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A CRITICAL REVIEW ON MOLECULAR DOCKING: CURRENT SCENARIO AND FUTURE SCOPE

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ABSTRACT

Molecular docking is a computer-based method used to study how two or more molecules interact with each other. It plays an important role in computer-aided drug design and structural biology. With the help of this technique, scientists can test thousands of chemical compounds on computers instead of in labs. The results show how well each compound fits and binds to a target molecule, such as a protein. Recent developments in drug design, especially for anti-infective medicines, have made molecular docking even more valuable. It helps researchers design new drugs based on the 3D structure of molecules. Docking predicts the best way molecules can fit together and how strongly they might bind. The quality of results depends on how accurately the input structures are prepared and on the sampling and scoring methods used. New software tools, like Local Move Monte Carlo, have improved the flexibility and accuracy of docking by allowing more realistic receptor movements. Overall, molecular docking helps scientists understand how ligands (small molecules) interact with proteins (targets). It is a reliable and efficient part of modern drug discovery, making it easier to find promising drug candidates and test large libraries of compounds quickly.

KEYWORDS: Molecular docking, Ligand, Receptor, Drug design, Docking tool, Mechanism of docking, Protein.

INTRODUCTION

Molecular docking is a commonly used method in molecular modeling that helps predict how one molecule attaches to another to form a stable complex. This process is shown in Figure 1.[1] It is an important part of structure-based drug design because it can predict how small molecules, known as ligands, fit into the binding sites of target proteins. Because of its usefulness, docking has become a popular and essential tool in drug discovery. Measuring how strongly molecules bind to each other is very important in developing new drugs and understanding basic biochemical processes.[2] The main goal of docking research is to predict the most likely three-dimensional structures formed when molecules interact. Docking software automatically finds the best positions for molecules to fit together. Today, there are many different computational methods and tools available for performing molecular docking studies.[3,4] In the field of molecular modeling, docking is a method used to predict how one molecule interacts with another to form a stable complex.[1] The information about the preferred orientation or direction of binding helps researchers estimate the binding strength or affinity between the two molecules.

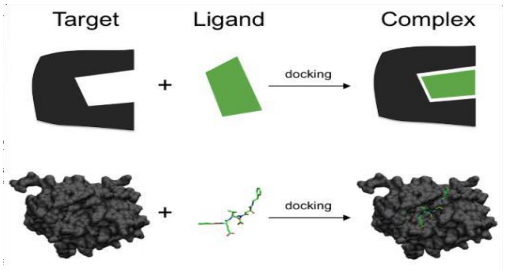

Fig. 1: Schematic diagram of docking a undersized molecule ligand (green) to a protein target (black) produce a steady compound.

Types of Docking

There are 2 types of docking(fig.2)

1. Rigid docking
2. Flexible docking

1. Rigid docking

In this type of docking, both the receptor and ligand molecules are treated as rigid structures. The process involves finding the best 3D orientation of one molecule so that it fits most effectively with the other, based on a scoring function. The ligand's structure or conformation can be generated either without considering the receptor or by including the receptor's binding site during the analysis**.**

2. Flexible docking

In this type of docking, both the ligand and the receptor can move, making the process flexible. During docking, the energy is calculated for each possible rotation or position. The surface interaction between the molecules is also measured After evaluating all the positions, the most stable and best-fitting binding pose is selected.[7]

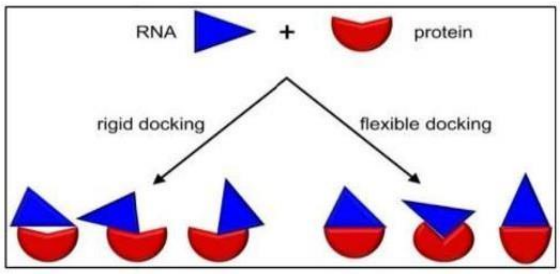

Fig. 2: Rigid and flexible docking.

Application of molecular docking Hit Identification

Molecular docking, along with a scoring function, helps in quickly screening large numbers of chemical compounds on a computer to find those that can strongly bind to a particular biological target such as a protein or enzyme. This process helps identify potential drug candidates at an early stage, saving time and cost compared to laboratory testing.

Lead Optimization

Docking also predicts how and where a ligand (a small molecule) fits into the active site of a protein — known as its binding pose. By understanding this interaction, scientists can modify the chemical structure of the ligand to improve its strength, selectivity, and effectiveness, creating a better version of the drug candidate.

Bioremediation

Molecular docking is used to study enzymes that can break down or remove pollutants from the environment. It helps identify how enzymes interact with harmful molecules, making it possible to design or select enzymes that can effectively clean up contaminated soil or water. It can also study protein–protein interactions important for biological restoration processes. (fig.3)

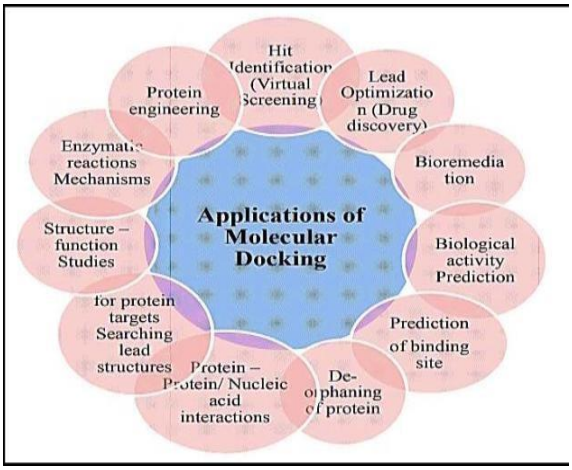

Fig. 3: Application of molecular docking.

Mechanism of molecular docking

The protein sequence is the first and most important requirement before starting a docking study. The 3D structure of the protein is generally determined using biophysical techniques such as *X-ray crystallography* or, in some cases, *Nuclear Magnetic Resonance (NMR) spectroscopy*.

In molecular docking, the software uses the protein's structural information and a database of chemical compounds as input data. The overall performance of the docking process depends mainly on three essential factors:

1. Search Algorithm – determines how different ligand positions and orientations are explored within the active site.
2. Scoring Function – evaluates and ranks the binding strength between the ligand and the protein, and
3. Docking Software – the computational tool that executes the entire docking process.[8]

Step I – Preparation of Protein

The process begins by obtaining the 3D structure of the target protein from the Protein Data Bank (PDB), an online structural database.

After downloading, the protein model needs to be cleaned and refined. This includes

- Removing all unnecessary water molecules.
- Adding hydrogen atoms to stabilize the structure.
- Filling missing residues.
- Assigning proper charges to atoms. This step ensures that the protein is in a suitable and accurate form for docking analysis.

Ligands can be downloaded from chemical databases such as ZINC or PubChem, or they can be manually designed using molecular drawing tools like *ChemSketch*.

Before docking, every ligand must be checked using Lipinski's Rule of Five, which helps determine whether a compound is likely to be a good drug candidate.

According to Lipinski's rule, a potential drug molecule should have

- No more than 5 hydrogen bond donors.
- Fewer than 10 hydrogen bond acceptors.
- Molecular weight below 500 Daltons.
- LogP value (lipophilicity) of less than 5.
- Molar refractivity between 40 and 130.[9]

Step III – Grid Generation

After preparing the protein and ligand, a grid box is created around the protein's active site. This grid defines the area where the ligand can move and bind during the docking process.

Important parameters such as position, rotatable bonds, and excluded volumes are fixed. The genetic algorithm parameters— including *crossover*, *mutation*, and *migration*—are used to improve accuracy when predicting the most suitable binding site.

Step IV – Active Site Prediction

The active site of the protein is then identified. This is the specific region on the protein where the ligand binds.

A protein may have multiple binding sites, but the one that plays a major role in biological activity is chosen for docking. Any water molecules or heteroatoms that do not participate in binding are usually kept inactive during this stage.[10]

Step V – Docking Process

Once both the protein and ligand are ready, the docking simulation is carried out. During docking, the software tries several orientations and conformations of the ligand in the active site to find the best possible fit.

Each position is scored based on its binding energy, and the pose with the lowest energy (most stable interaction) is selected as the best docking result.

Molecular docking approaches

1. Monte Carlo Approach

This approach generates random conformations of the ligand by changing its position, orientation, and structure within the active site of the target protein. Each new structure (configuration) is scored to estimate how well it fits. Using the Metropolis criterion, the system decides whether to accept or reject the new configuration. This helps the program explore many possible orientations and find the most stable one.

2. Metropolis Criterion

In this method, if a new conformation gives a better (higher) docking score than the previous one, it is automatically accepted. If it's worse, a Boltzmann probability function is used to check whether it should still be accepted (to avoid getting stuck in a local minimum). If the new structure passes this test, it's kept; otherwise, it's rejected. This allows both exploration and optimization of binding poses.

3. Matching Approach

This method focuses on complementarity between the ligand and receptor.

The ligand's atoms are positioned at the most suitable sites within the protein's binding pocket.

The final ligand–receptor complex may then undergo energy minimization or refinement to achieve a more accurate binding pose.

4. Ligand Fit Approach

This is a fast and reliable method for placing small ligand molecules into the active site of a protein. It analyzes the shape and size compatibility between the ligand and the binding pocket to predict the best docking pose. This approach is often used in high- throughput docking studies.

5. Point Complementarity Approach

This technique evaluates how well the shape and chemical features of the ligand and protein match each other.

It studies spatial alignment and interaction points like hydrogen bonds or hydrophobic contacts to identify the most compatible orientation.

6. Fragment-Based Method

In this approach, the ligand is divided into smaller fragments. Each fragment is docked individually into the protein's binding site. After determining the best positions, the fragments are linked together to form the complete ligand structure. This helps design new lead molecules by combining optimal binding fragments.

7. Distance Geometry Method

This method uses distances between atoms or molecular groups (intra-and intermolecular). These distances are used to build a 3D structure of the molecule that fits the experimental or theoretical distance data. It's useful for predicting possible conformations of ligands and proteins.

8. Blind Docking

Blind docking searches for potential binding sites without prior knowledge of the active site.

It scans the entire protein surface to find possible locations where the ligand can bind. This is particularly useful when the binding pocket is unknown or when exploring allosteric sites.

9. Inverse Docking

In this approach, a single ligand is docked into multiple protein targets.

It helps identify which proteins a drug might interact with — predicting off-target effects, toxicity, or side effects. This method is valuable for drug repurposing and toxicity prediction studies.

Theory of molecular docking

It mainly involves two key stages: Sampling Algorithm and Scoring Function.[14]

1. Sampling Algorithm

During molecular docking, a ligand can bind to a receptor in many possible ways, as both molecules can move and change shape.

Each molecule has six degrees of freedom — three for translation (movement in space) and three for rotation — along with many possible internal conformations.

Because of this, testing every possible configuration would require enormous computational power, so sampling algorithms are used to efficiently search for the best binding poses.

1. Matching Algorithms

These algorithms match the shape and chemical features of a ligand to the binding pocket of a protein.
They find the best geometric and chemical complementarity between the two molecules.
Common software that uses this approach includes DOCK, FLOG, LibDock, and SANDOCK.[16,17]

2. Incremental Construction Methods

In this approach, the ligand is built step by step inside the active site rather than docking it as a whole molecule.

Each fragment of the ligand is placed and optimized progressively, allowing better flexibility and accuracy.
Programs such as DOCK 4.0, FlexX, Hammerhead, SLIDE, and eHiTS use this incremental building strategy.

3. Monte Carlo Methods

The Monte Carlo approach generates random conformations of the ligand by rotating bonds or moving the molecule through translations and rotations.

Each new position is evaluated based on its energy value, and only favorable conformations (with lower energy) are selected.

This helps in exploring a wide range of possible ligand orientations.

Monte Carlo techniques are implemented in programs like AutoDock, ICM, QXP, and Affinity.

4. Genetic Algorithms

Genetic algorithms (GAs) are stochastic optimization techniques inspired by biological evolution.

They work by generating multiple ligand poses (a population), selecting the best ones, and combining their features through mutation and crossover to improve results over generations.

This process continues until the most stable ligand–protein binding mode is found.

Genetic algorithms are used in docking programs such as AutoDock.

2. Scoring Function

The scoring function in molecular docking is used to evaluate and rank the different ligand poses generated during docking.

Its main purpose is to identify the most accurate binding pose of a ligand and distinguish active binders (that interact strongly) from inactive compounds (that do not fit well). However, scoring functions only estimate how well a ligand binds to a protein; they do not give an exact prediction of the true binding affinity.

Because of the complexity of molecular interactions, scoring functions make several assumptions and simplifications to perform calculations quickly and efficiently.

Based on how they calculate the interaction energy, scoring functions are generally divided into three main categories:

1. Force-Field-Based Scoring

Uses physical energy terms such as van der Waals forces, electrostatic interactions, and bond energies. Estimates the total energy of the ligand– protein complex using classical molecular mechanics equations. Helps identify poses with the lowest potential energy, which indicates a stable binding configuration.

2. Empirical or Theoretical Scoring

Based on experimental data or regression models that relate certain interaction features (like hydrogen bonds, hydrophobic contacts, etc.) to known binding affinities. Parameters are determined from a large set of experimentally measured complexes.

3. Knowledge-Based Scoring

Derived from statistical analysis of known protein–ligand complexes available in structural databases (like PDB). Uses observed interaction frequencies between atoms to estimate how likely a ligand is to bind at specific sites. Provides a data-driven approach to scoring rather than relying purely on physics or empirical data.[19]

Model of molecular docking

1. Lock and Key Model

The Lock and Key Model was proposed by Emil Fischer in 1894 to explain how enzymes or proteins interact with their specific substrates or ligands.

According to this model, both the enzyme's active site and the ligand (or substrate) have specific and complementary shapes — similar to how a key fits perfectly into a lock.

In this model, the active site of the enzyme (or receptor) is considered rigid and pre- shaped, allowing only a specific ligand with a matching shape to bind.

When the correct ligand enters the binding site, it forms a stable enzyme–substrate or receptor– ligand complex through non- covalent interactions such as hydrogen bonds, ionic forces, and van der Waals interactions.

Because of its fixed shape, this model explains the high specificity of enzyme and receptor actions — meaning only one or a few ligands can bind effectively.

However, the Lock and Key Model does not account for flexibility or structural changes in the protein during binding, which are explained better by the Induced Fit Model.(fig.4)

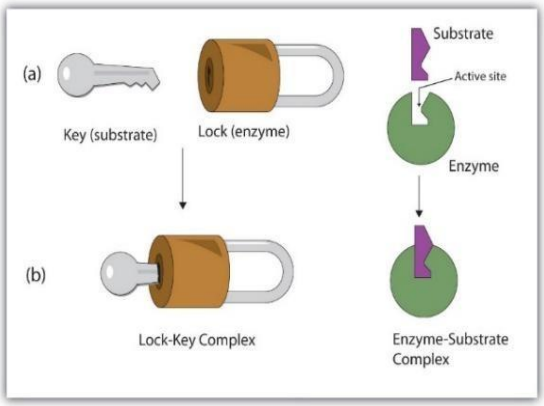

Fig. 4: Lock and key theory.

2. Induced Fit Model

The Induced Fit Model was proposed by Daniel E. Koshland in 1958 as an improvement to the Lock and Key Model.

This model suggests that the active site of the enzyme or receptor is flexible, not rigid. When a ligand (or substrate) approaches the binding site, the enzyme changes its shape slightly to allow a better fit.

This adjustment ensures stronger binding and greater catalytic efficiency.

The shape of both the enzyme and the ligand becomes complementary only after interaction, not before. This model explains how enzymes can sometimes bind to structurally similar ligands and how conformational changes occur during the binding process.

It also reflects a more realistic, dynamic interaction between proteins and ligands as seen in biological systems.(fig.5)

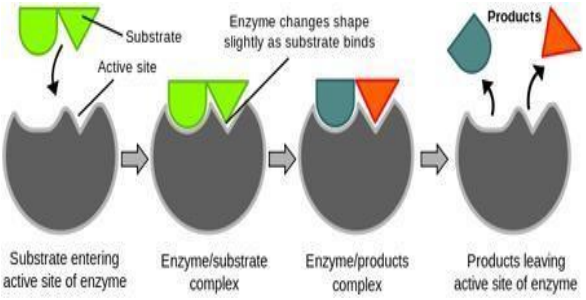

Fig. 5: Induced fit theory.

Current Scenario of Molecular Docking

Molecular docking is an important computer-based technique used in drug discovery and structural biology to predict how a small molecule (ligand) binds to a larger biomolecule, such as a protein or enzyme. In the current era, molecular docking has developed greatly because of improvements in computer speed, software design, and artificial intelligence. Modern docking tools such as AutoDock, AutoDock Vina, and Glide have become faster, more accurate, and user-friendly. The integration of machine learning (ML) and artificial intelligence (AI) has helped improve the prediction of ligand–receptor interactions, allowing researchers to identify potential drug candidates more efficiently. These advancements have also helped reduce the time and cost involved in the drug development process. Another major change is the introduction of cloud-based docking platforms, which allow scientists worldwide to perform complex docking studies without the need for expensive local hardware. Molecular docking is no longer limited to small molecule–protein studies; it now also includes protein–protein docking, protein–nucleic acid docking, and binding kinetics studies. During global health challenges, such as COVID-19, molecular docking played a major role in identifying potential antiviral compounds and understanding how drugs interact with viral proteins. Overall, molecular docking continues to evolve rapidly and is now a core tool in research areas like drug design, molecular mechanism studies, and computational biology. With the ongoing use of AI, big data, and high-performance computing, docking is becoming even more accurate, accessible, and essential for modern biomedical research.[18,19]

Challenges in Molecular Docking

1. **Scoring Functions** One of the major obstacles in molecular docking is the accurate estimation of binding affinity. Existing scoring functions often fall short because they do not fully consider important thermodynamic factors like solvation, enthalpy, and entropy. To overcome this, researchers are working on developing improved scoring models that can provide a more realistic representation of molecular interactions.

2. **Conformational Flexibility** Proteins and ligands are not rigid structures; they can change shape and orientation during interactions. Capturing this flexibility is essential for accurate docking

predictions. Techniques such as molecular dynamics simulations and ensemble docking are increasingly used to explore multiple conformations and enhance docking accuracy.

3. **Solvent Effects** The influence of water molecules and ions plays a crucial role in molecular binding. Accurately simulating solvent effects remains a challenge because solvent interactions can significantly alter binding behavior. New computational approaches, including implicit and explicit solvent models, are being developed to better mimic real biological conditions.

4. **Sampling Efficiency** The search for the optimal ligand-receptor binding pose requires exploring a large number of possible configurations. This process can be computationally demanding. To improve efficiency, advanced algorithms like Monte Carlo methods and genetic approaches are applied to sample the conformational space more effectively and identify the best docking orientations.

5. **Membrane Proteins** Docking studies involving membrane proteins are particularly complex due to their interaction with lipid bilayers and the unique environment they inhabit. Specialized computational tools and techniques are being created to handle the challenges of modeling these proteins while maintaining their structural and functional integrity.

Emerging Trends in Molecular Docking

1. Machine Learning Integration

Machine learning and deep learning are now being used in molecular docking to make results more accurate. These techniques analyze large amounts of experimental data to improve scoring functions and predict how well a ligand will bind to a protein.

2. Free Energy Calculation

Recent progress in free energy calculation methods has made it easier to predict binding strength more precisely. Approaches like thermodynamic and alchemical integration are becoming more common and accessible for researchers.

3. AI-Driven Drug Discovery

Artificial intelligence is playing a major role in modern drug discovery. Molecular docking is now part of AI-based systems that can identify new drug candidates, check for possible side effects, and predict how the drug will behave inside the body (ADMET – absorption, distribution, metabolism, excretion, and toxicity).

4. Fragment-Based Docking

This method focuses on using small molecular fragments instead of complete compounds. It helps in quickly screening fragment libraries to find new starting points for drug design and develop novel lead compounds.

5. Cryo-EM Integration

Combining molecular docking with cryo- electron microscopy (cryo-EM) allows scientists to study large biological molecules in great detail. This integration helps determine high-resolution structures and understand complex molecular interactions better.

Upcoming Difficulties, Future Initiatives, and Perspectives in Molecular Docking

Molecular docking is an essential computational approach widely used in drug discovery, bioinformatics, and structural biology to study how small molecules (ligands) interact with biological macromolecules (receptors). Although it has contributed significantly to understanding molecular recognition and drug design, several upcoming challenges and research directions continue to shape its evolution.

1. Improved Accuracy and Precision

Achieving higher accuracy in docking predictions remains a persistent challenge. Many current algorithms face limitations in correctly estimating binding affinities and identifying the most favorable ligand binding poses. Future research aims to develop enhanced scoring functions and advanced sampling algorithms that can improve prediction precision while reducing computational error.

2. Incorporating Flexibility

Biological macromolecules are not static; they exhibit conformational flexibility during ligand binding. Conventional docking methods often treat proteins as rigid structures, which can lead to inaccurate predictions. Integrating molecular dynamics (MD) simulations and conformational ensemble approaches can help capture the dynamic nature of both ligands and receptors, improving docking reliability.

3. Protein–Ligand–Water Interactions

Water molecules play a crucial role in stabilizing protein–ligand complexes. However, accurately modeling these interactions is still a major hurdle. Future efforts focus on predicting the location and energetics of water molecules during docking simulations, using improved solvent models and hybrid quantum–mechanical approaches to refine binding energy estimations.

4. Integration of Machine Learning and Artificial Intelligence

The incorporation of machine learning (ML) and artificial intelligence (AI) into molecular docking is revolutionizing prediction accuracy. AI models can analyze large datasets to optimize scoring functions, predict binding affinities, and automate docking workflows. These intelligent systems can significantly reduce computation time and increase prediction robustness.

5. Multi-Target Docking Approaches

In complex diseases involving multiple biological pathways, a single drug often interacts with more than one target. Multi- target docking aims to evaluate ligand binding across multiple proteins simultaneously. This approach supports polypharmacology and network pharmacology, enabling the design of multitargeted therapeutics.

6. Virtual Screening and Drug Repurposing

Molecular docking continues to be a cornerstone of virtual screening for large chemical libraries and drug repurposing efforts. Future developments will emphasize high-throughput docking, cloud-based computing, and improved ranking algorithms to accelerate the identification of potential lead compounds.

7. Personalized Medicine Applications

The integration of molecular docking with genomic and proteomic data can enhance personalized drug design. Future docking methods aim to predict how individual genetic mutations influence drug binding and therapeutic response, facilitating patient-specific treatment strategies.

8. Accessibility and User- Friendliness

For broader scientific adoption, docking software must become more accessible to non-specialists. Future initiatives focus on intuitive graphical user interfaces, web- based platforms, and cloud-based computational tools, allowing researchers with limited computational expertise to perform docking studies efficiently.

9. Utilization of Big Data and Structural Databases

The rapid expansion of structural databases such as the Protein Data Bank (PDB) and the rise of big data analytics present opportunities to enhance docking performance. By integrating AI-driven data mining with structural repositories, researchers can refine docking algorithms and identify novel binding trends.

10. Ethical and Regulatory Aspects

As AI becomes increasingly embedded in molecular docking and drug discovery, ethical considerations regarding data usage, model transparency, and bias must be addressed. Moreover, regulatory frameworks will need to adapt to evaluate drugs identified through computational predictions before clinical implementation.

CONCLUSION

Molecular docking is a powerful and useful tool in the field of drug design and discovery. It helps researchers and medicinal chemists easily study and visualize how small molecules interact with target proteins. This technique can accurately predict how a ligand fits and binds to a receptor, which saves both time and research costs.

Molecular docking plays an important role in developing new medicines by helping to identify and improve lead compounds before laboratory testing. However, some challenges still exist, such as optimizing lead molecules, studying complex biological pathways, and designing entirely new drugs from scratch.

Overall, this review highlights how molecular docking contributes greatly to modern drug research. It has been successfully applied in the study of diseases like malaria, heart failure, cancer, and various infectious disorders, showing its potential to accelerate the discovery of effective and safer treatments in the future.

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