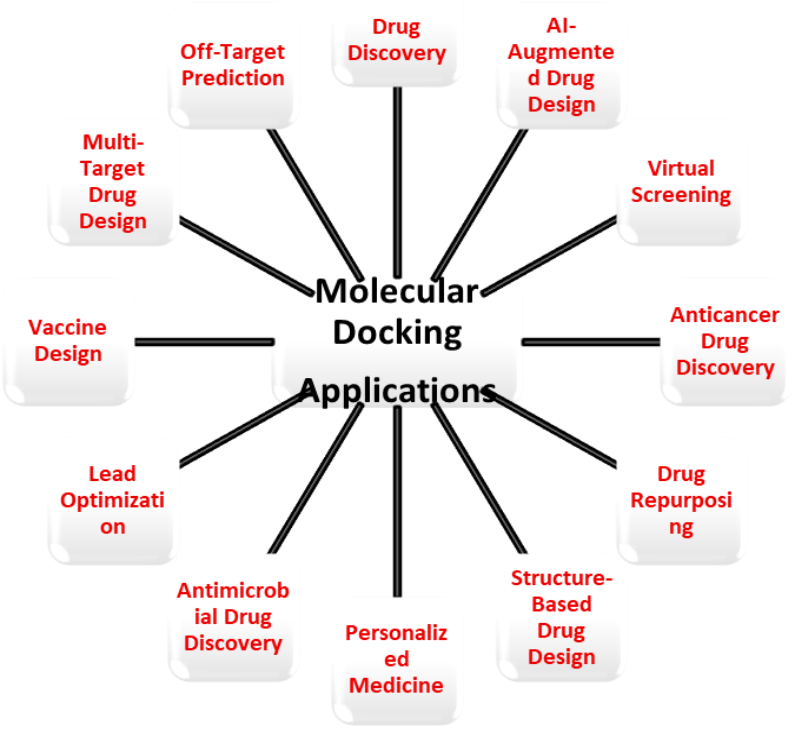

Figure 4: Applications of Molecular Docking in Drug Discovery and Development.

Challenges and Limitations of Molecular Docking

Despite significant advancements, molecular docking still faces several challenges that affect its accuracy, reproducibility and practical application in modern drug discovery. One of the major limitations is the inadequate prediction of binding affinity due to simplified scoring functions and incomplete representation of protein-ligand interactions. Current docking algorithms often fail to accurately model solvation effects, entropy, allosteric interactions and dynamic conformational changes of biomolecules.

Another critical challenge is protein and ligand flexibility. Many docking tools still treat receptors as rigid structures, whereas proteins frequently undergo conformational rearrangements during ligand binding. Similarly, insufficient conformational sampling of flexible ligands may lead to incorrect binding poses and unreliable docking outcomes.

The reliability of docking predictions is also limited by inaccuracies in scoring and ranking methods. High docking scores do not necessarily correspond to true biological activity and small score differences between compounds are often not meaningful. Consequently, molecular docking is more suitable for hypothesis generation and virtual screening than for precise quantitative prediction of binding free energies.

In AI-assisted docking workflows, dependence on large, high-quality datasets represents another important limitation.

Many machine learning models are trained on biased datasets dominated by well-studied protein families, reducing their ability to generalize to novel targets or rare molecular scaffolds. Furthermore, several AI models behave as “black boxes”, limiting interpretability, reproducibility and regulatory acceptance.

Computational demand is also a significant barrier. Advanced docking simulations, deep learning models and ultra-large virtual screening campaigns require high-performance computing infrastructure, GPU acceleration and substantial memory resources, making routine implementation difficult in resource-constrained environments.

Another major issue is interoperability and workflow reproducibility. Modern docking studies often combine multiple software tools for ligand preparation, docking, rescoring, visualization and post docking analysis. Differences in file formats, parameter setting and workflow design can reduce reproducibility and complicate cross platform integration.

Moreover, AI-based docking methods still face challenges related to physical realism and generalization. Recent benchmarking studies have shown that some deep learning approaches may generate physically implausible poses or fail when applied to unfamiliar targets outside their training distributions.

Overall, although molecular docking has become an indispensable tool in structure-based drug design, limitations related to scoring accuracy, molecular flexibility, computational cost, data bias, reproducibility and AI interpretability continue to restrict its full predictive potential. Continued development of hybrid approaches integrating docking, molecular dynamics, artificial intelligence and experimental validation is expected to improve the reliability and applicability of future docking workflows.[2,3,80,116]

AI Integration and Emerging Opportunities

Artificial Intelligence (AI) is rapidly transforming molecular docking by improving virtual screening, binding affinity prediction, and de novo drug design with greater speed and accuracy than convectional computational methods. Advanced deep learning, generative AI and graph neural network models are enabling the discovery of novel drug candidates and accelerating structure-based drug discovery workflows.[116]

One of the most promising future directions is the development of explainable AI (XAI), where techniques such as attention maps, SHAP and saliency analysis improve transparency and interpretability of docking predictions, thereby increasing trust and regulatory acceptance.[142]

Hybrid AI-physics frameworks integrating molecular docking, molecular dynamics and quantum mechanics are expected to provide more accurate and biologically realistic predictions by considering protein flexibility and dynamic molecular interactions.[116]

Generative AI and diffusion-based models are also revolutionizing ligand design by enabling real-time generation and optimization of novel molecular structures with improved pharmacological properties and target selectivity.[143]

Emerging technologies such as quantum computing, federated learning, digital twins and cloud-based AI platforms are expected to further accelerate molecular docking, enhance collaborative research, improve data security and support personalized medicine in future drug discovery pipelines.[144]

Future Perspectives in Drug Discovery

The future of drug discovery is moving from traditional computer-aided approaches towards fully AI-driven and computer-driven drug discovery systems. Advances in deep learning, protein structure prediction, molecular dynamics and high performance computing are expected to accelerate virtual screening, hit identification and lead optimization.[145]

Generative AI, graph neural networks and diffusion models may revolutionize ligand design by enabling rapid generation of novel molecules with improved pharmacological and ADMET properties, supporting precision and personalized medicine.[146]

Hybrid AI-physics models integrating molecular docking, molecular dynamics and quantum computing are expected to improve prediction accuracy, protein flexibility modelling and binding affinity estimation.[147]

Another major future direction is explainable and trustworthy AI, where techniques such as SHAP, saliency maps and attention mechanisms improve transparency, reproducibility and regulatory acceptance of AI-assisted drug discovery workflows.[148]

Cloud computing, federated learning and collaborative AI platforms are also expected to democratize access to advanced computational tools, enabling secure large-scale collaborative research and faster drug development.[148]

CONCLUSIONS

Molecular Docking has evolved into one of the most important tools in modern computer-aided drug discovery, significantly accelerating virtual screening, lead optimization and structure based drug design. The integration of artificial intelligence, machine learning, deep learning and advanced computational approaches has greatly improved docking accuracy, speed and predictive capability, transforming traditional drug discovery into a more data-driven and automated process.

Recent advancements such as AI-assisted scoring functions, generative molecular design, protein structure prediction, molecular dynamics integration and cloud-based computational platforms have expanded the potential of molecular docking beyond conventional applications. These technologies are enabling faster identification of novel drug candidates, improved prediction of protein-ligand interactions and the development of more personalized therapeutic strategies.

Despite these advancements, important challenges remain, including scoring inaccuracies, protein flexibility, limited interpretability of AI models, data bias, reproducibility concerns and high computational demands. Addressing these limitations through explainable AI, standardized benchmarking, hybrid AI-physics models and collaborative open-source frameworks will be essential for improving the reliability and real-world applicability of molecular docking workflows.

Overall, the convergence of molecular docking, artificial intelligence, structural biology and high-performance computing is expected to reshape the future of pharmaceutical research by making drug discovery faster, more accurate, cost-effective and increasingly personalized.

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