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Original Article

A Comprehensive Review on Molecular Docking in Drug Discovery

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ABSTRACT

Molecular docking is a pivotal computational technique in drug discovery and development, enabling the analysis of interactions between small molecules (ligands) and target proteins. This review aims to explore the evolution of molecular docking methodologies, examine their current applications, and anticipate future directions in the field. By synthesizing insights from recent literature and technological advancements, we highlight the transition from traditional rigid docking approaches to more sophisticate flexible and ensemble docking techniques, discussing their respective advantages and limitations. At its core, molecular docking evaluates the spatial and energetic compatibility between a ligand and the active site of a receptor, playing a critical role in identifying new drug candidates, optimizing existing compounds, and elucidating drug-receptor interactions. The use of accurate scoring functions is essential to effectively rank ligand-receptor conformations based on binding affinity, thereby prioritizing compounds for experimental validation. Molecular docking is integral to various stages of drug development, including structure-based drug design, virtual screening, and lead optimization. In structure-based approaches, the three-dimensional structure of the target biomolecule guides the selection of ligands that interact with the active site. Virtual screening accelerates the identification of promising candidates by rapidly evaluating large chemical libraries. As docking technologies continue to evolve, their integration with other computational and experimental methods holds promise for more efficient and precise drug discovery pipelines.

Keywords: Molecular docking, Drug discovery, Ligand-receptor interaction, Structure-based drug design, Virtual screening, Scoring functions, Flexible docking, Ensemble docking, Computational drug design, Lead optimization

INTRODUCTION

The completion of the human genome project marks a significant breakthrough for human civilization in its attempt to understand the enigmas of nature. This biological study provided a fresh direction to the conventional view on drug design, in specific, the choice of therapeutic targets, where we may consider of the genome as a pharmacological target [1]. These days, it's straightforward to attain these goals with accurate techniques like high throughput protein purification, crystallography, and NMR (Nuclear Magnetic Resonance) spectroscopy. Even for tiny features of molecules and their complexes, the structural details produced by these methods have greatly enhanced human knowledge. This process easily creates huge quantities of data that must be stored methodically and retrieved as required. Robust computational methods are necessary for the storage, organization, and exploration of more than one million high-resolution 3D protein structures. The drug discovery process has been enhanced with approaches including virtual screening, lead identification, and optimization generated via computational models [2, 3]. Since its inception in the 1960s, docking has demonstrated itself to be a useful instrument and a crucial strategy in drug screening, protein-protein interactions, and nanomaterial behavior. That's owing to the incredible developments in physics, chemistry, information technology, biochemistry, and computers. Technologies that dock tiny compounds into macromolecules, especially protein targets, dominate the modern area of computer-aided drug design (CADD), and their

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application is growing constantly. Structure-based medicines design nowadays CADD is vital [4–7], and this department is present in the majority of large pharmaceutical corporations. Many pharmaceuticals sold in stores are directly created using the CADD approach [8]. It is certain that docking approaches are essential advances in science for grasping chemical molecules, particularly considering the fact that three eminent computational scientists received the 2013 Chemistry Nobel Prize. Protein–ligand, referred to as protein–protein docking, is an algorithmic approach that anticipates a ligand's orientation upon docking to an enzyme or protein receptor. Most of the time, one can select the most potent ligand for future biochemistry research and development based on its "binding affinity. “Due to the ease of use and minimal equipment needed (it even functions well on a Computer), docking Over the past ten years, the number of linked studies has greatly risen. A comprehensive examination reveals that accuracy is an important concern with docking investigation, as these articles will be of little benefit if the docking is not done precisely. The accuracy of docking can occasionally even fluctuate between 0% and 92.66%. [9] The field of docking between molecules faces barriers that must be dealt with in order to boost predictive capacity and expand the computational field's utilize. Docking has shown remarkable development as a field of study since its inception. The underlying algorithms do not always predict the proper binding modes of a ligand because they merely reflect approximations of the real world. As a result, the docking score ranks the various docked positions that are produced by each docking run in a sequential manner. Only specific characteristics—such as tiny ligands, sufficient to occupy the binding site, receptor knowledge, a lower threshold for binding locations, and—above all—expert handling—can accurately predict the binding modes [10]. The development of drugs and design depend heavily on molecular docking, a computer algorithm that predicts the optimal orientation of small molecules once they are bound to target proteins. This process aids in understanding the interactions between chemicals and proteins, which facilitates the development of new treatment medicines. The history of molecular docking began in the 1980s, when algorithmic advancements persisted. Boost processing power to increase accuracy and efficiency. These days, a fundamental tool in pharmaceutical research is molecular docking, allowing the recognition of interesting drug candidates and the optimization of their interactions during binding. The relevance and development of molecular docking in drug discovery is briefly outlined in this text [11]. In order to find possible binding sites and improve the medication's binding affinity and specificity, researchers can use it to model and examine the connections among the proposed drug and the protein of interest. A useful technique for screening sizable chemical libraries and forecasting their potential as therapeutic candidates is molecular docking. However, manual drug study employs more conventional methods in which researchers can model and examine the binding between the drug candidate and the target protein, assisting in the identification of possible binding sites and the improvement of the drug's binding specificity and affinity. Molecular docking is a useful tool for a useful method for evaluating sizable chemical libraries and forecasting their potential as therapeutic candidates is docking [12]. Experiments like crystallography and biochemical assays are frequently used in this procedure to comprehend the binding mechanisms and maximize the drug's effectiveness. Manual drug study offers more thorough and precise information regarding drug-target interactions, even if molecular docking is a quicker and more economical method of screening and analyzing possible drug candidates [13]. The choice between molecular docking and manual drug study ultimately depends on the particular research goals, available resources, and the complexity of the drug-target interactions being studied.

The basic theory of molecular docking

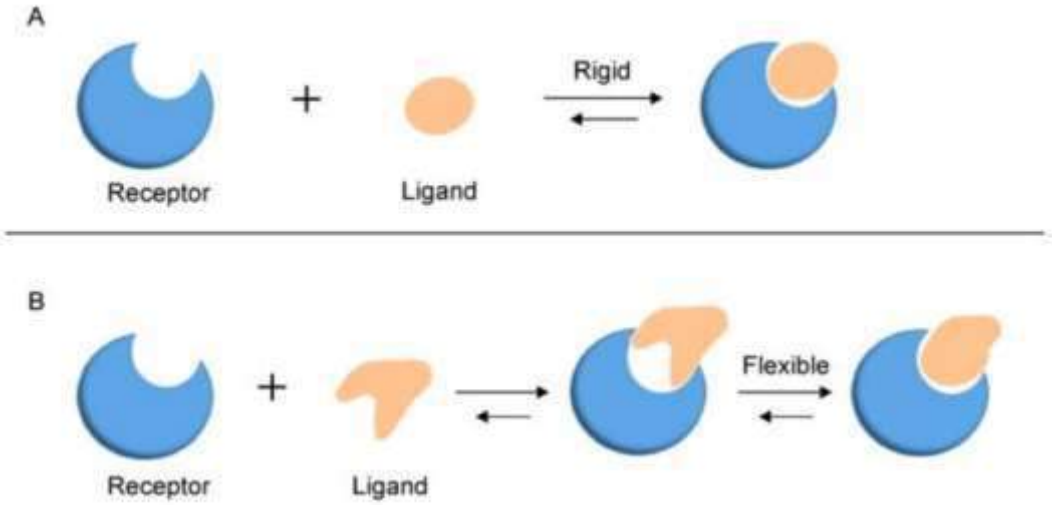

Figure 1: Two models of molecular docking. (A) A lock-and-key model. (B) Induced fit model.

In order to predict and determine the binding affinity with interaction form among ligands and receptor is molecular docking models a desired conformation based on complementarity and pre-planning [14]. Figure 1A illustrates the first suggested "lock-and-key model," which calls for the rigorous docking of ligands and receptors to ascertain the ideal orientation for the "key" that will open the "lock." The importance of geometric complementarity is demonstrated by this model. [15]

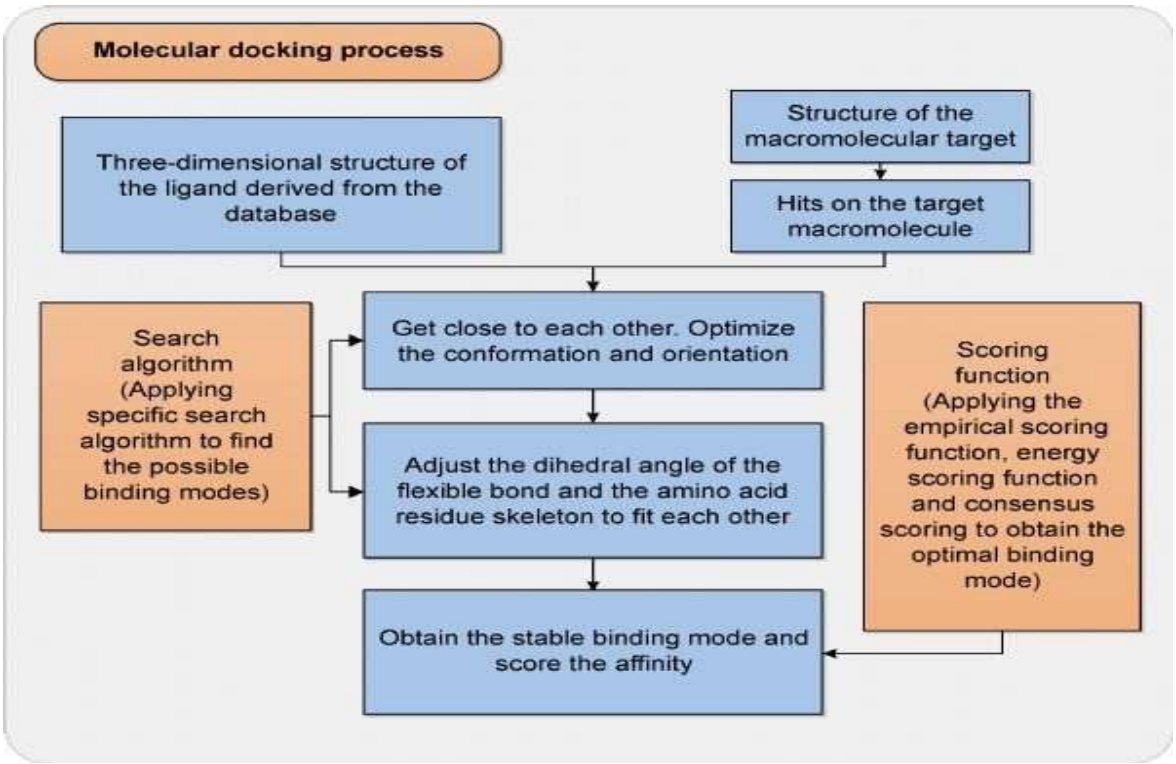

Figure 2: Molecular docking process

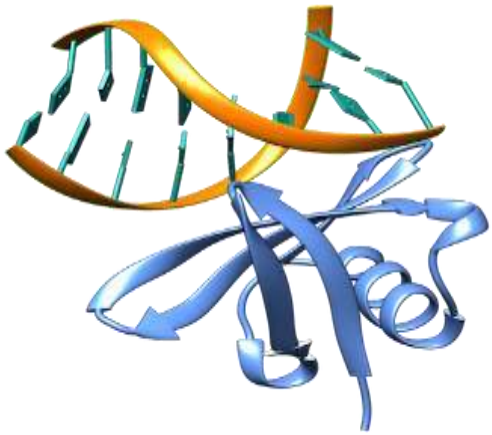

Figure 3: The protein-DNA docking.

Consequently, we generate an "induced fit model" to ensure that conformations match each other appropriately (Figure 1B) [16]. In order to decrease free energy, ligands and receptors will acquire a more stable structure via energy complementarity and pre-organization, which depend on geometric complementarity. The molecular docking program, demonstrated in Figure 2, can help us determine the best orientation and conformation based on pre-organization and cooperation by applying a specific algorithm. The interactive mode is then examined and the binding affinity is predicted using a score formula. In Figure 3, the protein-DNA docking using Auto dock Vina is displayed. [17]

Approaches of Molecular Docking [18]

Simulation Approach	Shape Complementarity Approach
This method calculates the interaction energy for each ligand-receptor pair.	This method suggests estimating the complementarity between the receptor surface and the ligand**.**
The ligand is permitted to fit into the receptor's groove based on least energy consideration in order to produce the optimal docked conformer of the ligand and receptor.	This method describes solvent exposed topographic aspects of the receptor and its ligand in terms of corresponding surface in order to obtain the docked conformer. The calculation of shape complementarity between interacting molecules is then performed in order to determine the best groove or pocket for ligand binding to its target.
Each time the ligand is moved into the receptor's pocket for optimal fit, an energy known as the Gross Energy of System is produced. This energy is then compared to determine the best docking conformer with a small quantity of energy.	This approach includes calculating features and curvature, expressing the receptor and ligand surfaces (i.e., surface creation and smoothing), docking, and scoring based on favorable geometric criteria.
This method allows for a more accurate evaluation of molecular perception and the interaction between ligand and receptor molecules since it is more compatible with ligand flexibility in molecular modeling tools.	Flexible and rigid docking are each possible using the shape complementarity technique. Conformational adjustments may occur between bound and free molecules that engage in the case of flexible or soft docking. Together with this, the two interacting molecules overlap and approach into another. However, during molecular modeling, secure docking eliminates spatial shifts to the form of interacting molecules.
This technique takes quite longer to finish molecular modeling because it needs to calculate a massive energy spectrum. Grid-based tools and swift methods for optimizing, however, have substantially modified the issue.	This technique delivers rapid and dependable answers by rapidly scanning an enormous amount of ligands for binding on a specific object in just a few of seconds.

Algorithms, Scoring Functions and Tools

Three clinical and three rotating DOFs (Degree of Freedoms) are available to bring two molecules closer together for docking, and the likelihood of this happening may grow exponentially as the number of components increases [19]. For instance, it could take up to 107 trails for a molecule to cover every patch of a protein [20]. When protein flexibility or screening big drug or protein databases are taken into account, this issue becomes much more sensitive. A full solution space search and a guided partial search are the two methods used to accomplish this search for the global minimum. With the goal to find the best fit solution, search methods can be categorized into three primary types: deterministic, systematic, and stochastic. Certain techniques also combine elements of these three groups. Algorithm classifications that are utilized extensively.

Types of molecular Docking

Rigid docking

This kind holds the receptor (target protein) and the ligand (small molecule) stationary throughout the docking process. Although this approach is quicker, it might not take into consideration how the protein's structure changes as it binds to a ligand [21]. In molecular modeling, rigid docking—also described by the terms straight-body coupling or geometric docking—is a computer method that predicts, at the atomic level, the mechanism of attachment and propensity involving a ligand, or small molecule, and a receptor, or typically a protein. This method ignores any changes in conformation that could take place upon binding and alternatively assumes that the ligand that the receptor both remain their rigid structures over the procedure of docking [22].

Flexible docking

Flexibility in the ligand, receptor, or both during the docking process can be rendered available by flexible docking. This may lead to accurate predictions of binding modes by including conformational changes into consideration. A computational tool used in molecular modeling to project the mechanism of attachment and affinity between a ligand and a receptor while considering into thought flexibility in both the ligand and receptor structures is called flexible docking, occasionally referred to as flexible ligand docking or induced-fit docking. Unlike rigid docking, which assumes that both the ligand and receptor maintain rigid conformations during binding, flexible docking considers the conformational changes that may occur in both the ligand and receptor upon binding [23].

Induced fit docking

Induced fit docking combines aspects of both rigid and flexible docking. It involves initial docking with rigid structures followed by refinement of the complex with flexible side chains or backbone movements to account for induced fit effects. It is a computational technique used in molecular modeling to predict the binding mode and affinity between a ligand and a receptor while explicitly considering conformational changes in both the ligand and receptor structures upon binding. The unpredictable nature of biomolecular interactions and the induced-fit phenomenon seen in ligand-receptor binding is taken account of with induced fit docking, as opposed to rigid docking, which makes the assumption that the two molecules the ligand and the receptor maintain rigid conformations during binding [24].

Ligand-based docking

In ligand-based docking, the docking process is guided by the properties of the ligand molecule rather than the receptor structure. This method is useful when the receptor structure is unknown or difficult to obtain. Ligand based docking, also known as ligand-centric docking or structure-based pharmacophore modeling, is a computational technique used in molecular modeling to predict the binding mode and affinity of a ligand to a target receptor or enzyme without explicit consideration of the receptor structure. Contrasting to receptor-based docking methods which necessitate an awareness of the receptor's structure, ligand-based docking relied purely on data collected from the ligand, notably its structure, chemical features, and connections to the object of interest [25].

Protein-protein docking

The associations amongst the two molecules of protein have been predicted by means of protein-protein docking. It is required for comprehension of signaling pathways and protein complexes. In molecular modeling, peptide-protein 1mooring is a computerized approach that the predicts the three-dimensional structure and mechanism of cooperation among two or more protein molecule. It is essential for knowing the mechanisms governing protein-protein relationships (PPIs), which are essential for many biological functions include gene regulation, inflammatory response, and signal transduction. The basic principles, treatments, applications, and boundaries of protein-protein docking in biological modeling will all be addressed within this essay [26].

Blind docking

Blind docking is the technique of attaching a ligand to a receptor's broad surface without determining a binding site. Exploring probable attachment areas and interactions is a breeze using this method of research. Blind docking, sometimes referred to as global docking or blind protein-ligand docking, is a molecular modeling computational technique whereby estimates the binding procedure as well as sensitivity between a ligand and a receptor without knowing the receptor's binding site ahead. Blind docking searches the entire receptor surface to determine candidate binding sites and determine the most beneficial ligand binding positions, in contrast to conventional docking algorithms generally rely upon understanding of the receptor's anatomy to control the docking process. [27]

Key stages in docking

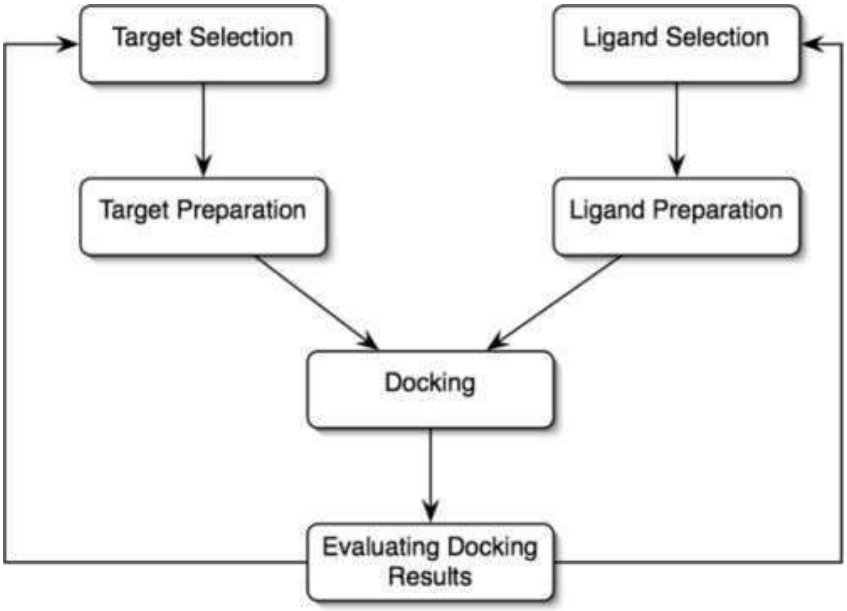

Figure no:4 Docking workflow

Target Selection and Preparation

The target structure should ideally be established experimentally, often using nuclear magnetic resonance or x-ray crystallography. Although docking against homology models has been achieved successfully [28], the accuracy and skew of the helix model exert a major effect on how accurate the docking results remain. The target structure has to have suitable symmetry-related molecules while in some cases the biological unit, or the physiologically necessary version of the target structure, is a multimer. In this regard, target structures may be found as a biological unit ideal for docking examinations in the online database of Binding MOAD.

Ligand Selection and Preparation

The goals is to determine the variety of ligands which are chosen to undergo docking; for lead discovery, the number of molecules requiring to be docked can be reduced through adding fundamental filters which includes net impose, molecular weight, polar surface area, commercial availability and price-per-compound. Filters like synthetic accessibility,

pharmacophores, similarity levels, and distribution, absorption, metabolism, excretion, and toxicology (ADME-Tox) features are also used for lead optimization. A special library of analogs related to the lead substance or compounds is often developed for docking in order to help guide and prioritize drug discovery endeavors for targeting lead optimization [29].

Docking

When trying to discover the most suitable binding mode, molecular docking includes computationally navigating a search space defined by the molecular model the method uses and ranking potential solutions. Therefore, a scoring system and a search technique are both needed for docking. The two primary types of search techniques are stochastic and systematic. The fineness of the search space sampling impacts the degree of precision of the solution in the former the situation, while the found solution is deterministic. Because stochastic approaches depend on an element of whim, conclusions are not all exactly the same. Programs notably DOT, GRAMM, and ZDOCK commonly use systematic methods of searching in rigid proteins–rigid protein docking that provide just six degree of freedom [30].

Evaluating Docking Results

The chemical complementarity between the ligand and the protein should be brought seriously whenever interpreting docking information irrespective of the ligand–protein docking approach that has been deployed. Could the ligand have all of the potential donors and acceptors of hydrogen obligations? Would the ligand's charged groups interact with the receptor's oppositely charged side chains, or have they shrouded in aqueous pockets? Do the ligand's hydrophobic groups become trapped in the receptor's hydrophobic pockets? Furthermore, whenever the geometry of the agonist–protein complex is known, the docking tool's capacity to replicate the binding mode of a ligand to protein can be exploited as an indicator of the parameters employed for the docking.

Recent software and webservers for docking [31]

Program name	Novel features
Autodock	EA-based docking software that's completely open source. pliable ligand. Side chains of proteins that are flexible. held up current by the Scripps Research Institute's Molecular Graphics Laboratory in La Jolla.
DOCK	applications for anchor-and-grow docking. Academic use remains free. protein ligand. Protein that is flexible. maintained by the School of Medicine of California San Francisco's (UCSF) Soichet group. docking program based on GOLD GA. hydrophilic ligand.
Glide	robust docking program based on search. offers in virtual high-throughput screening, standard precision (SP), and extra precision (XP) modes. Antibodies and receptors are flexible. permission of Schro Dinger.
SCIGRESS	Software suite for desktop/server molecular modeling which employs semi-empirical quantum algorithms using linear scaling for ligand docking and protein optimization. Fujitsu developed and distributed it.
Glam Dock	software suite for desktop/server molecular modeling which employs semi-empirical quantum algorithms using linear scaling for ligand docking and protein optimization. Fujitsu developed and distributed it.
GEMDOCK (generic evolutionary method for molecular docking)	A program for estimating the orientation and shape of a ligand having relation to the target protein's active site.
Flex X, Flex-Ensemble (Flex E)	Docking program built around incremental builds. pliable ligand. The ensemble of structures of protein gives proteins versatility. Bio Solve IT is the provider.
Autodock Vina plugin for PyMOL	Docking runs can be initiated initiated with Autodock or VINA from inside of the add-on, binding sites can be defined and supplied to Autodock and VINA input files, multiple ligands can be managed and virtual screenings can be configured up, docking runs with flexible side chains can be set up, and Autodock or VINA grid maps are visible in PyMOL.

DockoMatic	GUI software designed to facilitate developing and handling AutoDock is jobs for high-throughput ligand/receptor interaction screening relatively predictable.
Ligand Fit	docking program based on CHARMm. Shape-based docked for ligand conformations generated using Monte Carlo techniques into an active site is followed by subsequent CHARMm minimization. uploaded by Accelrys
HYBRID	The docking tool looks similar to FRED, nonetheless it incorporates a scoring function based on the chemical Gaussian overlsy (CGO) ligand generated using the scientific software Open Eye
Swiss Dock	A web-based tool for anticipating putative chemical interactions between a small pharmaceutical and an undesirable gene.
Docking Server	provides an easy to use, web-based interface that coordinates each aspect of molecular docking, commencing with the setup of compounds and proteins.
Blaster	A structure-based ligand discovery service that is accessible to all. uses several ZINC Information groups as the database and MOOR as the docking usage. offered by UCSF's Department of Pharmaceutical Chemistry's Shoichet Laboratory
Id Target	A web server which utilizes a divide-and-conquer docking algorithm as well as powerful scoring functions to discover actual biomolecular targets of minuscule chemical compounds. The National Taiwan University maintains
Flex Pep Dock	Rosetta framework-based excellent quality peptide docking (refinement) techniques. A PDB file based on the relationships between the protein's receptor and a determined peptide conformation functions to represent the server's input.
GPCRautomode	A service on the internet that (i) deposits odorants on the six new three-dimensional structures of G-Protein coupled receptors (GPCRs) presently accessible and (ii) simplifies the homologous modeling or mammalian receptors for odor (ORs) by grading the complexes using the colony energy concept. sponsored by INRA.
Pose & Rank	Protein-ligand complex scoring web server. supplied by Andrej Sali's laboratory.

Application of molecular docking

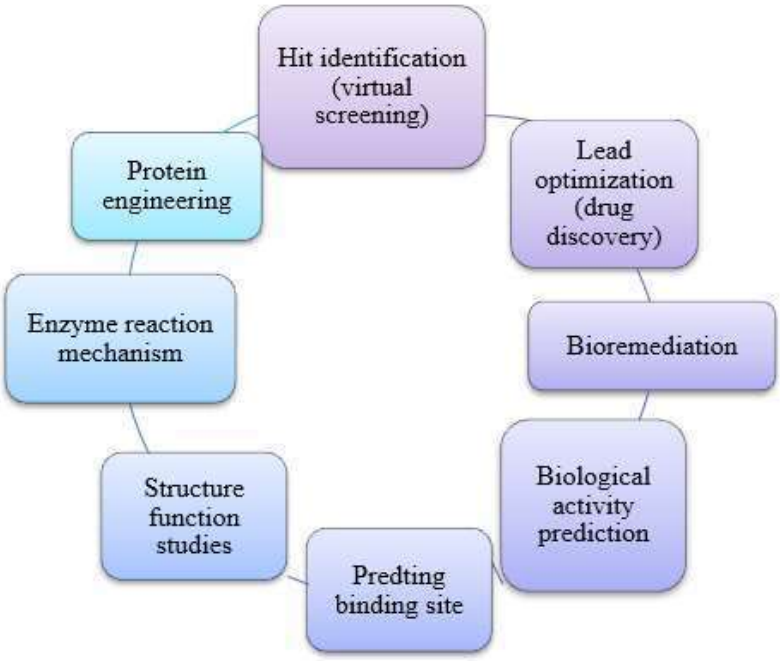

Figure No 5: Application of docking

Hit identification

When integrated with a scoring function, docking provides swift in silico screening of an enormous

number of potential therapeutics to locate molecules able to bind to a single target of interest.

Lead optimization

Docking, frequently referred to as the binding mode or pose, is a tool for anticipating the exact location and distance of a ligand's bond to a protein. Greater precision and strong mimics can be created based on the prior supplied information.

Drug discovery

By estimating the way tiny molecules will link to a polypeptide or receptor, molecular docking is being used for discovering viable pharmaceutical alternatives. In order to improve a lead compound's binding affinity and selectivity, its structure can also be changed.

ADMET prediction

Small molecule features such as Shock Absorption, Distribution of Benefit, Metabolism, or Flushing, and Neurotoxicity (ADMET, which stands) can possibly be simulated via molecular docking.

Structure elucidation

Antibodies with unclear geometries may get their structures confirmed with the aid of molecular docking.

Target fishing

Specific proteins that the medication might function through can be established utilizing the use of molecular docking.

Nutraceutical research

Defining the cellular targets of nutraceuticals to medical use can be improved by the practice of molecular docking.

Bioremediation

Molecular docking may be utilized to uncover enzymes and their means of activation. It is also essential to discover interactions among proteins. Molecules are evaluated electronically using the restoration treatment. Figure 5 exhibits further molecular docking uses.

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