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Framework of Network based Studies and Molecular Docking in Pharmacology

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Abstract: *Over the past few decades, there has been an emphasis on combinatorial and multi-target medicines. By modifying the activity of the targets in complicated diseases like HIV-1 infection, cancer, and diabetes, these strategies demonstrated significant therapeutic success. Since most diseases entail the disruption of the coordinated activity of various gene groups, they cannot be effectively treated with a single gene target. The majority of cellular components function effectively through interactions with other cellular components, which collectively form an interactome. This interconnectedness demonstrates that a gene malfunction may propagate throughout the network rather than being limited to the gene product itself. A computer method for predicting the binding affinity of ligands to receptor proteins is called molecular docking. Despite its potential use in nutraceutical research, it has evolved into a powerful tool for drug development. Nutraceuticals are bioactive compounds that can be utilised to treat illnesses and are found in dietary sources. Identifying their molecular targets can aid in the development of novel treatments tailored to individual diseases. This review's goal was to investigate the use of molecular docking in the research of dietary supplements and illness treatment.*

Keywords: Network pharmacology , molecular docking, biological target , Bioinformatics

I. INTRODUCTION

NETWORK PHARMACOLOGY

Combining computational analysis with in vitro and in vivo experiments and integrating a lot of data is how network pharmacology, a research field based on systems biology, genomics, proteomics, and other disciplines, finds new drug targets and molecular mechanisms.. The calculation methods mainly include network topology information calculation, random network generation and comparison, network layering and clustering, and network visualization technologyIn vitro biology and pharmacology studies, as well as a variety of high-throughput omics techniques, are examples of experimental methods. . Experimental methods ; Methods used in network pharmacology for TCM research include network-based disease gene prediction, drug targets , drug function prediction to specific diseases , network construction of Chinese herbal medicine , and construction and analysis of drug-gene-disease network [1].The interconnection of biological systems is studied in network pharmacology, an interdisciplinary field that finds key signal nodes for pharmacological molecule design. It integrates the core ideas and research techniques of computer science, mathematics, network science, and bioinformatics. It is a broad, multidisciplinary area that uses systems-based methods to study how medications interact with their targets. This presents a fresh perspective on medication development that could result in important breakthroughs [2].

MOLECULAR DOCKING

Docking is a technique used in molecular modelling that predicts the direction a molecule will prefer to go in when it jumps to another molecule to create a stable complex . To predict the degree of involvement or binding affinity between two molecules, information about the rotation's selected direction can be worn, such as in a scoring function [3]
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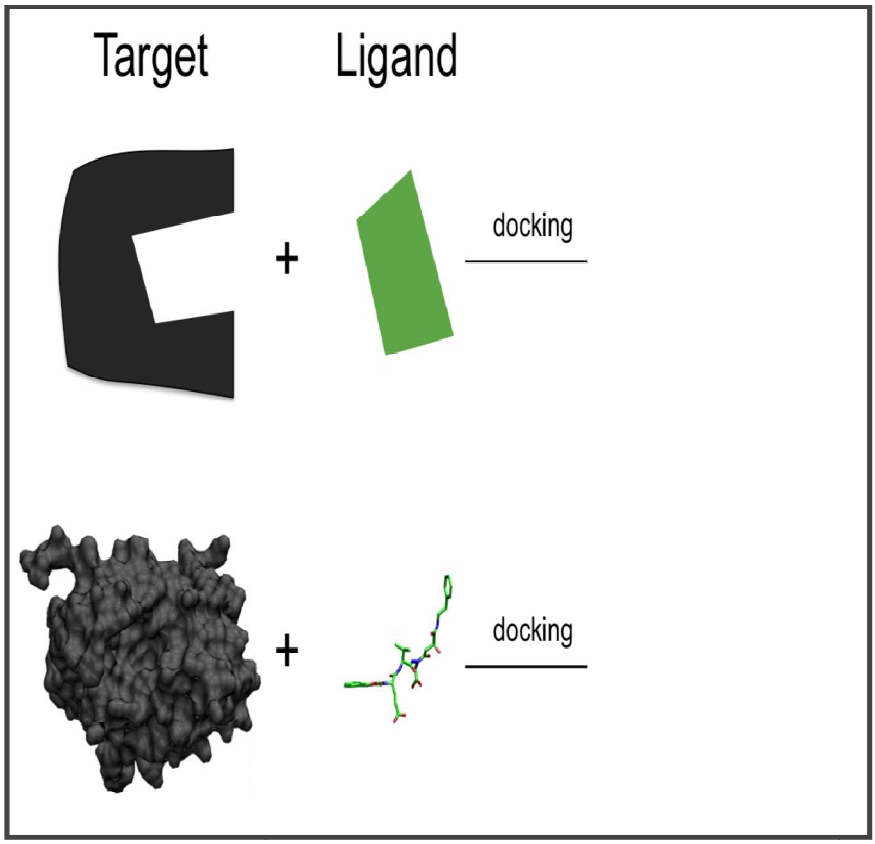

Fig. 1 .Molecular docking

The preferred orientation of a small molecule (ligand) when attached to a target macromolecule (often a protein or nucleic acid) to create a stable complex is predicted using a potent computational method called molecular docking. By assisting researchers in comprehending the molecular interactions between ligands and their biological targets at the atomic level, it plays a critical role in contemporary drug discovery. Finding a ligand's binding affinity and ideal binding position within a receptor's active site is the primary objective of molecular docking, which offers important insights into structure–activity relationships (SAR) and directs the creation of novel therapeutic compounds (Morris & Lim-Wilby, 2008) [4]. Molecular docking is now a crucial part of structure-based drug design (SBDD) thanks to developments in computational biology and bioinformatics. In order to model and assess ligand-target interactions, it combines computational techniques with experimental structural data, such as X-ray crystallography and NMR spectroscopy (Meng et al., 2011). According to Pagadala et al. (2017), docking algorithms typically consist of two primary steps: sampling the ligand's conformational space and rating each posture according to expected binding energy or interaction potential [5].

TYPES OF MOLECULAR DOCKING :

There are two types of docking :-

Rigid docking

Flexible docking

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1. Rigid docking :

We are seeking for a conversion in 3D space of one of the molecules that brings it to the best fit with the other molecules in terms of a scoring function if we believe that the molecules are rigid. The ligand may be creating its conformation while there is no receptor present or when there is receptor binding activity.

2. Flexible docking :

Our goal is to find the confirmations of the receptor and ligand molecules as they evolve in complex situations by considering molecular flexibility in addition to transformation.[3]

In flexible docking, the ligand and/or receptor can undergo conformational changes during docking to identify the optimum binding pose. It delivers more realistic results. [6]

3. Blind docking :

When the active site is unknown, blind docking searches the entire protein surface for possible binding sites .

Key Features:

No specific binding site.

beneficial for unidentified proteins or new targets.

computationally challenging [7].

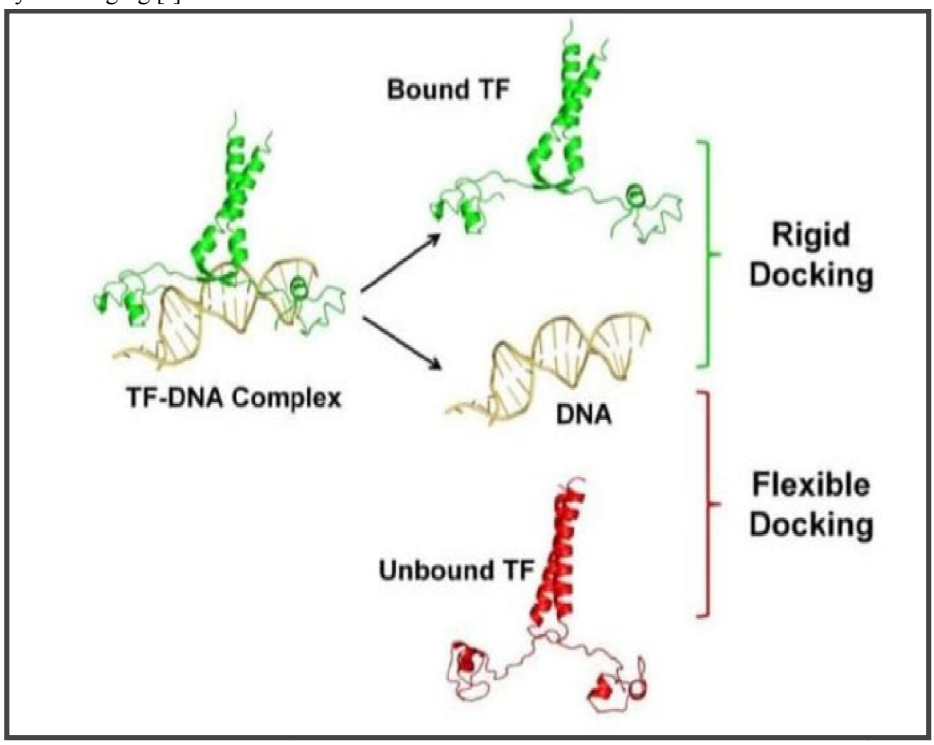

Fig.2 Structural Rigid docking and flexible docking.

APPROACH FOR MOLECULAR DOCKING:

1. Monte carlo approach :

The molecular docking problem, which involves predicting which way a molecule would like to face one another while uniting to form an enduring structure, was resolved using the Monte Carlo approach. To create ligand randomised conformation, Monte Carlo (MC) techniques employ rigid-body translation, bond rotation, or rotation in an active site.

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We use an energy-based decision criteria to evaluate the conformation learned by this change. It will be kept and used to generate the subsequent confirmation if it meets the requirements.

2. Metropolis Criteria :

The Metropolis criterion evaluates the necessity of maintaining an updated configuration. This criterion states that a new approach is instantly adopted if it outperforms the old one.[8]

3. Fragment base method:

The fragment base approach involves splitting the ligand into fragments or divide protons, docking the pieces, and then joining them.[3]

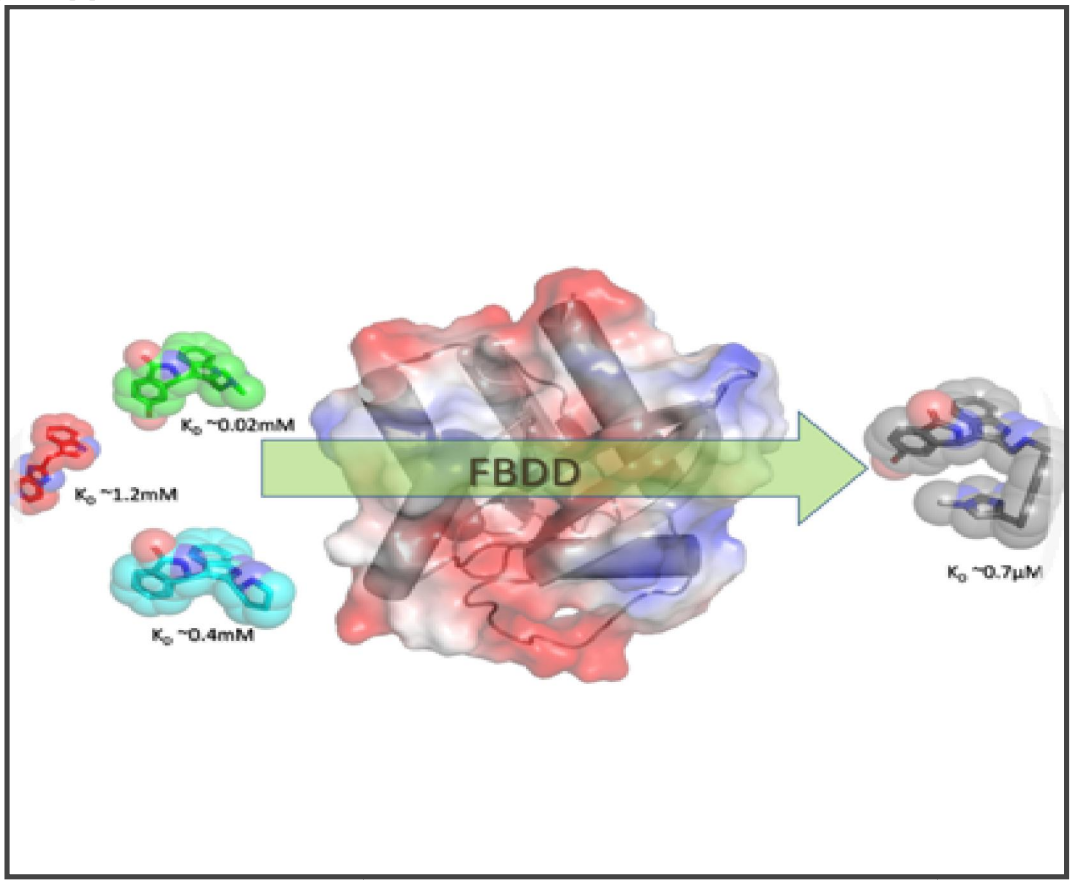

Fig.3 Fragment based method

Key Role of TCM in the Origin and Development of Network Pharmacology

TCM is a national treasure and the core of the Chinese people's millennium-long experience in disease prevention. People's livelihoods and the country's economy both depend on medical research. It has long been a major engine for advancing technical and scientific change and innovation. Through years of clinical experience, TCM has developed a large number of treatments. Many natural chemical components included in TCM prescriptions, like arsenic trioxide and artemisinin, are also important sources of novel drug development in China. It is important to remember that TCM is a traditional, systematic medicine, and that one of its distinguishing characteristics is its holistic approach to diagnosis and therapy.Treatment for complex diseases must evolve from single-target therapy to comprehensive, methodical network regulation. Nevertheless, there are currently no recognised research methodologies that align with the holistic characteristics of TCM. The comprehensive therapy features of TCM are very distinct from the reduction

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and trial-and-error analysis techniques frequently employed in contemporary science. Additionally, the "single target, single disease, and single drug" approach to medical research now in use leads to higher expenditures and a lower success rate, making it challenging to adjust to the treatment requirements of complex disorders. As a result, both TCM and contemporary medicine anticipate the development of novel study paradigms and techniques.

TCM's holistic methods also draw attention to the shortcomings of reductionist research and medicine. In order to comprehensively uncover the molecular underpinnings of TCM's entire diagnosis and therapy, Tsinghua University Professor Shao Li spearheaded the development of a novel idea known as the "network target." Prior to the advent of network pharmacology, the theories, techniques, and case studies pertaining to network targets were put forth globally, and a number of Chinese and US innovation patents have been granted in this area. A series of exploratory investigations on the entire examination of the complex system of TCM started in 1999 when Professor Li proposed a theory regarding the relationship between biomolecular networks and TCM .Consequently, a number of preliminary investigations into the comprehensive examination of the intricate TCM system were initiated. The entire regulatory influence of TCM prescriptions on complicated diseases and syndromes was illustrated in 2002 using the functional gene network. Through network regulation of "multi-cause and micro-effect," TCM prescriptions were found to interfere in diseases and syndromes, ultimately achieving an "emerging" impact January 2007: [9]

Table. 1 The key role of TCM in the origin and development of network pharmacology

Country	Study type	Publication date	Study aim
China	Experiment	1999	Mechanism of TCM injection-induced nephrotoxicity
China	Retrospective	1982	Investigate effect of TCM decoction on ADRs
China	Experiment	January 2007	Establish LD50 for TCM injection
China	Experiment	October 2007	Evaluate allergic mechanism
China	Experiment	October 2008	Allergic effect evaluation
China	Experiment	2009	Sensitization analysis
USA	Case Report	Current medicine 2004	Case of TCM injection reaction
USA	Case Report	Current medicine 2009	Detailed ADR case
China	Review	2011	Comprehensive ADR analysis
USA	Case Report	Journal of Clinical Medicine, 2015	Single case study

BUILDING A COMPOUND TARGET NETWORK :

Using Cytoscape V3.10.1 , the compound-targets network was built to examine how active compounds interact inside the complicated biological system. The chemical components and targets are represented by nodes in this network, and their interactions are depicted by edges. The core features of the network were assessed using the network analyser tool. The network was then filtered according to the "degree," a node attribute that indicates how many connected nodes are associated with a particular network node . [10]

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SOFTWARE TOOLS FOR MOLECULAR DOCKING :

A wide range of software and tools, including PyRx-Virtual Screening Tool, Discovery Studio Visualizer 2020, AutoDock Vina, PyMOL, MGL Tools, the Protein Data Bank (PDB), and PubChem, were used to carry out the molecular docking analyses. Desmond (Schrodinger LLC) was used to run the MD simulation on a 64-bit operating system with a Core i7 processor, 12GB RAM, and an NVIDIA RTX 4090 graphics card. [[11]]

MOLECULAR DOCKING SIMULATION :

Molecular docking was used to dock the core protein targets from the protein-protein interaction (PPI) implicated in the bioactive-targets-pathways network and the primary bioactive compounds of A. laxiflora from the bioactive-target network. Additionally, by confirming the binding affinity of A. laxiflora's bioactive phytoligands, molecular docking helps anticipate the antidepressant efficacy of these compounds.

The RCSB PDB database provided the three-dimensional protein structures of the top six hub genes as a result of network pharmacology (Berman et al., 2000). The following are the selection criteria for the target protein 3D structures: Target structures with bound ligands are chosen with high priority; (a) X-ray solved crystal structures with a better resolution or up to 2.5 Å were included; (b) if two or more 3D structures are available in the database, the better resolution is taken into consideration for the selection; (c) the proteins isolated from humans as an organism are preferred.

The two-dimensional (2D) structures of the core phytoligand were obtained from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/), transformed into three-dimensional (3D) structures using Chem3D 20.0 version software, and stored in PDB format. Water and other non-protein molecules were eliminated, the cognitively attached ligand was separated from the protein's binding site, residues' missing atoms were fixed, and polar hydrogens were added using PyMOL 2.4.0 software (Mooers, 2020). Lastly, the molecular docking operations were performed using AutoDock 4.2.1 and AutoDock Vina 1.1.2 software (Morris et al., 2009; Trott and Olson, 2010). For each target protein's binding sites, a grid box for docking was created and saved in pdbqt format. the details of protein targets, including centre coordinates and PDB IDs.[[12]]

MOLECULAR DOCKING USING AUTODOCK VINA :

We employed the AutoDock Vina module of the PyRx tool (0.8) for molecular docking . Open BabelTM and AutoDock Vina were used to convert protein and compound structures to PDBQT files, respectively. For the molecular docking investigation, a grid box with an exhaustiveness value of 8 was made using AutoDock Vina to predict the protein binding site. Further analysis was conducted on the top interacting compounds that had binding affinities of −6.0 kcal/mol and less against each of the five target proteins. BIOVIA Discovery Studios® was then used to visualise the 2D and 3D compound-target interactions.[13]

CONCEPT AND SIGNIFICANCE OF NETWORK PHARMACOLOGY :

Pharmacology Large amounts of data have been made available by molecular biology and genomics research, which has aided in the acquisition of fresh perspectives on drug discovery procedures. A single medication can target several nodes in the disease network, according to Hopkin, the pioneer of network pharmacology. The foundation of network pharmacology is the integration of several disciplinary ideas, including molecular biology, biochemical biology, and bioinformatics. The high success rate in clinical research, fewer or less expensive side effects, improved drug efficacy, regulation of the signalling pathway with multiple channels, and interaction of multiple genes and proteins that could be easily targeted to cause the disease have all contributed to the increased interest in network pharmacology. Furthermore, network pharmacology aids in identifying the disease node, which is a crucial disease node [[14]].

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METHODS IN NETWORK PHARMACOLOGY :

Identification of drug target Intraction :

One of the main areas of interest in genomic drug discovery is the identification of drug target interactions. Small compounds interact with several pharmaceutically significant protein targets to regulate their activity. The identification of medications with diverse targets was made possible by the high throughput screening of huge chemical databases using a variety of biological assays. The goal of chemical genomic research was to establish a connection between chemical and genomic worlds, however there isn't much of one. For instance, millions of chemicals are listed in the PubChem database, yet there is relatively little information available regarding how these compounds interact with their targets. It takes a lot of effort and money to determine compound-protein interactions or possible drug-target interactions through experimentation. Thus, the development of an efficient in silico prediction approach is necessary .

Prediction of Drug–target Interaction Networks Through Side Effect Similarity :

When certain medications are used to treat human diseases, side effects are carefully documented. These side effects appear to be among the most significant situations and are directly linked to drug interactions with primary targets and off targets (extra targets). Drug interactions with off-target substances can have unanticipated and detrimental effects. However, these interactions can occasionally be advantageous and open up new treatment avenues for medications. For instance, sildenafil was used to treat angina, but it caused extended penile erections in human volunteers. This led to the development of a new therapeutic area for sildenafil .

Prediction of Drug–target Interaction Via Chemical protein Interactome (CPI) :

Roughly 90% of medication candidates fail in the various stages of development before they are introduced to the market. The research and development process becomes more costly and time-consuming as a result. The cost of research and development may be reduced if a unique indication for the currently marketed medication is found. A drug's de novo development, which involves risks related to quality, efficacy, and regulations, takes ten to seventeen years. Because of the previously gathered pharmacokinetic, toxicological, and safety data, repurposing the medications provides the benefit of lowering research and development costs with launch time. The drug's negative side effects have been widely reported as the primary cause of hospitalised patients' deaths [15].

NETWORK CONSTRUCTION AND ANALYSIS TOOLS IN NETWORK PHARMACOLOGY :

In network pharmacology research, network creation and analysis are essential phases. These techniques make it possible to visualise and investigate biological interactions, offering insights into disease pathways, drug-target correlations, and protein-protein interactions (PPIs). The following are important resources that are frequently used to create and examine biological networks:

1. Cytoscape :

Description of Cytoscape An effective open-source tool for analysing and visualising intricate networks of molecular interactions.

Features:

Allows biological data from different databases to be integrated. provides hub node analysis and functional enrichment plugins such as ClueGO and CytoHubba. permits pathway enrichment and dynamic network analysis.

2. STRING :

A database for predicting PPIs based on established and anticipated protein relationships is called STRING (Search Tool for the Retrieval of Interacting Genes/Proteins).

Features:

Integrates literature mining, computational forecasts, and experimental data. gives interaction confidence scores.

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3. Gephi:
A tool for network analysis and visualisation that works especially well for big networks.
Features:
Allows for temporal and dynamic network analysis. incorporates modularity and clustering methods. interactive interface for manipulating data in real time. 4. Pajek Description: A large-scale network analysis tool [16].

Design of molecular docking programmes :
Molecular docking has been essential in many drug development efforts, particularly for the virtual screening of phytochemicals or nutraceuticals as potential medicinal compounds. The first docking programme was developed in the mid-1980s by Irwin Kuntz of the University of California, and docking computations are continuously improved. In order to predict an enzyme's capacity, current advancements in docking techniques determine the enzyme's natural substrates36. Protein complexes can be effectively predicted by restricting the search for likely substrates and reaction types to that region if it has been shown that the protein of interest
belongs to a particular superfamily37 [17] .

MECHANISM OF MOLECULAR DOCKING :
The sequence of the particular protein is the first prerequisite for performing a docking screen. A biophysical method like x-ray crystallography or, less frequently, NMR spectroscopy is used to find the structure. This protein function and a chemical database are inputs used by a docking tool. The search algorithm and the scoring mechanism are the three components that determine the success of a docking programme. When examining the conformational space of a protein
attached to a ligand, the search space includes all possible protein orientations and conformations[18].A computer method for predicting the preferred orientation, binding affinity, and interactions between a ligand and a target macromolecule is called molecular docking. Several methodical phases are involved in its mechanism:

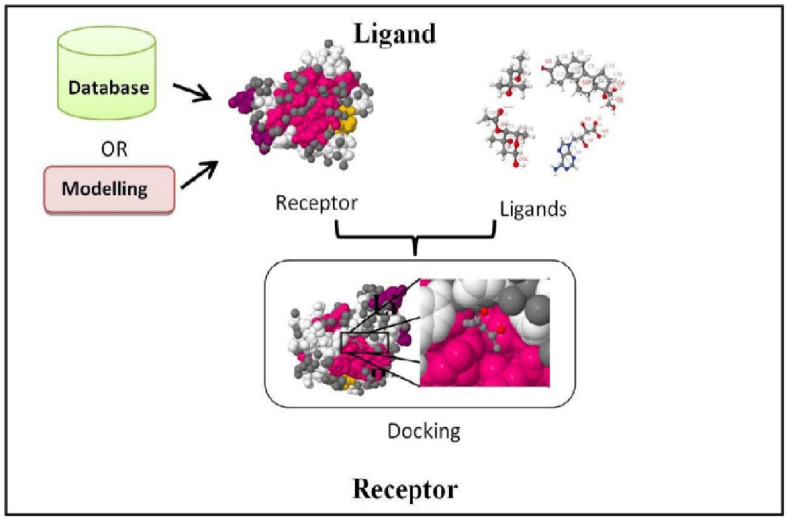

Fig.4 Mechanism of molecular docking

1. Preparation of Target and Ligand :
Water molecules are eliminated in order to prepare the ligand and protein structures :
adding atoms of hydrogen.
Protonation states are assigned.
geometry optimisation [19][20] .

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2. Identification of Binding Site :
The docking programme either:
Uses a known active site (derived from crystallographic data).
Uses algorithms to predict a potential binding pocket [21].

3. Scoring Function Evaluation :
A score function is used to assess each ligand posture, estimating binding affinity depending on:
1. Hydrogen bonding .
2. Hydrophobic interactions .
3. Van der Waals forces .
4. Electrostatic interactions .
5. Desolvation energy [22][23].

4. Ranking and Selection of Best Pose :
The lowest energy pose is chosen as the projected binding mode after the scoring mechanism ranks every stance. The outcome is verified by visual inspection and interaction analysis (H-bonds, π–π stacking, salt bridges) [23].

APPLICATION OF MOLECULAR DOCKING :
1. Drug Discovery and Lead Identification :
Molecular docking is a popular technique for screening vast chemical libraries to find possible therapeutic candidates and aids in predicting how small molecules (ligands) interact with biological targets. For instance: Finding inhibitors for enzymes like GPCRs, proteases, and kinases [24].

2. Virtual Screening (VS) :
In virtual screening (high-throughput or targeted) to select active compounds from millions of molecules prior to laboratory testing, molecular docking is essential [25].

3. Drug Repurposing / Repositioning :
Docking speeds up research and lowers costs by enabling the screening of current medications against novel targets [26].

APPLICATION OF NETWORK PHARMACOLOGY :
1. Drug Discovery and Development :
Network pharmacology helps identify potential active compounds, map their targets, and anticipate therapeutic pathways in the early stages of drug discovery. This reduces laboratory work and expedites the discovery of lead compounds [27].

2. Drug Repositioning (Drug Repurposing) :
By finding common pathways or illness networks, network-based similarity research can uncover new therapeutic applications for currently available medications [28].

3. Precision Medicine and Personalized Therapy :
Customised treatment approaches for complicated illnesses including cancer, diabetes, and cardiovascular conditions are made possible by combining patient-specific genomic data with network models [29] .

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4. Understanding Multi-Component Herbal Medicines :

Complex formulations are frequently used in Ayurveda and Traditional Chinese Medicine (TCM). Network pharmacology facilitates the scientific validation of conventional methods by connecting phytoconstituents to biological targets and pathways [30].

FUTURE PROSPECTIVE

Network pharmacology and molecular docking have a bright future thanks to the quick developments in computational biology, systems medicine, and artificial intelligence. In order to improve personalised medicine approaches and provide more precise disease-target-drug interaction maps, network pharmacology is anticipated to advance towards multi-omics data integration—combining genomics, proteomics, metabolomics, and transcriptomics [31][32].Target prediction, drug-disease association modelling, and network building will all be enhanced by the use of machine learning and deep learning algorithms, speeding up and lowering the cost of drug development [33] .Additionally, new scoring functions, physics-based simulations, quantum mechanical approaches, and validation methodologies will promote molecular docking and increase the precision of binding affinity and ligand specificity predictions [34].Furthermore, the discovery of bioactive chemicals from medicinal plants will be accelerated by the quick development of systems biology databases and cloud-based docking pipelines, making the method essential for finding new treatments for complicated illnesses [35].

II. CONCLUSION

When combined, network pharmacology and molecular docking offer a potent integrative approach to contemporary drug development, especially when it comes to comprehending the multi-component, multi-target, and multi-pathway processes of complicated disorders. By integrating systems biology, chemoinformatics, and network analysis, network pharmacology makes it possible to systematically identify important bioactive substances, possible targets, and biological pathways. By forecasting binding affinity and molecular recognition between phytoconstituents and medicinal targets, molecular docking further confirms these relationships at the structural level. The integrated strategy offers a dependable foundation for setting lead molecule priorities, cutting down on experimental workload, and quickening the creation of synthetic or plant-based treatments.

REFERENCES

[1]. Li Zhao , Hong Zhang , Ning Li et.al , Network pharmacology a promising approach to reveal medicine formula , Journal of Ethnopharmacology . Volume 309, 12 June 2023 , 116306.

[2]. Neera Bhanwala , Raunak Katiyar , Submit Kumar et.al , Network pharmacology and in silico investigation into the therapeutic potential of phyto constituents of peucedanum ostruthium as anti tuberculosis agents.Health Sciences Review (2025) , 100219.

[3]. Khemnar Manisha Dyandev , Galave Vishal Babasaheb Kulkarni Vaisha Chandrasekhar et.al Review on molecular Docking , International Research Journal of pure and applied chemistry 20 may 2021 , 2231-3443,60-68 .

[4]. Morris, G. M., & Lim-Wilby, M.(2008). Molecular Docking. In Molecular Modeling of Proteins (pp. 365–382).

[5]. Meng, X. Y., Zhang, H. X., Mezei et.al . Molecular Docking: A powerful approach for structure-based drug discovery. Current Computer-Aided Drug Design,

[6]. 7(2), 146–157.

[7]. Morris GM et al. "AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility." Journal of Computational Chemistry. 2009;30(16):2785–2791.

[8]. Hetényi C, van der Spoel D. "Efficient docking of peptides to proteins without prior knowledge of the binding site." Protein Science. 2002;11(7):1729–1737.

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International Open-Access, Double-Blind, Peer-Reviewed, Refereed, Multidisciplinary Online Journal
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Impact Factor: 8.2

[9]. M. Chaudhary , K. Tyagi , A review on molecular docking and its application, International Journal of Advanced Research, 2320-5407 ,1141-1153 .

[10]. Shao Li , Qingyang Ding and Xin Wang , Network pharmacology 978-981-16-0753 , 1-465 .

[11]. Zainab Shahzadi , Zubaida Yousaf, Irfan Anjum , Network pharmacology and molecular docking: Combined computational approaches to explore the antihypertensive potential of face species , (2024) . 10.1186/s40643-024-00764-6.

[12]. Ansar vikhar Danish Ahmad , Subur W. khan , Syed Ayaz Ali et.al Network pharmacology combined with molecular docking and experimental verification to elucidate the effect of flavan-3-ols and aromatic resin on anxiety , scientific reports , (2024)14-9799 , 1-19 .

[13]. Nem Kumar Jain, Mukul Tailang , Balakumar Chandrasekaran et.al Integrating network pharmacology with molecular docking to rationalize the ethnomedicinal use of Alchornea laxiflora (Benth.) Pax & K. Hoffm. for efficient treatment of depression , Frontier in Pharmacology ,10.3389/fphar.2024.1290398 .

[14]. Anathi Msobo , Manamele Dannies Mashabela , Gerrit Koorsen et.al , Molecular docking and network pharmacology highlight salvianolic acids as potential inhibitors and therapeutic agents for COVID-19 treatment , Science Direct, (2025), 102991 , 1-9 .

[15]. Mohammad Junaid, Abbas Khan, Arif Ali et.al Network Pharmacology: Exploring the Resources and Methodologies Research geat (2018)18, 000-000 .

[16]. Akash Jain , Huzaif Mohd.khan , Jintendrasingh Rampure et.al NETWORK PHARMACOLOGY : A New Avenue For Drug Development , International Journal of Research Publication and Reviews , (2022)2582-7421, 552-572.

[17]. Shreyash S.Chavan , Shweta Gite Tools and Software used in Network pharmacology Studies , International Research Journal of Modernization in Engineering Technology and Science , (2024) 2582-5208 .

[18]. P.C.Agu , C.A.Aflukwa , O.V.Orji et.al ,Molecular docking as a tool for the discovery of molecular targets of nutraceuticals in disease management , Scientific reports,(2023)13398 .

[19]. Keval Raval , Tejas Ganatra Basics, types and applications of molecular docking: A review , IP International Journal of Comprehensive and Advanced Pharmacology , (2022)

[20]. 10.18231 .

[21]. Morris, G. M., et.al . Automated docking using a Lamarckian genetic algorithm and empirical binding free energy function. Journal of Computational Chemistry, (1998)19(14), 1639–1662.

[22]. Kim, S., et.al. PubChem substance and compound databases. Nucleic Acids Research,(2016) 44(D1), D1202–D1213.

[23]. Laskowski, R. A. SURFNET: A program for exploring molecular surfaces. Journal of Molecular Graphics, (1995)13(5), 323-330.

[24]. Trott, O., & Olson, A. J. . AutoDock Vina: Improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. Journal of Computational Chemistry,(2010) 31(2), 455-461.

[25]. Lengauer, T., & Rarey, M . Computational methods for biomolecular docking. Journal of Molecular Biology, (1996),280(3), 317-336. (Docking theory and scoring) .

[26]. Kitchen, D. B., Decornez, et.al ,Docking and scoring in virtual screening for drug discovery: methods and applications. Nat Rev Drug Discov, (2004) 3(11), 935–949.

[27]. Ferreira, L. G., Dos Santos, R. N., et.al , Molecular docking and structure-based drug design strategies. Molecules, (2015)20, 13384–13421.

[28]. Pushpakom, S., et.al , Drug repurposing: progress, challenges and recommendations. Nat Rev Drug Discov,(2019) 18, 41–58 .

[29]. Hopkins, A.L. “Network Pharmacology: The Next Paradigm in Drug Discovery.” Nature Chemical Biology,(2008) .

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International Open-Access, Double-Blind, Peer-Reviewed, Refereed, Multidisciplinary Online Journal
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Impact Factor: 8.2

[30]. Pushpakom, S. et al. "Drug Repurposing: Progress, Challenges and Recommendations." Nature Reviews Drug Discovery, (2019) .
[31]. Chen, R., Snyder, M. "Systems Biology and Precision Medicine." Science, 2019.
[32]. Zhao,S. et.al , TCM Network Pharmacology: A New Trend Towards Combining Computational and Experimental Technologies. Journal of Ethnopharmacology, (2021).
[33]. Hopkins, A.L. Network pharmacology: The next paradigm in drug discovery. Nat Chem Biol. 2008.
[34]. Li, S., et.al . Systems approaches to traditional Chinese medicine. Am J Chin Med. 2013.
[35]. Chen, H., et.al . Artificial intelligence in drug discovery. Drug Discov Today. 2018.
[36]. Meng, X.Y., et.al . Molecular docking: A powerful approach for structure-based drug discovery. Curr Comput Aided Drug Des. 2011.
[37]. Zhang, R., Zhu, X., Bai, H., et.al . Network pharmacology databases for traditional Chinese medicine: review and assessment. Frontiers in Pharmacology, (2019)10, 123.
[38]. Fig.1 https://share.google/images/x2kbDMHuyif87gh2x (4/Nov/2025).
[39]. Fig.2 https://share.google/Cgp31tsV1m0Wp12ua (2/Nov/2025).
[40]. Fig .3 https://share.google/wjLHZp7jl2LY4nk2m (7/Nov/2025).
[41]. https://share.google/images/WGjOAhGIXy1hAHeLL(7/Nov/2025)