Molecular Docking and Simulation in Drug Discovery: A Review

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ABSTRACT

Drug discovery is a complex, time-consuming, and costly process that requires the identification and optimization of potential therapeutic compounds. In recent years, computational approaches such as molecular docking and molecular dynamics (MD) simulation have significantly transformed modern drug design. These techniques, which fall under the domain of Computer-Aided Drug Design (CADD), provide efficient and cost-effective strategies for analyzing molecular interactions and predicting drug behavior.Molecular docking is widely used to predict the binding orientation and affinity of ligands toward target proteins, thereby facilitating the identification of promising lead compounds. On the other hand, molecular dynamics simulation provides detailed insights into the structural flexibility, stability, and dynamic behavior of biomolecular systems under physiological conditions. Additionally, structure-based and ligand-based drug design approaches further enhance the efficiency of identifying and optimizing drug candidates.The integration of molecular docking with MD simulation has emerged as a powerful strategy, combining the speed of docking with the accuracy of dynamic simulations. This combined approach improves the reliability of predicting protein-ligand interactions and reduces the need for extensive experimental validation. Overall, these computational tools play a crucial role in accelerating the drug discovery process, minimizing costs, and enhancing the success rate of developing effective therapeutic agents.

INTRODUCTION

Drug discovery involves identifying new therapeutic compounds and bringing them to market. Traditional methods are costly and time-intensive computational techniques; particularly, molecular docking and molecular dynamics (MD) simulation have emerged as an essential tool in modern drug design. These approaches fall under computer-aided drug design (CADD), which accelerates the identification and optimization of lead compounds.[1]

Molecular docking works on the principle of “lock and key” or “induced fit” theory

- The proteinacts as the lock.
- The ligand acts as the key.

The docking software predicts how well the ligand fits into the active site of the protein and calculates a binding energy (docking score).

Lower (more negative) binding energy indicates stronger binding affinity and better stability of the complex.

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Two or more molecular structures that fit together are called a molecular docking.

Molecular docking = Target + Ligand as shown in Fig. 1[2]

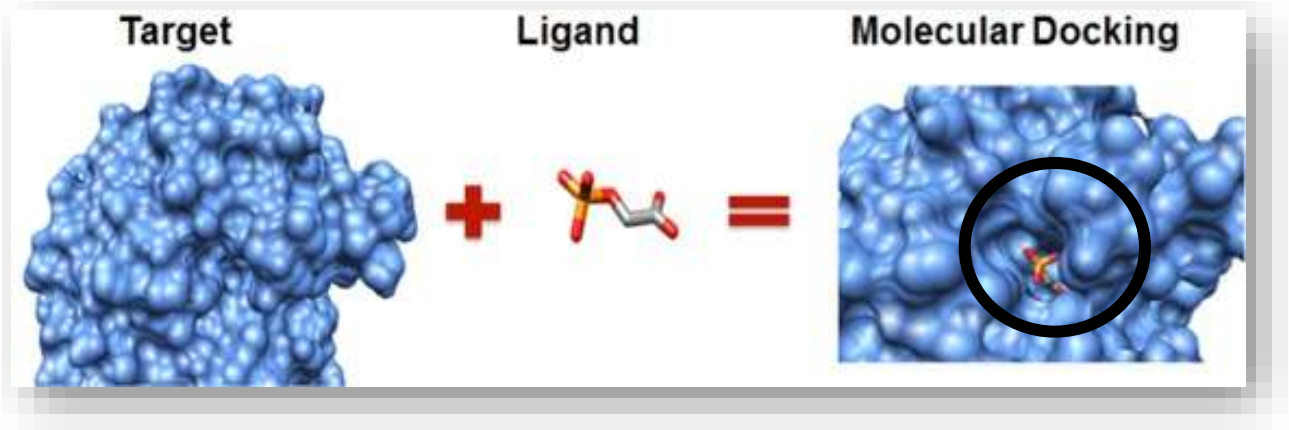

Fig:1 Molecular docking

Computer-aided drug design (CADD) techniques have been widely utilized in drug discovery over the past two decades.[3]Approaches such as molecular modeling, molecular docking, and simulation were initially based on the assumption of a rigid interaction between the receptor and ligand, supported by computational tools. Molecular docking primarily focuses on understanding how two or more molecular entities-such as proteins or enzymes, nucleic acids, and small drug molecules-interact and fit together.[4] Different types of docking, including protein-ligand (small molecule), protein-nucleic acid, and protein-protein docking, are crucial for predicting the orientation and binding affinity of a ligand within the active site of a target protein. These studies provide valuable insights into the intermolecular interactions occurring between small molecules and the binding site of the target receptor.[5]

Molecular Docking Studies

Molecular docking is a computer-aided drug design (CADD) technique used to predict the interaction between a small molecule (ligand) and a target protein (receptor). It helps in identifying the binding orientation, binding affinity, and stability of a ligand–protein complex. Docking studies are widely used in drug discovery to design new compounds with potential antimicrobial, anti-inflammatory, anticancer, and antiviral activities. Molecular docking is a computational technique used to predict the interaction between a small molecule (ligand) and a target protein (receptor). It is widely used in drug discovery, especially for studying compounds like 1,2,4-triazole derivatives.

Recent Comparative Studies

As we know the number of programs available on the market, the aim should be to achieve the accuracy of the objective of the project based on the choice of docking tool for virtual screening of corporate libraries consisting of millions of compounds. The key criterion is a reasonable timeframe. The consumer will start with a fast tool, followed by more detailed ones. Similarly, simple ligand docking aiming at Project De Novo of drugs and their optimization requires the use of a more accurate tool.

It's not easy when compared with protein-ligand docking systems. Each program has advantages and disadvantages in terms of docking accuracy, ranking accuracy, and computational time consumption. But in recent comparisons, some general strengths and disadvantages of existing docking devices can be found.

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Computer-Aided Drug Design.

Computer-aided drug design (CADD) is a computer-based technique used in computational chemistry to discover, design, and study drugs and other biologically active molecules[6]. It plays a crucial role in modern drug discovery by facilitating the development of new therapeutic agents through a deeper understanding of the chemical and biological properties of ligands and their corresponding targets. This approach enables the identification and optimization of novel drug candidates by employing advanced computational tools, including in silico screening and predictive modeling.

Such techniques allow early evaluation of undesirable properties, such as low biological activity, poor pharmacokinetic profiles, and potential toxicity, thereby reducing the risk of late-stage failure. Furthermore, it supports the optimization of drug targets and the identification of promising hits through the use of chemical scaffolds and virtual screening strategies, ultimately accelerating the discovery of effective and safe drug molecules [7].

Structure-Based Drug Design

Structure-based drug design (SBDD), as shown in Fig 2,relies on detailed knowledge of the three-dimensional structure of the target protein to evaluate and calculate interaction energies with potential drug candidates.Structural databases contain crystallized forms of target proteins, which are used as templates for designing new compounds. The primary objective of structure–based design is to develop molecules that bind specifically, strongly, and with minimal energy to the target site.[8]

A broader concept associated with this approach is virtual high-throughput screening, a computational technique used to screen large libraries of chemical compounds for potential biological activity.[9] The application of computational tools during the lead optimization phase of drug development is highly beneficial and cost-effective. These tools assist in hit-to-lead optimization by reducing the number of compounds that need to be synthesized and experimentally tested in vitro, thereby saving time and resources.[10]

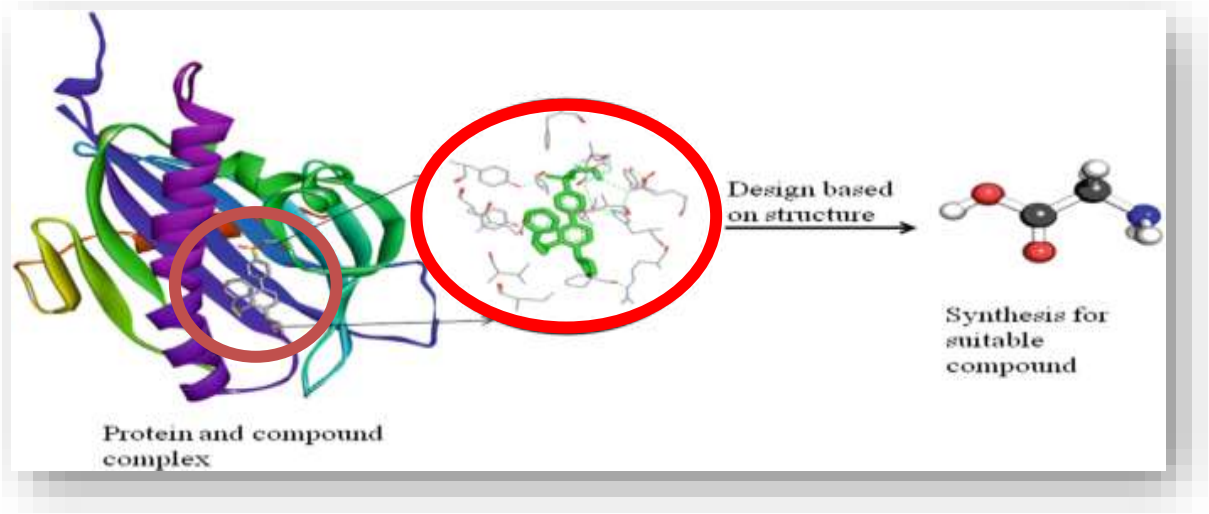

Fig 2 Structure-based drug design

Ligand-Based Drug Design

Ligand-based drug design (LBDD), as shown in Fig 3, utilizes information from known active and inactive compounds to identify new drug candidates. It mainly relies on techniques such as chemical similarity searching and quantitative structure-activity relationship (QSAR) analysis. This approach is especially useful when the three-dimensional structure of the target protein is not available.[11]

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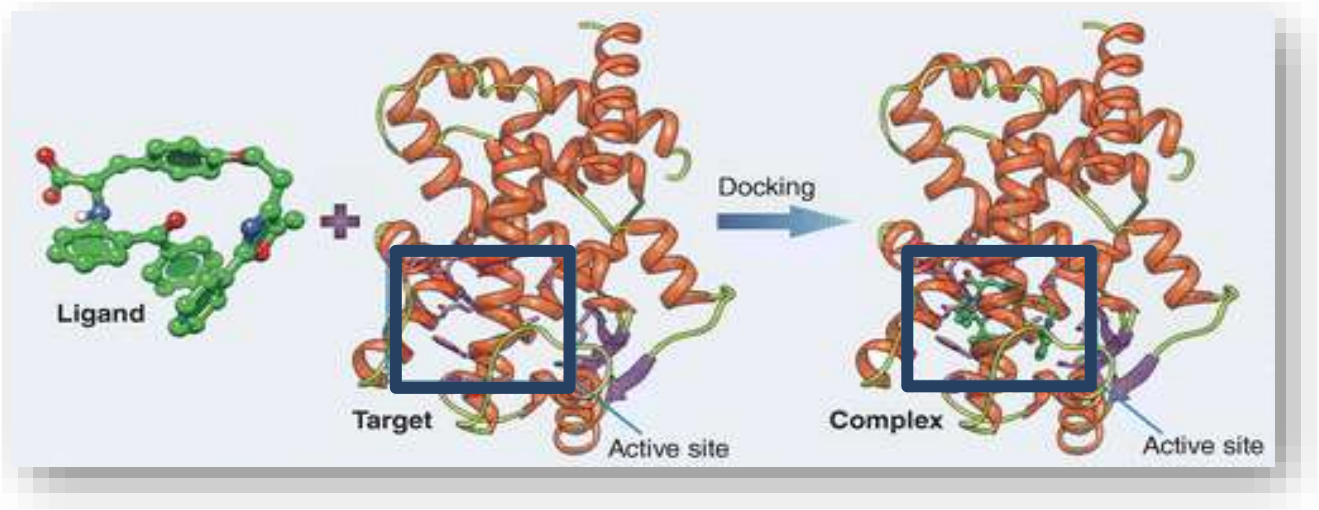

Fig 3 Ligand-based drug design

Types of Molecular Docking

Molecular Docking can be Broadly Classified into two main Types: -

Rigid docking: In rigid docking, mentioned in Fig 4, both the ligand and the receptor are considered as fixed structures with no flexibility. This approach simplifies the calculations, making the process faster and less computationally demanding. However, it does not fully capture the dynamic behavior of molecules during binding. Rigid docking is most appropriate when the ligand and the binding sites of the receptor are known to undergo little or no conformational changes [12].

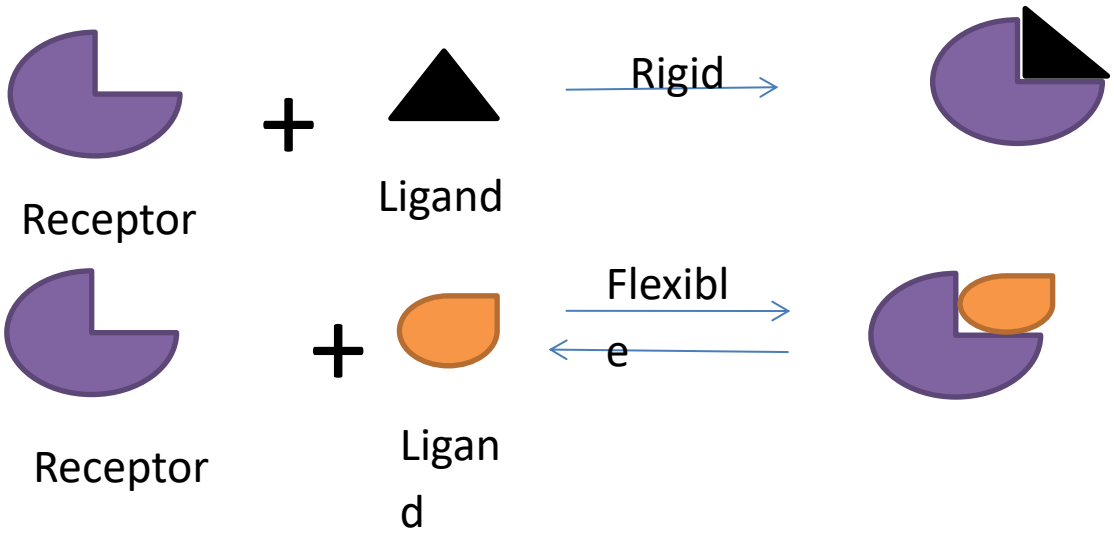

Fig 4 Rigid and Flexible docking

Semi-Flexible Docking: This method allows the ligand to change shape or conform during docking, while the receptor remains static. It strikes a practical balance between speed and precision and is frequently used in large-scale virtual screening studies.

Flexible docking: Flexible docking, in contrast, mentioned in Fig 2, allows the ligand to adopt multiple conformations, and in some advanced methods, the receptor can also exhibit limited flexibility. This results in a more accurate and realistic simulation of molecular interactions. Ligand flexibility is typically achieved by

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exploring various conformations, while receptor flexibility may involve adjustments in side chains or the use of induced-fit models.[13]

Molecular docking process

Step 1: Protein Preparation

The three-dimensional structure of the selected target protein is retrieved from the Protein Data Bank (PDB). The protein is prepared by removing water molecules and any co-crystallized ligands, adding missing hydrogen atoms, assigning appropriate charges, and saving the structure in the required docking format.

Step 2: Ligand Preparation

The chemical structure of the ligand (e.g., synthesized compound) is drawn using chemical drawing software and converted into a 3D structure. The molecule is then energy minimized to obtain a stable conformation, hydrogen atoms are added, charges are assigned, and the file is saved in a compatible format for docking.

Step 3: Grid Box Setting

A grid box is defined around the active site of the protein to specify the region where docking will occur. The grid center coordinates (x, y, z) and dimensions are set to cover the binding pocket properly.

Step 4: Docking Simulation

Docking is performed using software such as AutoDock Vina. The program generates multiple binding poses of the ligand within the active site and calculates binding affinity values (kcal/mol) for each pose.

Step 5: Result Analysis

The best docking pose is selected based on the lowest binding energy. The protein-ligand interactions, including hydrogen bonds, hydrophobic interactions, and amino acid residues involved, are analyzed to evaluate the potential biological activity of the compound.

Molecular docking software

Molecular docking software plays a vital role in the evolving field of computational biology and drug discovery. It enables researchers to simulate and predict how small molecules interact with target proteins, providing a clear understanding of molecular binding mechanisms.[14] Using advanced algorithms, this software evaluates binding strength, identifies possible binding patterns, and offers valuable insights that help make the drug development process more efficient and effective.[4] Some of the software used in molecular docking are shown in Table 1

Table 1:Software Used In Molecular Docking

S. no	Software's	Application
1.	Autodock Vina	Docking
2.	Discovery Studio	Visualization tools
3.	Open Babel	Files transferred and Preparation of Ligand
4.	PyMol	Visualization and Interaction Study
5.	Chimerax	Visualization tools
6	GROMACS SOFTWARE[15]	Biomolecular Simulation[16]

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Application of Molecule Docking

Applications of molecule docking are as follows: Computational and integrative approaches play a significant role across multiple domains of pharmaceutical and biotechnological research, including target identification and validation, lead compound identification, and subsequent lead optimization to enhance efficacy and safety. These methods also contribute to bioremediation by enabling the design and analysis of biological systems for environmental detoxification.

Additionally, predictive tools are widely used for biological activity prediction and binding site identification, facilitating a better understanding of ligand-target interactions. Advanced computational strategies further assist in the de-orphaning of proteins by assigning functions to previously uncharacterized proteins. Moreover, such approaches support protein engineering efforts to design proteins with improved or novel functions, as well as the elucidation of enzymatic reaction mechanisms at the molecular level. Beyond drug discovery, these technologies are also applied in the production and development of nutraceuticals, thereby expanding their impact across healthcare and environmental applications [17], [18], [19], [20].

Definition of Simulation

Simulation technology is a technique used to forecast future outcomes by imitating real-world systems, processes, or events. It is widely applied in areas such as military operations, business management, public policy, and many other sectors, making it a valuable tool for decision-making and risk evaluation.[21]

Simulation technology involves the use of computer-based models and tools to replicate the behavior and development of complex systems.[22] Defining initial conditions, parameters, and governing rules, it helps predict possible outcomes and assess the impact of different decision –making strategies. It is a comprehensive approach that combines qualitative insights with quantitative analysis, integrating expert knowledge with data-driven methods.[23]

Early Development of Simulation

The origins of modern simulation technology can be traced back to the use of operations research during World War II, where it was applied to solve complex military problems. With the advancement of computers in the 1950s, researchers began utilizing Monte Carlo simulation techniques to build and analyze military models. In 1957, the U.S. Air Force initiated the “Linear Programming-400 Project,” which marked an important step toward computer-assisted analysis of military operations.[3]

During the 1960s, several important theories, including game theory and inventory theory, were incorporated into military simulation. At the same time, in the business sector, IMB’s Geoffrey Gordon developed GPSS(general-purpose simulation system).

Over time, the development of advanced approaches such as system dynamics, agent-based modeling, and object-oriented simulation languages significantly expanded the application of simulation technology across various industries, making it a powerful tool for decision-making and system analysis.[24]

Molecular Dynamics Simulation

Molecular dynamics (MD) is a computational simulation technique used to study the structure, motion, and thermodynamic behavior of molecular systems,as shown in Figs. 5 and 6.These systems usually include biomolecules like proteins, enzymes, or lipid membranes placed in a water or electrolyte environment.[24] Molecular DynamicsSimulation typically beginswith experimentally determinedstructures available in the Protein Data Bank (PDB). If such structures are not available, they can be predicted using methods like homology or comparative modeling.[3] In all atoms is calculated using Newton’s law of motion over small time steps (1-2 femtoseconds).

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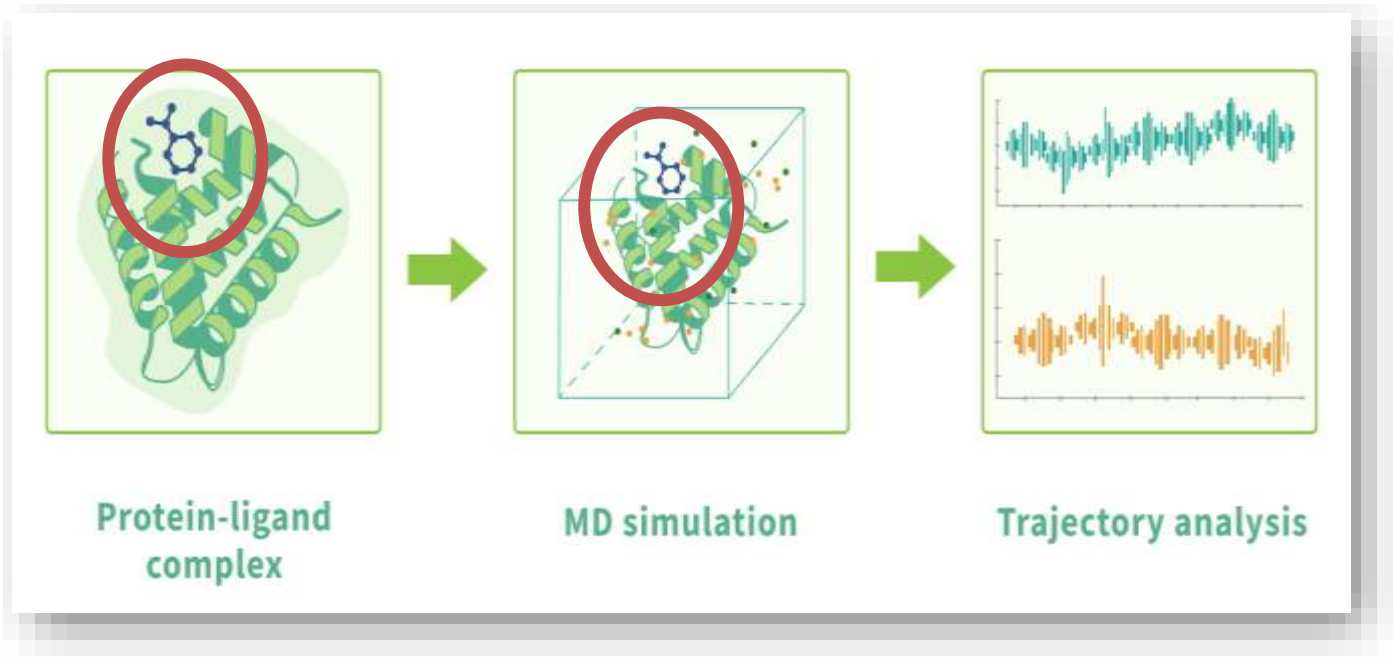

Fig 5 Molecular dynamics simulation

Algorithms such as velocity-verlet or leap-frog are used to update the positions and velocities of atoms. The forces acting on atoms are calculated using a force field, which includes bonded interactions (bonds, angles, dihedrals) and non - bonded interactions (electrostatics and van der Waals forces). These force fields help maintain the structural stability of the biomolecules.[25] Simulations are usually performed under constant temperature and pressure. To mimic large systems, periodic boundary conditions (PVC) are applied, where the simulation box is surrounded by its replicas. Large-range interactions are handled using methods like Ewald summation. Finally, the simulation generates a trajectory of atomic moments over time, which is analyzed to understand molecular behavior.[26] Common molecular dynamics software includes GROMACS, AMBER, NAMD, and CHARMM, as shown in Table 2

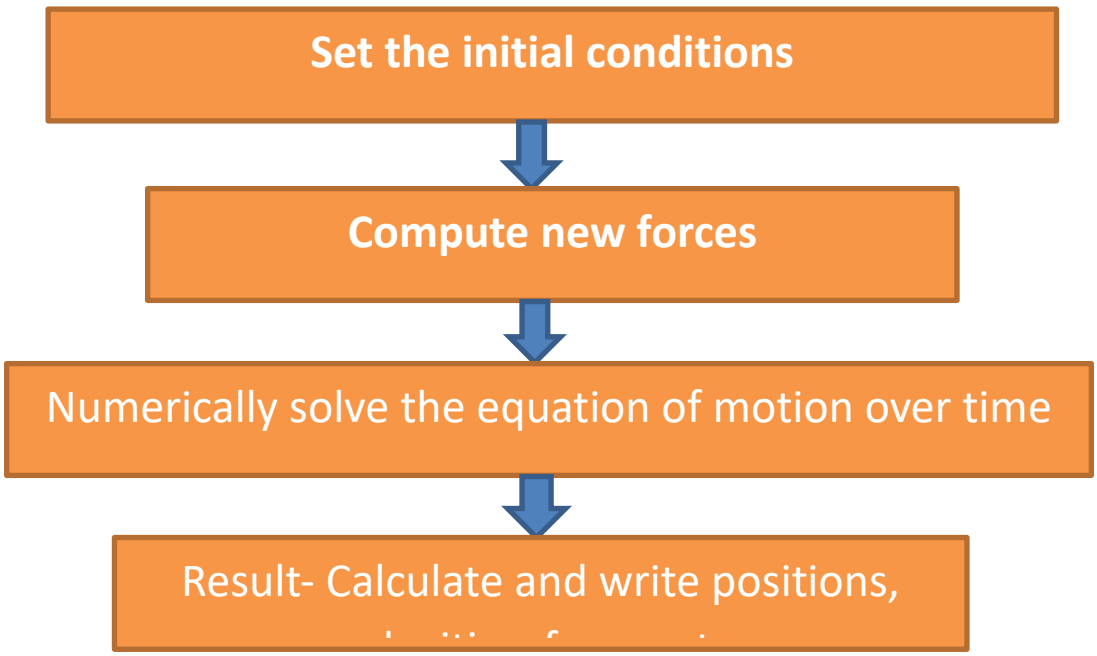

Fig 6 Molecular dynamics simulation algorithms

Table 2 Algorithms used in molecular dynamic simulation

S. no.	Algorithms	Characteristics
1.	Matching algorithms	Geometry- based
2.	Incremental construction	Fragment-based and docking incrementally
3.	MCSS	Fragment-based methods for de novo design
4.	LUDI	Fragment-based method for de novo design
5.	Monte Carlo	Stochastic search[27]
6.	Genetic algorithms	Stochastic search
7.	Molecular dynamics	For further refinement

Simulation in Drug Discovery

Modern drug discovery usually begins with identifying and validating, as mentioned in Fig 6, a biological target that can be influenced by drug molecules to prevent, treat, or reduce the symptoms of disease.[28] These targets are commonly proteins such as enzymes or receptors, but they can also include DNA or RNA. One of the main challenges in drug design is protein confirmation, as proteins are not rigid structures-they are dynamic and constantly changing shapes.[29] Even small changes, like the movement of amino acid side chains, can significantly affect how well a drug molecule (ligand) binds to the target site. Because protein flexibility plays a crucial role in ligand binding, molecular dynamics (MD) simulations are very useful.[30] They help in understanding the dynamic behavior of the target protein and provide valuable insights for designing effective drugs.[31]

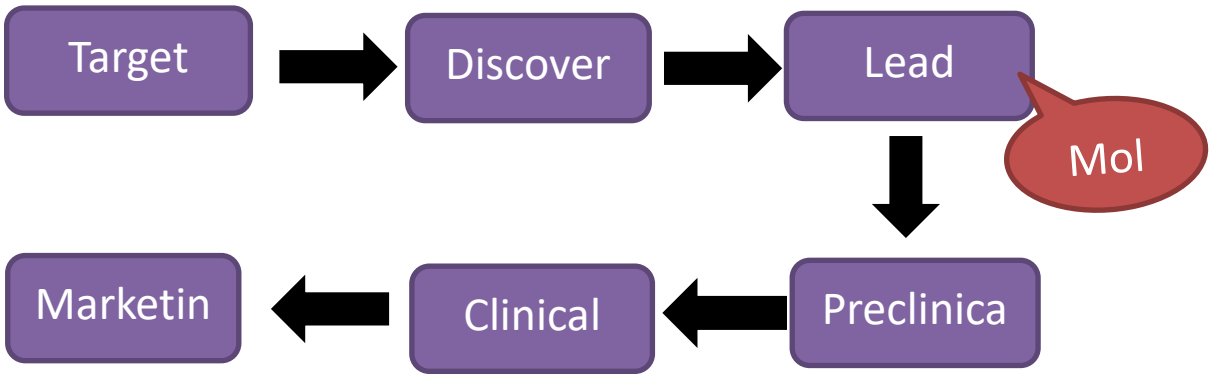

Fig 7 Phases of drug discovery

Methods for Performing Molecular Dynamics

Many software tools are available for performing molecular dynamics simulations of biomolecules, such as GROMACS, Open Babel, VMD, and UCSF Chimera. Any of these can be used depending on the requirement, but it is important to note that each software uses different force fields.[32]

Molecular Dynamics simulations are generally carried out in three major steps:

1. Model Selection
2. Energy Minimization, Heating, and Equilibration
3. Production Run and Analysis

In Chimera, Molecular Dynamics Simulation is linked to minimization and dynamics function provided by the molecular mechanics toolkit (MMTK). Standard residues are assigned amber force field parameters, whilenonstandard residues are treated using the antechamber module.[33]

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Model selection: First, an appropriate molecular model must be selected. Using the complete structure as available, but if any part is missing, it must be reconstructed and proper protonation states assigned. All relevant atoms must be included at this stage, as anything excluded will not be considered later.

The prepared structure is typically saved in POB and PSF file formats. Most simulations begin withcrystal structures obtained from the protein data bank. Important information included atom names, residue names, coordinates, occupancy, temperature factor, and segment ID.[34]

Energy Minimization, Heating, and Equilibration: This step ensures that the system reaches a stable and low-energy state using the selected force field. Initially, the system is minimized to remove stains and unfavorable interactions.

Table 3: Common minimization algorithms include:

Algorithms	Uses
Steepest Descent	For constrained systems
Conjugate Gradient	For large systems
BFGS method	Quasi-Newton approach
Newton-Raphson method	Energy derivatives

After minimization, the system is gradually heated by adjusting particle velocities. Equilibration is then performed until system properties become stable over time.[35]

Important consideration

Periodic Boundary Conditions (PBC): Used when simulating systems with solvent; the cutoff distance must be less than half the box size.

Fixed Atoms: Some atoms can be held stationary if needed, though all atoms still contribute to energy calculations.[36]

Translation and Rotation Removers: These eliminate the overall movement of the system during simulation.[37]

Files used

Topology files: Define atom types, charges, and connectivity.

Parameter files: Provide force constants for bonds, angles, torsions, and non-bonded interactions.

Solvation: Since biological processes occur in aqueous environments, solvation is essential. It can be done in two ways:

Explicit solvation: Adding water molecules directly

Implicit solvation: Treating solvent as a continuous medium

Production Run and Analysis

After equilibration, the system is simulated under specific conditions such as constant temperature (NVT) or constant pressure (NPT). This phase generates trajectory data over time.[24]

The simulation length and time intervals for recording data are defined in this step. The generated trajectories are then analyzed to study properties like structural stability, interactions, and conformational changes.[38]

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Applications of molecular dynamics

Modulation- Molecular dynamics simulations are widely used to evaluate protein stability under both native and non- native environmental conditions.[39] By analyzing the dynamic behavior of unstable residues, valuable insights can be obtained to guide rational protein design. Furthermore, simulations of mutated protein structure enable the assessment of how specific alterations influence overall stability.[40]

Engineering of functional regions-Molecular dynamics simulation plays a crucial role in understanding the dynamic behavior of functional regions within proteins. By capturing functional motions and analyzing key residues involved in activity, these simulations help in optimizing protein function. Additionally, simulation of designed variants allows researchers to evaluate the effects of mutations on the structural integrity and functionality of this region.[31]

Insights from folding pathways- Molecular dynamics simulation provides detailed insights into protein folding and unfolding mechanisms by exploring conformational trajectory and identifying intermediate states.[41] These simulations can be used to partition folding pathways into distinct conformational states, offering a deeper understanding of structural transitions. Such insights are valuable for guiding protein design, as they allow the evaluation of how mutations affect the folding landscape and overall protein behavior.[42]

Limitation of Molecular Docking Simulation

Over the last two decades, more than sixty molecular docking software programs have been created. [43] , including SLIDE [44] X-CSCORE [45] , and ConsDock [46]. Typically, most docking procedures treat ligands as flexible molecules, whereas proteins are treated as rigid bodies since proteins comprise thousands of atoms. However, several approaches allow protein side-chain optimization to account for protein flexibility to some extent, e.g., GalaxyDock.[47].

Protein flexibility and induced-fit effects can also be considered by using multiple protein conformations. Such ensembles can be generated using computational approaches such as molecular dynamics (MD) simulations or experimental data such as NMR or X-ray crystallography. The MDock program implements the "ensemble docking" approach by introducing protein conformation as another variable in docking optimization and accounting for protein movement implicitly. This method remains computationally efficient by providing similar performance speeds as single-structure docking[48].

Other programs used different approaches to address protein flexibility issues. For example, Mizutani et al. enlarged the binding cavity in their docking application ADAM by expanding the Van der Waals energy potential between atom pairs, thereby uniformly enlarging the pocket. Then, the generated structure was refined to eliminate overlapping atoms and improve interactions. Bottegoni et al. developed the SCARE protocol.[49]

Integration of Molecular Dynamics Simulation and Docking in Drug Design

To achieve more reliable and accurate characterization of protein-ligand complexes, an integrated approach combining molecular docking and molecular dynamics simulations is widely employed. This hybrid strategy leverages the complementary strengths of both techniques while compensating for their individual limitations. Molecular dynamic methods are computationally efficient and enable rapid exploration of the conformational space of ligands. They are particularly useful for high-throughput screening of large compound libraries, such as potential drug candidates, at a relatively low computational cost.[50] However, docking approaches often suffer from limitations, including inadequate representation of protein flexibility and the lack of a universally reliable scoring function for accurate ranking of ligand-protein complexes. In contrast, molecular dynamics simulations provide a more detailed and dynamic representation of biomolecular systems by allowing full flexibility of both the ligand and the protein. This enables better characterization of conformational changes, particularly within the receptor binding site, and improves the understanding of ligand-induced structural adaptations. Despite their accuracy, molecular dynamic simulations are computationally intensive and less suitable for large-scale screening.[14] Therefore, the integration of docking and molecular dynamics simulations

represents a rational and effective strategy in drug design. Typically, docking is employed for the rapid initial screening of large compound libraries, followed by molecular dynamics simulation to define binding poses, optimized protein-ligand interactions, and calculate more precise binding energies. This combined approach significantly enhances the reliability and efficiency of the drug discovery process.[21]

CONCLUSION

Computational techniques have revolutionized the field of drug discovery by providing efficient, accurate, and cost-effective alternatives to traditional experimental methods. Molecular docking and molecular dynamics simulation are two fundamental approaches within Computer-Aided Drug Design that contribute significantly to understanding protein–ligand interactions and optimizing drug candidates. Molecular docking enables rapid screening of large compound libraries and identification of potential lead molecules, while molecular dynamics simulation offers deeper insights into molecular behavior, stability, and conformational changes. Each method has its own strengths and limitations; however, their integration provides a comprehensive understanding of drug-target interactions. The combined use of docking and MD simulation enhances the reliability and accuracy of drug design by allowing both efficient screening and detailed refinement of molecular interactions. This integrated approach not only reduces time and resources but also increases the likelihood of successful drug development.

In conclusion, the application of advanced computational tools in drug discovery continues to expand, offering promising opportunities for the development of safer, more effective, and targeted therapeutic agents. Future advancements in computational power and algorithms are expected to further improve the precision and efficiency of these techniques.

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