International Journal of Pharmacy and Industrial Research (IJPIR)

IJPIR |Vol.16 | Issue 1 | Jan - Mar -2026

www.ijpir.com

ISSN: 2231-3656

DOI : https://doi.org/10.61096/ijpir.v16.iss1.2026.164-173

Review

An Overview of Molecular Docking

Deepa. R, Govindamy. S, Sujith Kumar. S, Dhamodhara Prsad*, Vigneshwaran L.V

RKP College of Pharmacy, Krishnagiri, Tamilnadu, India.

*Corresponding Author: Dhamodhara Prasad
Email: dhamodharaprasad490@gmail.com

Published on: 14.02.2026

Published by:
Futuristic Publications

Abstract

Molecular docking is a crucial computational method used to predict the preferred orientation of one molecule to another when bound together to form a stable complex. This technique plays a vital role in virtual screening and database exploration to identify novel therapeutic candidates from a range of chemical scaffolds. There are two primary types of molecular docking: rigid docking and flexible docking. Rigid docking assumes that the molecules are stiff and searches for a 3D transformation that yields the best fit between two molecules based on a scoring function. This approach can be applied in the absence of a receptor or when receptor-binding activity is present, allowing for the generation of ligand conformation. In contrast, flexible docking takes into account the flexibility of molecules, enabling a more accurate prediction of molecular interactions. This abstract provides an overview of the types of molecular docking, highlighting the importance of this technique in drug discovery and development.

Keywords: Molecular docking, Types, Approaches, Software docking, Virtual screening.

1.INTRODUCTION

Molecular docking is a technique used in molecular modeling that predicts a molecule's preferred orientation when attached to another molecule to form a stable complex.[1] The intensity of connection or binding affinity between two molecules is predicted using scoring systems based on the preferred orientation. . Signal transduction relies heavily on the connections between biologically significant substances such proteins, nucleic acids, carbohydrates, and lipids. Additionally, the kind of signal generated may depend on the relative direction of the two interacting partners. (e.g. agonism/ antagonism). as a result, docking is helpful for forecasting the kind and strength of signal generated. In order to estimate the affinity and activity of the small molecule, docking is often utilized to predict the binding orientation of drug candidates to their

protein targets. Docking is therefore crucial to the logical design of pharmaceuticals. Making predictions about the desired three-dimensional configurations is the main goal of docking research. Docking automatically creates suitable incentive structures. Numerous computational docking techniques are available for use.[2]

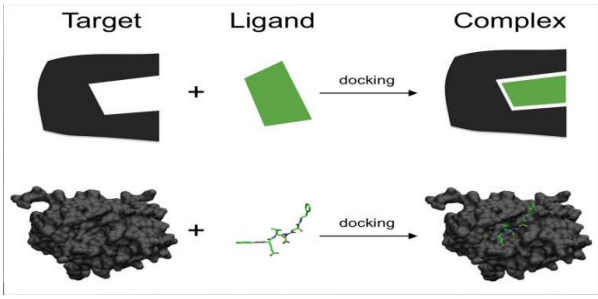

Fig 1: Structure of molecular docking [3]

2. TYPES OF MOLECULAR DOCKING :

There are two kinds of docking :

1. Inflexible docking
2. Docking flexibility

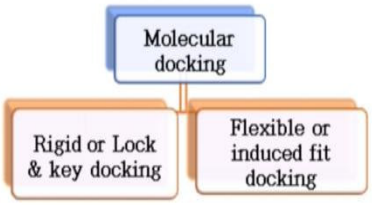

Fig 2 : Docking Methods[2]

2.1 Rigid docking or inflexible docking

If we believe that the molecules are stiff, we are searching for a 3D conversion of one of the molecules that brings it into the best possible fit with the other molecules in terms of a scoring function. When there is no receptor or when there is receptor binding activity, the ligand's conformation may be produced.[4] Assuming molecules are stiff, we look for a three-dimensional transformation of one molecule that yields the best fit between it and another molecule in the form of a scoring function . Without a receptor or with a receptor-binding activity present, ligand conformation can be generated. Innovative therapeutic candidates from a range of chemical scaffolds are found by virtual screening and database exploration .[5]

Eg : Induced fit model

Eg : lock and key docking method

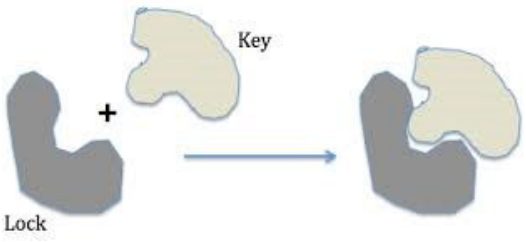

Fig 3 : Structure of lock and key method[6]

2.2 Docking flexibility

Both the ligand and the receptor can move in this docking. It is versatile in terms of conformity. The energy is computed for every rotation. The occupancy of each configuration surface cell is determined. The most ideal binding position is then chosen.[7] Typically, ligands are freely docked onto a rigid receptor in virtual docking experiments. But it's becoming more and more obvious that side chain flexibility is important in ligand-protein interactions. These modifications enable the receptor to modify its binding location in response to the ligand's orientation.[8]

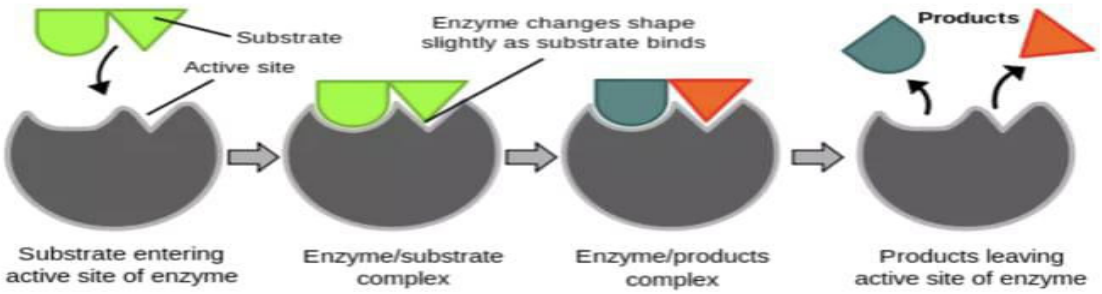

Fig 4 : Structure of induced fit model [9]

Mechanism action of induced fit model :

Substrate binds to the enzymes active site .As substrate binds, the shape of the active site changes slightly. If the substrate enables the active site's shape to change in the right way then the reaction takes place and an enzyme - product complex is formed. The products are then released from he active site .[9]

Table 1. Types of molecular Docking their method, application & limitation

S. No.	Types of Molecular Docking	Method	Application	Limitation
1.	Rigid Docking	a. Preparation	a. Post-processing and Analysis	a. Neglect of Flexibility
		b. Search Algorithm	b. Protein-Protein Interactions	b. Scoring Function Accuracy
		c. Scoring Function	c. Enzyme Mechanisms	c. Computational Cost
		d. Post-processing and Analysis	d. Virtual Screening	d. Treatment of Solvent Effects
2.	Flexible Docking	a. Docking Algorithm	a. Computational Cost	a. Computational Cost
		b. Scoring Function	b. Scoring Function Accuracy	b. Scoring Function Accuracy
		c. Induced-Fit Modeling	c. Conformational Sampling	c. Conformational Sampling
		d. Post-processing and Analysis	d. Modeling Receptor Flexibility	d. Modeling Receptor Flexibility

Table 1 : Types of molecular docking [10]

3.Steps involved in molecular docking:

3.1.Ligand preparation: Prior to docking, the ligand molecule must be ready. This entails acquiring the ligand's three-dimensional structure, refining its geometry, adding hydrogen atoms and allocating partial charges.

3.2.Protein preparation: The target protein structure must be ready for docking. In order to do this, the protein structure must be optimized, hydrogen atoms must be

added, partial charges must be assigned and any ligands or water molecules must be eliminated.

3.3 Grid generation: The protein's active site is surrounded by a grid of spots. This grid is used to specify the ligand's sample region during docking.

3.4. Ligand positioning: The ligand is positioned close to the active site of the protein inside the designated grid space. Different ligand conformations and orientations are investigated using a variety of methods

3.5. Scoring: The fitness of each ligand conformation inside the binding site is assessed using a scoring function. By taking into account elements like hydrogen bonds, van der Waals forces and electrostatic interactions, this function determines the interaction energy between the ligand and protein.

3.6.Refinement and optimization: To increase their accuracy and solidify the interactions, the top-ranked ligand conformations are put through refinement procedures such energy minimization or molecular dynamics simulations.

3.7. Analysis and visualization: To determine the binding mode and the most promising interactions between the ligand and protein, the docking results are examined and visualized. Examining hydrophobic interactions, hydrogen bonds and other crucial elements may be part of this.[11]

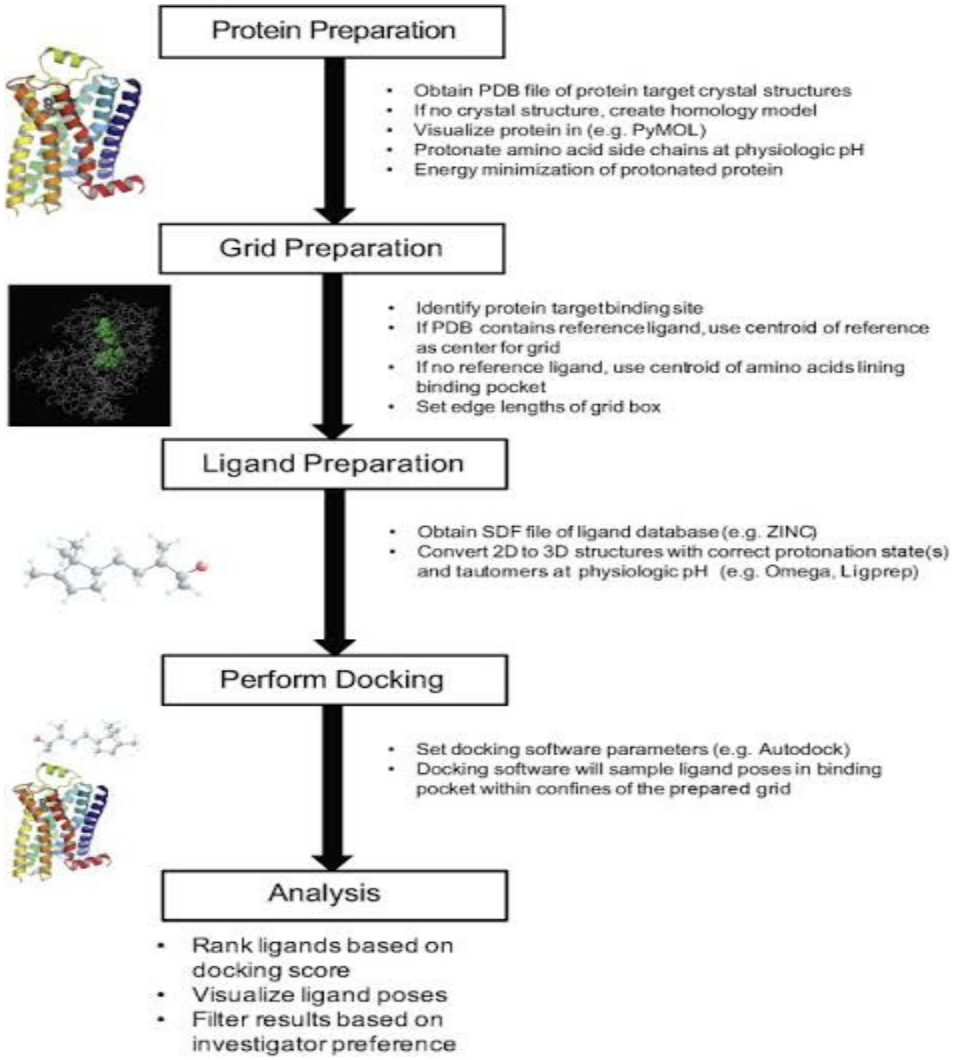

Fig 5 : Steps involved in molecular docking [12]

4.Approaches of Molecular docking :

4.1.Monte Carlo Approach

It provides a randomized conformation, translation, and rotation for a ligand in an active site. It gives the configuration a beginning value. It then builds a fresh configuration and scores it. Using the Metropolis criterion, it decides whether to sustain the new configuration.

Metropolis criterion: If a new method out performs the old one, it is immediately approved. If the arrangement is not novel, a Boltzmann's law-focused likelihood study is used. The arrangement is approved if the solution satisfies the probability function test; if not, it is rejected.

4.2.Matching Approach

The ligand-receptor arrangement established by this technique, which emphasizes redundancy and selects the optimal spot for the ligand atom in the site, might also be enhanced.

4.3.Ligand Fit Approach

A quick and accurate approach for docking small molecule ligands into protein active sites while taking form complementarity into consideration is referred to as "ligand fit".

4.4.Point Complimentarily Approach

These techniques focus on comparing the physical or chemical properties of several substances. Blind docking is a method for screening the complete interface of target molecules to uncover potential peptide ligand binding sites and mechanisms of action.

4.5.Structure based complimentary approach

This technique employs ligand and target as a set of surface structure properties that promote their molecular docking. The target's molecular surface is explained in terms of its solvent-accessible surface area in order to accomplish molecular docking, while the ligand's molecular surface is described in terms of matching surface illustration. The complementarity between two molecular surfaces is evaluated based on shape matching depiction, which assist in locating the complementary groove/pocket for ligand docking on target molecular surface. In instance, for protein target molecules, hydrophobicity is also calculated applying number of twists in the main-chain atoms. Geometric complementarity between protein and ligand utilizing search method . Mostly search strategies such as monte carlo ,genetic algorithm and exhaustive approaches are employed to anti capte alternative conformations of ligand.[13]

5.Application molecular docking :

"While ligand binding can result in agonism or antagon ism, molecular docking interactions can either activate or inhibit the protein.
Perhaps using molecular docking to:

1.Hit identification (virtual screening)

2.Lead optimization (drug discovery)

3 Bioremediation

4.Remediation

5.Binding site prediction (blind docking)

6.Protein – protein/ nucleic acid interactions

7.Mechanisms of enzymatic reactions

8.Protein engineering

9.Molecular dynamics simulation

10.Structure elucidation

5.1 Hit identification (Virtual screening)

Identifying Hits (Virtual Screening) Hit identification is the first step in any successful drug discovery project. During this process, the right small molecules—often referred to as hits—are discovered that bind to the target and change its function. Drug discovery efforts are accelerated and attrition rates are decreased by high-quality initial hits. After a hit discovery campaign finds several hit series, a variety of orthogonal methods, such as biophysical assays, are employed for hit qualification and characterization in order to choose the most promising hit series for the beginning of the hit-to-lead (h2l) process. Using computer techniques like molecular docking and molecular dynamics simulations, virtual screening predicts which compounds in a large library are most likely to bind to a target protein.

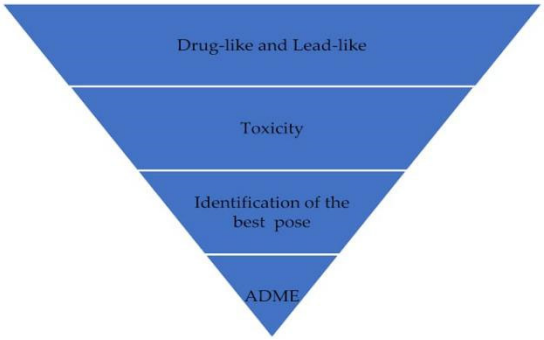

Fig 6 : Steps involved virtual screening [15]

5.2 Lead optimization

The process of creating and improving a lead compound that has already been identified is called "lead optimization." It involves changing the molecule in a number of ways through chemical modifications. Throughout this process, synthetic changes are performed to optimize the compound's ADMET (absorption, distribution, metabolism, excretion and toxicity) properties as well as its activity, potency and selectivity. The compound's capacity to enter the bloodstream (absorption), travel throughout the body to its intended location (distribution), decompose once inside the body (metabolism), eliminate the compound and any metabolites from the body (excretion) and have any negative effects on the body (toxicity) are all examples of ADMET characteristics. However, these features are monitored not just during the lead optimization stage of drug development but also during the earlier stages.

5.3 Bioremediation

Biomedicine In bioremediation, molecular docking is used to forecast how well tiny molecules will bond to enzymes that break down environmental contaminants. To improve the effectiveness of bioremediation, docking can be used to create inhibitors or activators of these enzymes.

5.4 Remeadiation

Enzyme-degradable pollutants can be predicted using protein-ligand docking. It can be used to gather both the intended location and the most effective drug. Molecular docking can be used to identify enzymes and their modes of activity. Determining the relationships between proteins is another application for it. The remediation is used for virtual screening of compounds.

5.5 Blind site prediction

Comprehending biological processes requires an understanding of the specific sequence regions known as binding sites that facilitate interaction. Experimental methods can report incorrect binding locations, while computational approaches often require data that is not available at the proteome-scale due to experimental limitations. This method is also essential when targeting locations other than the original substrate binding site. Finding the allosteric binding site that controls the activity of the target protein is one of the most important goals in drug discovery.

5.6 Protein protein /nucleic acid interactions

A remarkable range of protein–nucleic acid interactions facilitate the transfer of genetic information between DNA, RNA and proteins. The reviews in this section of current opinion in structural biology cover a wide range of gene expression, including RNA synthesis mechanisms and regulation, DNA packaging, unwinding and repair, post-transcriptional modification, the start of protein synthesis and the selection of newly formed polypeptides for secretion or membrane insertion.

5.7 Protein engineering

The process of creating new proteins or enzymes with desired or novel functionalities is known as protein engineering. It is predicated on altering amino acid sequences using recombinant DNA technology. Enzymatic Reaction Mechanisms To perform enzymatic processes, site-directed mutagenesis, protein structure

determination, quantum mechanical, classical mechanical and statistical mechanical techniques have been integrated with quick computers and algorithms.

5.8 Molecular dynamic simulation

The dynamic behavior of protein–ligand complexes can be studied by combining molecular docking with molecular dynamic simulations. Understanding the conformational changes that take place upon ligand binding and the complex's stability can be aided by the simulations. Molecular docking and dynamics simulation are combined in a number of software applications. These include popular programs like Gold, Vina, Auto dock and Glide. They offer the ability to do molecular dynamics simulations in addition to molecular docking, which enables the investigation of protein-ligand interactions throughout time and the examination of their dynamic behavior.

5.9 Structure elucidation

Structure Clarification Proteins with unknown structures can also have their structures clarified through the use of molecular docking. The binding modes of small compounds to proteins can be predicted via docking and a homology model of the protein can be produced based on the binding mode prediction. An accurate protein structure can then be obtained by refining the produced model with experimental data.[11]

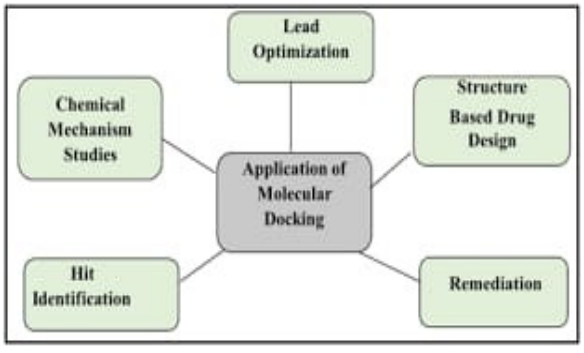

FIG 7 : Application of Molecular docking [16]

6.SOFTWARE FOR MOLECULAR DOCKING:

By modeling their interaction and evaluating binding affinity, molecular docking software forecasts how tiny molecules (ligands) will attach to target proteins. AutoDock (and its quicker replacement, Auto Dock Vina), UCSF Dock, DOCK, GOLD and the Schrödinger commercial suite are popular choices. These resources are essential for computational biology and drug discovery since they aid in the identification of possible therapeutic candidates.[17]

6.1 Widely used molecular docking software

- Popular molecular docking programs Auto Dock and Auto Dock Vina:

Auto Dock is a traditional program that use a Lamarckian genetic algorithm and a grid-based energy evaluation approach. Virtual screening is made easier by Auto Dock Vina, a faster, more accurate version that takes less input files. [18] A novel molecular docking and virtual screening program called Auto Dock Vina is introduced. According to our tests on the training set used in the development of Auto Dock 4, Auto Dock Vina significantly improves the accuracy of the binding mode predictions while achieving a speedup of about two orders of magnitude over the molecular docking software previously developed in our lab (Auto Dock 4). By employing multithreading on multi-core computers, parallelism can be further accelerated. In a transparent manner for the user, Auto Dock Vina automatically computes the grid maps and clusters the results.[29]

- **Dock:**

One of the first and most popular docking programs is called DOCK [19].Fragmentation algorithm molecular force field fast flexible docking, it is widely applicable and always used between flexible proteins and flexible ligands [14]

- **Gold:(Genetic optimization for ligand docking)**

A well-known program with virtual screening and lead compound optimization features [20].Based on a genetic algorithm, GOLD is a well-known protein–ligand docking program. It is renowned for its flexibility in managing various drug research protein docking scenarios and its high accuracy in predicting ligand binding. By anticipating how small compounds, or ligands, interact with their target proteins, the program, which has a worldwide reach, assists researchers in identifying and optimizing possible medication candidates. It is well known for its adaptability in managing a variety of docking situations. Four scoring

functions—ChemPLP, ChemScore, GoldScore, and ASP—as well as a number of heuristics and cutting-edge docking technologies are used by GOLD, a leading molecular docking engine, to produce bioactive poses.[26]

- **UCSF Dock:**

The University of California, San Francisco created the UCSF Dock program.[21] UCSF DOCK predicts small molecule binding mode using geometric methods. DOCK was co-developed by Robert C. Rizzo, David A. Case, and Brian K. Shoichet. The docking program is currently being developed in two versions: DOCK 6 and DOCK 3. The UCSF DOCK algorithm solves rigid body docking difficulties by superimposing ligands onto the binding pocket's negative picture using a geometric matching approach. Important features have been added to improve the algorithm's ability to find the lowest energy binding mode, including force field-based scoring, dynamic optimization, an improved rigid body docking matching algorithm, and a flexible ligand docking alogrithm called anchor and grow (v4-v6), and hierarchical docking of databases.[28]

- **Schrödinger (Glide):**

Industry leading ligand receptor docking solution. It augments and accelerates structure based drug design across range of applications , including virtual screen in binding mode prediction and inter active 3D molecular design.[27] Molecular docking tools, molecular dynamics simulations and other computations are all included in this commercial suite.[22]

S.no	Program	Application
1.	Auto Dock	It is employed in molecular docking.it predicts the binding capacity of tiny chemical and assigns a target protein to a 3D structure
2.	Schrodinger	Comprehensive molecular modelling and CADD tool [30]
3.	GOLD	It is genetic algorithm based docking software .it uses force field based scoring function for the evaluation of docking.[31]
4.	DOCK	Force field [32]

Table 2 : List of software uses in molecular docking [22]

7. Current status of molecular docking :

With its current state characterized by sophisticated algorithms (AI/ML integration), enhanced scoring functions, and difficulties in accurately modeling protein flexibility and water molecules, all driven by increased computational power and structure data, molecular docking is a mature but quickly developing core tool in drug discovery. It is essential for finding drug candidates, comprehending target interactions and even investigating nutraceuticals.[23]

8.Advanced techniques molecular docking:

In order to simulate realistic protein-ligand interactions, account for flexibility, integrate experimental data (Cryo-EM, NMR) and quickly screen large libraries for highly accurate drug discovery, advanced molecular docking goes beyond simple prediction and incorporates machine learning, deep learning, fragment-based techniques and improved scoring/sampling (like Molecular Dynamics). This results in improved lead identification and optimization in contemporary computational drug design (CADD). [24]

9.Key advancements & techniques:

- **AI & Machine/Deep Learning:**

Makes docking quicker and more precise by using algorithms (such as Genetic Algorithms) to search conformational space, forecast binding and enhance scoring.

- **Scoring Functions:**

Creates increasingly complex functions to differentiate active from inactive molecules and more accurately predict binding affinity.

- **Flexible docking:**

Flexible docking simulates more realistic binding by allowing flexibility in both the ligand and certain regions of the protein, going beyond rigid models.[25]

CONCLUSION

The molecular docking method serves as a crucial tool in drug discovery, enabling researchers to predict the interaction between molecules and biological targets, thereby facilitating the design of more effective therapeutic agents. Its application not only enhances our understanding of molecular interactions but also accelerates the development of innovative treatments.

REFERENCES:

1. 1.De M, Rego V, Jacques J. Tropical Diseases: An Overview of Major Diseases Occurring in the Americas. Bentham Science Publishers; 2017.
2. Tiwari S, Prakash K. Unrevealing The Complex Interplay: Molecular Docking: A Comprehensive Review On Current Scenario, Upcoming Difficulties, Forthcoming Initiatives, And Viewpoints. International Journal of Chemistry Research [Internet]. 2024 Jan 1 [cited 2024 Jul 31];1–9. Available from: https://ijcr.info/index.php/journal/article/view/226
3. Docking (molecular) - Wikipedia. Docking (molecular) - Wikipedia [Internet]. www.google.com. 2024 [cited 2025 Dec 7]. Available from: https://share.google/6YNZTszXHQivc0L39
4. Dnyandev KM, Babasaheb GV, Chandrashekhar KV, Chandrakant MA, Vasant OK. A Review on Molecular Docking. International Research Journal of Pure and Applied Chemistry. 2021 May 20;60–8.
5. Fan J, Fu A, Zhang L. Progress in molecular docking. Quantitative Biology [Internet]. 2019 Jun;7(2):83–9. Available from: https://link.springer.com/article/10.1007/s40484-019-0172-y
6. Lock. Lock and Key Model. | Download Scientific Diagram [Internet]. www.google.com. 2024 [cited 2025 Dec 8]. Available from: https://share.google/0W4mqDGaFfJSJ1fSP
7. Bhagat RT, Butle SR, Khobragade DS, Wankhede SB, Prasad CC, Mahure DS, et al. Molecular Docking in Drug Discovery. Journal of Pharmaceutical Research International. 2021 Jun 3;46–58.
8. Pagadala NS, Syed K, Tuszynski J. Software for molecular docking: a review. Biophysical Reviews. 2017 Jan 16;9(2):91–102.
9. Study. Enzymes: Mechanism of Action (A-level Biology) - Study Mind [Internet]. www.google.com. 2022 [cited 2025 Dec 8]. Available from: https://share.google/enkvOUNHHvqgU5nAG
10. Sahu MK, Nayak AK, Hailemeskel B, Eyupoglu OE. Exploring Recent Updates on Molecular Docking: Types, Method, Application, Limitation & Future Prospects. International Journal of Pharmaceutical Research and Allied Sciences [Internet]. 2024;13(2):24–40. Available from: https://ijpras.com/storage/files/article/f1d817cc-40f0-4732-917b-aec9cb6976c8-Quf8v5mnwpnSPpLz/DYRiBWP5RhTc9l7.pdf
11. Deepak Venkataraman N, Bharathwaj J, Charumathi P, Lakshminarasimman S, M PV, Sudharsan S. An Overview of Basics, Types, Approaches, Applications, Advantages and Disadvantages of Docking. International Journal of Pharmaceutical Sciences [Internet]. 2025 Mar 7 [cited 2025 May 7]; Available from: https://www.ijpsjournal.com/article/An+Overview+of+Basics+Types+Approaches+Applications+Advantages+and+Disadvantages+of+Docking
12. Dermatology in. Research Techniques Made Simple: Molecular Docking in Dermatology ... [Internet]. www.google.com. 2024 [cited 2025 Dec 8]. Available from: https://share.google/TISVxlbmStOubEBr4
13. Tripathi A, Misra K. Molecular Docking: A Structure-Based Drug Designing Approach. JSM Chemistry [Internet]. 2017 May 15 [cited 2025 Dec 8];5(2):1–5. Available from: https://share.google/kIWrzh6qTqZlKO8Ys
14. Sawhney SK, Singh M. Molecular Docking Software's Applications And Basic Challenges Faced: A Review. International Research Journal of Pharmacy. 2020 Mar 21;11(2):15–9.

15. Drug in. Virtual Screening Algorithms in Drug Discovery: A Review Focused ... [Internet]. www.google.com. 2024 [cited 2025 Dec 8]. Available from: https://share.google/t5uvmSFbdQUFIPupI
16. Application of molecular docking | Download Scientific Diagram. Application of molecular docking | Download Scientific Diagram [Internet]. www.google.com. 2024 [cited 2025 Dec 8]. Available from: https://share.google/sBqCRZlCis3wVdBmW
17. Butt SS, Badshah Y, Shabbir M, Rafiq M. Molecular Docking Using Chimera and Autodock Vina Software for Nonbioinformaticians. JMIR Bioinformatics and Biotechnology. 2020 Jun 19;1(1):e14232.
18. Mohd Mursal, Ahmad M, Hussain S, Mohemmed Faraz Khan. Navigating the Computational Seas: A Comprehensive Overview of Molecular Docking Software in Drug Discovery. IntechOpen eBooks. 2024 Apr 29;
19. Molecular Docking Software - CD Computa Bio [Internet]. Computabio.com. 2019 [cited 2025 Dec 8]. Available from: https://www.computabio.com/molecular-docking-software.html
20. GOLD: The All In One Molecular Docking Package | CCDC [Internet]. www.ccdc.cam.ac.uk. Available from: https://www.ccdc.cam.ac.uk/discover/blog/gold-the-all-in-one-molecular-docking-package/
21. UCSF DOCK [Internet]. Share. google. 2025 [cited 2025 Dec 8]. Available from: https://share.google/DH9XwrwPHNaz2065c
22. cnapolitan2. Docking and scoring [Internet]. Schrödinger. 2021. Available from: https://www.schrodinger.com/life-science/learn/white-papers/docking-and-scoring/
23. Stefaniu A. Molecular Docking and Molecular Dynamics. BoD – Books on Demand; 2019.
24. Fatima K, Ashfaq UA, Muhammad, Asif M, Haque A, Qasim M, et al. Advanced network pharmacology and molecular docking-based mechanism study to explore the multi-target pharmacological mechanism of Cymbopogon citratus against Alzheimer's disease. South African Journal of Botany. 2024 Jan 10;165:466–77.
25. Prieto-Martínez F, Arciniega M, Medina-Franco J. Molecular docking: current advances and challenges-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/). TIP Revista Especializada en Ciencias. 2018;21:65–87. Available from: https://www.medigraphic.com/pdfs/revespciequibio/cqb-2018/cqbs181h.pdf
26. Protein–Ligand Docking with GOLD | CCDC [Internet]. Share.google. 2022 [cited 2025 Dec 10]. Available from: https://share.google/WxC6Vj0blpGDhIKID
27. Glide | Schrödinger [Internet]. Schrödinger. 2025 [cited 2025 Dec 10]. Available from: https://share.google/JFwEqQj86yNdP94zI
28. Applications of UCSF DOCK Software - CD ComputaBio [Internet]. Share.google. 2025 [cited 2025 Dec 10]. Available from: https://share.google/dbZnLDdr2qSxTKhAK
29. \Trott O, Olson AJ. AutoDock Vina: Improving the Speed and Accuracy of Docking with a New Scoring function, Efficient optimization, and Multithreading. Journal of Computational Chemistry. 2009;31(2).
30. The. Summary of the most widely recognized molecular docking software ... [Internet]. www.google.com. 2024 [cited 2025 Dec 10]. Available from: https://share.google/a5zQXTrOS3BOAbEkk
31. List. List of Docking tools and web servers | Download Scientific Diagram [Internet]. www.google.com. 2024 [cited 2025 Dec 10]. Available from: https://share.google/MXo1wt7XJkGk0oN75
32. List. List of common molecular docking software | Download Scientific ... [Internet]. www.google.com. 2024 [cited 2025 Dec 10]. Available from: https://share.google/SYbIiujlbCUJbMoPF