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REVIEW ARTICLE

Insight of Computational Tools, Software and Databases in CADD

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ABSTRACT

Considering the emergence of several different computational tools, databases and software the process of drug study and development has become substantially easier. The novel development of drugs method is transformed by computer- aided drug design because it is rapid, economically viable, and efficient in terms of time and it has higher levels of pharmacological activity. It includes molecular docking, molecular dynamic simulations, quantitative structure activity relationship (QSAR) modelling. Uses several software platforms for virtual screening, lead optimization, designing novel chemotypes, emphasizes its application in rational drug design. It also underscores the significance that specialized databases are for supplying vital information for drug development, such chemical libraries, protein target repositories, Absorption, Distribution, Metabolism, Excretion, Toxicity (ADMET) databases.[1]

KEYWORDS

• CADD • Computational tools • Molecular docking

INTRODUCTION

CADD is a technologically advanced computational method used to find and develop a possible lead in the process of developing drugs. The following three phases are often included in the process involved in developing novel drugs, and they are as follows: Search for a novel substance with the requisite pharmacological action. Pharmacological and toxicological examinations additionally to expressional studies. The approval of an ideal pharmacological committee for the agents' clinical testing.

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The process of bringing a novel medication to market is extremely difficult, dangerous, and expensive in terms of labour, money, and time. On an average, the medication discovery and development process require 10 to 14 years and more than $1 billion in total funding.

The novel drug discovery and design widely uses different techniques such as rational drug design and structure-based drug design.

Rational drug design begins by developing understanding the nature of certain specific chemical interactions in the target organism or body, then modifying combinations of them to suit a therapeutic profile. It functions as

Discover an enzyme or receptor that is associated with the illness. Examine the receptor's or enzyme's structure and functionality. Develop a medication molecule that has advantageous interactions with the receptor or enzyme.[2]

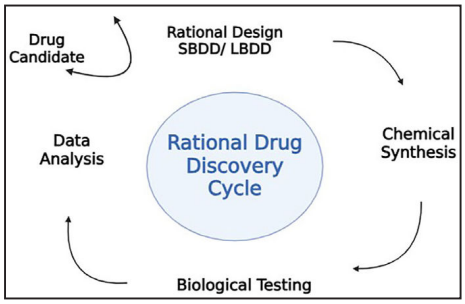


Figure 1: Rational Drug Discovery Cycle

Structure-based drug design is the process of designing new pharmaceuticals (ligands) using three-dimensional structures (proteins, enzymes, and receptors), and rational drug design is the innovative process of developing novel drugs based on biological target data. The surrounding amino acids determine the binding site, which is the location of the targeted protein. Molecular docking is the term used to describe the process of computationally creating molecules that "fit" the binding site. This determines the compounds' orientation and conformation at the desired binding site, often known as their "docking pose." The most likely stable interaction is predicted using a range of scoring parameters, and the best compounds are designed or chosen for experimental testing against the target protein. Through an understanding of how the intended structural alterations affect biological activity or the structure-activity relationship, these experimental data will enable subsequent rounds of SBDD. The target protein's optimal binder's co-crystal structure can verify thecomputationally predicted interactions between the molecule and the target protein.[3] It functions as

Determine which compounds bind to the target. Compile these molecules into a model of a pharmacophore. Utilize the pharmacophore model to forecast the molecular properties of compounds capable of binding to the target. Utilize a quantitative structure activity relationship (QSAR) to forecast novel compounds' activities. Utilize the QSAR model to create more potent analogs. Check the analogues' bioactivity.[4]

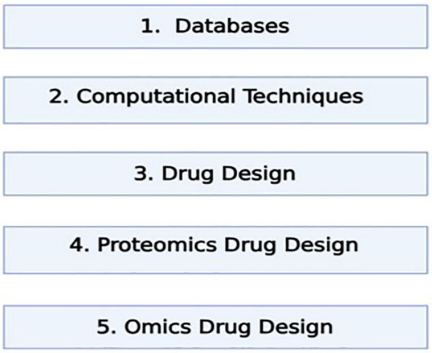


Figure 2: Structure based drug design paradiagram

Also, Ligand-based drug design in this method target is a ligand to correlate the chemical structure and biological activity (SAR, or Structure Activity Relationship), LBDD uses the chemical data of the active and non-active drugs in a tested series. Bioactivity screening and chemical synthesis are iterative processes used in LBDD. It is presumed in LBDD that substances with structural similarities also interact with the target protein and have the same biological activity.[5]

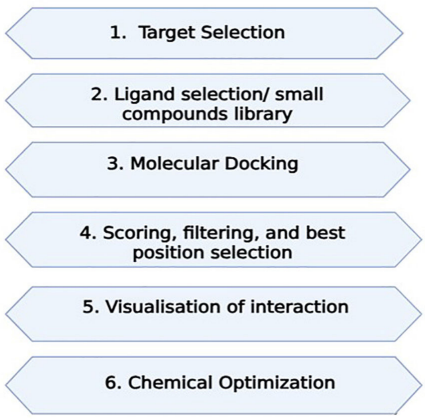


Figure 3: Flowchart of ligand based drug design steps

These methods function with the help of computational techniques and different software's by verifying receptor drug binding affinity. In the contemporary drug development process, computational techniques are essential for target identification, chemical screening, drug optimization, and safety profile prediction. They substantially accelerate up the development of new medical therapies while lessening the time, expense, and hazards connected with conventional approaches by simulating intricate biological processes, forecasting drug interactions, and improving lead compounds.[6]

1. Molecular modeling and visualization tools

Molecular modeling is an algorithm for identifying out the fundamental shape of any unknown molecule, no matter how big or little. In order to find novel potential therapeutic compounds, the methodology includes screening ligand libraries. It is the process of developing, adjusting, or depicting three-dimensional molecular structures and the corresponding physico-chemical characteristics.[7] Molecular visualization is critically important part of comprehending biomolecules is visualization. It renders difficult 2D or 3D chemical structures readily accessible and interactive by utilizing computer graphics techniques. It functions in helping to figure out molecular properties by providing structural information in a manner that is accessible.[8]

2. Techniques for molecular modeling

There are now two significant methodological strategies utilized in the development of novel medications**;**

Drug design from direct method - The X-ray crystallographic structure of the receptor is used in the direct drug design approach for identifying the ligand's mechanism of binding to the macromolecules' active site. The results of the indirect design structural model led us to validate the model using the direct drug design.[9]

Drug design from indirect method - The phenotypic of drug-treated cells and untreated cells can frequently be compared to ascertain a drug's method of action. There may be a limited number of possible pharmacological targets that could cause the specified phenotype in some situations; thus, a targeted examination of those prospective targets is probably appropriate. To identify the drug targets, however, worldwide analyses are necessary since in the majority of cases, the number of potential targets that could result in the phenotypic, like cell death, is potentially huge.[10]

3. Molecular Modeling Softwares

Avogadro - It is a comprehensive molecular editor optimized for various platforms in bioinformatics, molecular modeling, and computational chemistry. It provides a strong plugin architecture together with a versatile rendering foundation. Development of chemical structures, input file formatting, and output analysis of a broad range of computational chemistry tools are typical applications. Using the CML file format as its native document type, Avogadro aims to improve chemical data types' semantic accessibility.[11]

Schrodinger - The extensive software program known as Schrödinger's Molecular Modeling Suite was created by Schrödinger, Inc. It is intended for use in simulations, computational chemistry research, and molecular modeling. Numerous tools and algorithms are included in the suite for understanding the interactions, structures, and characteristics of molecules.[12]

MODELLER - It is used to model protein three-dimensional structures for homology or comparison. Computes a model with all non-hydrogen atoms automatically once the user aligns a sequence to be modeled with known related structures. By satisfying spatial constraints, Itcarries out comparative protein structure modeling. It is also capable of performing a wide range of other tasks, such as de novo modeling of loops in protein structures, optimizing different protein structure models in relation to a flexible objective function, multiple alignment of protein sequences or structures, clustering, searching sequence databases, protein structure comparison, etc.[13]

Visualization Softwares - Software frequently incorporates analytical and molecular visualization techniques to provide a thorough depiction of the structure and characteristics of molecules.

VMD - The purpose of VMD is to model, visualize, and analyze biological systems, including lipid bilayer assemblies, proteins, and nucleic acids. VMD can read standard

Protein Data Bank (PDB) files and show the contained structure, therefore it can be used to view more general molecules. Simple lines and dots, CPK spheres and cylinders, licorice bonds, backbone tubes and ribbons, cartoon designs, and more are just a few of the many ways that VMD can depict and color molecules. Molecular dynamics (MD) simulations can be animated and their trajectory examined using VMD. Specifically, by showing and animating a molecule undergoing simulation on a distant computer, VMD can serve as a graphical front end for an external MD program.[14]

PyMol - is a cross-platform molecular graphics application that has been widely used for 3D visualization of surfaces, trajectories, electron densities, proteins, nucleic acids, and tiny molecules. Furthermore, it can create movies, modify molecules, and trace rays. Along with several Python plugin tools, this Python-based program was created to improve its functionality and make drug design in PyMOL easier. Includes information on drug screening, molecular simulations, protein-ligand modeling, and visualization and analysis improvement.[15]

UCSF Chimera – It is sometimes known as "Chimera," is a molecular graphics program that maximizes interactive visualization and collaboration. It also makes it simple for users to createnew tools to expand its functionality. Initially it identifies active sites, optimizes proteins for docking, designs new drugs, analyze interactions.[16]

YASARA - In biocatalysis, structural understanding of the interactions between an enzyme and its substrates supports and directs experimental research. Computational methods like homology or molecular modeling can be used to produce structural information about an enzyme or a biocatalytic reaction system. A computer program designed for protein molecular modeling is necessary for this kind of computational work; we utilize YASARA Structure.[17]

COMPUTATIONAL TOOLS

Molecular Docking - is a method of computing that statistics the extent to which ligands will bind to receptor proteins. The approach entails forecasting the atomic level interaction between a protein and an extremely small chemical. A high-resolution three-dimensional representation of the target protein, acquired by means of methods such as X-ray crystallography, nuclear magnetic resonance spectroscopy, or cryo-electron microscopy, is necessary for the structure-based method. The docking programs AutoDock Vina, Discovery Studio, Surflex, AutoDock GOLD, Glide, MCDock, MOE-Dock, FlexX, DOCK, LeDock, rDock, ICM, Cdcker, LigandFit, FRED, and UCSF Dock are among the most widely used ones. AutoDock Vina, Glide, and AutoDock GOLD have been shown to be the best scoring options among the programs.[18]

Discovery Studio - Dassault Systèmes BIOVIA created the molecular modeling and simulation software program Discovery Studio. A variety of tools for protein modeling, virtual screening, molecular docking, and molecular dynamics simulation analysis are included. The molecular docking component is used to evaluate the intensity of the contact between a ligand (small molecule) and a target protein, as well as to forecast the mechanism of binding.[19]

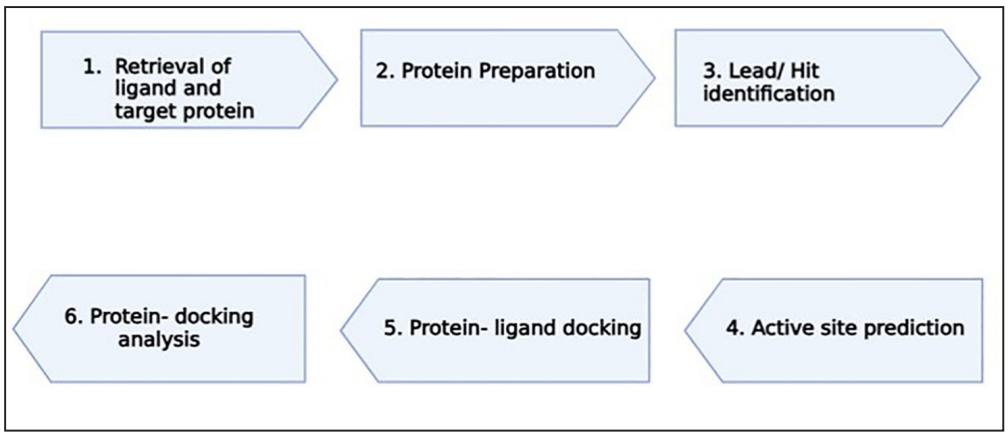


Figure 4: Flowchart of Molecular docking study

Molecular Dynamic (MD) Simulation - In a biomolecular system, such as a protein encased in water and maybe a lipid bilayer, the locations of every atom allow one to determine the force that each atom receives from the other atoms. Newton's equations of motion can therefore be used to forecast each atom's spatial location over time. Specifically, time is stepped through, with the forces acting on each atom being repeatedly calculated and then used to update the atoms' position and velocity. The trajectory that is produced is essentially a three-dimensional film that depicts the system's atomic-level configuration at each moment of the simulated time period. A model called a molecular mechanics force field is used to compute the forces in an MD simulation. This model is fitted to the outcomes of quantum mechanical computations and, usually, to specific experimental observations. In lead optimization, where a ligand is modified to enhance its efficacy or other characteristics, MD simulation is especially useful. On a qualitative level, simulations can offer a range of insights to direct the ligand optimization process: they can be used to determine the important interactions a ligand has with the binding pocket, forecast binding pocket rearrangements brought on by a ligand, or test and improve possible ligand positions.[20]

GROMACS is intended to carry out quick and effective MD simulations of biomolecular systems, including membranes, proteins, and nucleic acids. GROMACS supports coarse-grained and polarizable models and can handle a variety of force fields, including AMBER, CHARMM, OPLS, and GROMOS. Normal mode analysis, free energy calculations, improved sampling, and QM/MM calculations are just a few of the MD simulation types that GROMACS can do.

Proteins and nucleic acids in particular may be accurately and reliably simulated using AMBER's MD capabilities. For biomolecular simulations, AMBER's unique force fields such as AMBER, ff99SB, and ff14SB are frequently employed and verified. A variety of MD simulations, including increased sampling, free energy calculations, normal mode analysis, and QM/MM calculations, can also be carried out using AMBER. Additionally, AMBER is designed for high-performance computation and is capable of operating on clusters, multiple CPUs, and GPUs. Modern hardware technologies like multi-core processors, CUDA cores, and SIMD instructions are also available for AMBER to utilize. AMBER has the accuracy and stability to manage big, complicated systems.[21]

Quantitative Structure - Activity Relationship (QSAR) Modeling - is a computer technique used to ascertain how chemical structures and biological activity are related. The premise that alterations in bioactivity are linked to structural and molecular alterations in a class of chemicals forms the basis of QSAR studies. Drug discovery commonly uses QSAR (non-specific activity) to identify chemical compounds that may have strong inhibitory effects on certain targets while being low toxicity.[22] QSAR models are used to forecast the biological characteristics of new substances once they have been created and verified. Despite not being a fundamental component of QSAR approach, experimental testing of computational hits is highly desired and ought to be carried out as a last validation of generated models.[23]

Virtual Screening - The drug discovery approach uses Virtual screening, an in-silico technique. It involves the automatic evaluation of vast databases of molecular structures by computational techniques. Finding compounds that are more likely to bind to the molecular target usually a protein or enzyme receptor is envisaged when VS is used. Functions as a filter, getting rid of more molecules so that there are significantly fewer final candidate molecules that could be turned into drugs. The initial selection of molecules that have the potential to be useful medications is based on their similarity to known functioning pharmaceuticals or on their features that support their action. Following analysis of the candidate ligands, compounds with pharmacophoric groups that suggest a high probability of toxicity are removed. Finding the ideal positions for potential ligands is the next stage. In a database of structures, VS enables the selection of compounds that are more likely to exhibit biological activity against a target of interest.[24]

A wide spectrum of VS applications and tools are available: Structure based LiSiCA, SABER, ViCi, LigCSRre, SurflexSim, Pharma, as well as ligand based VS; VS—PyRx, AutoDock Vina, Schrödinger, Discovery studio, DOCK Blaster, DockoMatic, iGemDock, and GOLD.[5]

A new method for drug development has

been brought about by recent advances in the molecular disease pathways inside the cell as well as growing knowledge about protein binding partners. Rather than focusing only on the catalytic active site of a single enzyme or protein, there is interest in developing medications that alter protein-protein interactions. In order to aid in the discovery of medications that effectively disrupt and inhibit protein-protein interactions, computational techniques to forecast protein-protein interaction modes and protein interface hot spots have gained a lot of consideration.[26]

Protein Databases

Protein databases are a treasure trove of possible novel therapeutic targets. Drug discovery pipelines benefit most from early access to a comprehensive grasp of all facets of protein biology. Collecting universal proteins (like UniProt), identifying protein families and domains (like Pfam), reconstructing evolutionary trees (like TreeFam), and analyzing protein structures (like PDB) are all goals of building protein databases. PDB is the classic instance of a protein database; it is the principal database for 3D structures of biological macromolecules as established by NMR and X-ray crystallography. The protein sequence and functional information offered by UniProt is extensive, of excellent quality, and publicly available. Three member databases are currently part of UniProt: UniProt Archive (UniParc), UniProt Knowledgebase (UniProtKB), and UniProt Reference Clusters (UniRef).[27]

Chemical Databases

The foundation of computer aided drug development, whether it be bioinformatics or chemoinformatics, is chemical databases and resources. These databases provide data that can be utilized to create knowledge based models for drug compound discovery and design.

ChEMBL extensive database of bioactivity information for a wide range of chemical substances that is openly accessible. It offers useful data for studies on computationally assisted drug design (CADD) and is run by the European Bioinformatics Institute (EBI). Data from experimental assays and bioactivity measurements, particularly those pertaining to the interaction of small compounds with biological targets like proteins and enzymes, are the main emphasis of it. The database currently includes 5200 protein targets and 5.4 million bioactivity measurements for over 1 million chemicals. There is a web-based interface for access.[28]

DrugBank - Combining extensive drug target (i.e., sequence, structure, and pathway) information with detailed drug (i.e., chemical, pharmacological, and pharmaceutical) data makes the DrugBank database a unique bioinformatics and cheminformatics resource. For example, the database's overall number of experimental medications has increased by about 300%, drug-drug interactions by nearly 600%, and SNP-associated pharmacological effects by more than 3000%.[29]

5. Challenges and prospects

Boosting the effectiveness of virtual screening; increasing the quantity and caliber of online computing resources, advancing computational chemo-genomics, fortifying medication design targeting many molecular targets, In order to maximize the search for bioactive substances for the treatment and/or prevention of diseases, toxicity models and side effects should be improved, and interactions with other disciplines should be strengthened. A new push to push the limits of drug discovery is being driven by ongoing improvements in informatics infrastructure and methodological advancement. Molecular property and behavior prediction is one area where AI-related methods are becoming increasingly important due to the volume of data available. On the structure based side, methods for AI rescoring, delta learning, and deep learning based 3D pocket mapping have been created and reported recently. The prioritization performance provided by traditional scoring procedures has been surpassed by these new techniques.[30]

CONCLUSION

The pharmaceutical sector has undergone a remarkable transformation thanks to the combined strength of CADD's databases, software, and computational tools. These technologies have increased medication development's speed and cost-effectiveness while also broadening the range of possible outcomes. The combination of computational methods with clinical data and experimental research will enable more individualized and

efficient treatments as they develop further, spurring healthcare innovation for years to come. As new advancements are anticipated to result in tools for illness identification and the screening of possible lead compounds, new technologies and computational algorithms are needed to advance the CADD method.[31]

Conflict of Interest: Nil

REFERENCES

1. Niazi, S.K., & Mariam, Z. (2024). Computer-Aided Drug Design and Drug Discovery: A Prospective Analysis. Pharmaceuticals, 17(1), 22.
2. Soma Mandal, Mee'nal Moudgil, Sanat K. Mandal, Rational drug design, European Journal of Pharmacology, Volume 625, Issues 1–3, 2009, Pages 90-100, ISSN 0014-2999.
3. Batool, M., Ahmad, B., & Choi, S. (2019). A Structure-Based Drug Discovery Paradigm. International Journal of Molecular Sciences, 20(11), 2783. https://doi.org/10.3390/ijms20112783
4. Prajapat, P., Agarwal, S., &Talesara, G. L. (2017). Significance of computer aided drug design and 3D QSAR in modern drug discovery. J Med Org Chem, 1(1), 1.
5. Vivek Yadav, Jurnal Reang, Vinita, Rajiv Kumar Tonk, Chapter 3 - Ligand-based drug design (LBDD), Editor(s): Mithun Rudrapal, ChukwuebukaEgbuna, In Drug Discovery Update, Computer Aided Drug Design (CADD): From Ligand-Based Methods to Structure-Based Approaches, Elsevier, 2022, Pages 57-99, ISBN 9780323906081
6. Hemant Arya, Mohane Selvaraj Coumar, Chapter 4 - Lead identification and optimization, Editor(s): Tarun Kumar Bhatt, Surendra Nimesh, The Design & Development of Novel Drugs and Vaccines, Academic Press, 2021, Pages 31-63, ISBN 9780128214718
7. Temitope Isaac Adelusi, Abdul-Quddus Kehinde Oyedele, Ibrahim DamilareBoyenle, Abdeen Tunde Ogunlana, RofiatOluwabusola Adeyemi, Chiamaka Divine Ukachi, Mukhtar Oluwaseun Idris, Olamide Tosin Olaoba, Ibrahim OlaideAdedotun, Oladipo Elijah Kolawole, Yin Xiaoxing, Misbaudeen Abdul-Hammed, Molecular modeling in drug discovery, Informatics in Medicine Unlocked, Volume 29, 2022, 100880, ISSN 2352-9148
8. Keil, Matthias & Marhoefer, Richard & Rohwer, Andreas & Selzer, Paul & Brickmann, Jurgen & Korb, Oliver & Exner, Thomas. (2009). Molecular visualization in the rational drug design process. Frontiers in bioscience: a journal and virtual library. 14. 2559-83. 10.2741/3398.
9. Tulloch L.B., Menzies S.K., Coron R.P., Roberts M.D., Florence G.J., Smith T.K. Direct and indirect approaches to identify drug modes of action. IUBMB Life. 2018 Jan; 70(1): 9-22. doi: 10.1002/iub.1697. Epub 2017 Dec 6. PMID: 29210173.
10. Ashish A. Gawai, Kailash R. Biyani, Sanjib Das, Ganesh G. Tapadiya, Santosh N. Mokale, Sachin A. Dhawale, Design, Synthesis, Molecular Docking, and Preliminary Pharmacological Screening of some New Benzodthiazol-2-ylamino Containing Chromen-2- one Derivatives with Atypical Antipsychotic Profile, Current Computer-Aided Drug Design, 10.2174/1573409919666230202105207, **19**, 6, (465-475), (2023).
11. Hanwell, M.D., Curtis, D.E., Lonie, D.C. *et al.* Avogadro: an advanced semantic chemical editor, visualization, and analysis platform. J Cheminform **4**, 17 (2012).
12. Schrodinger Molecular Modelling Suite – DUCC. ducc.du.ac.in/wp3/schrodinger-molecular-modelling-suit.
13. Sanne Abeln, Klaas Anton Feenstra, Jaap Heringa, Protein Three-Dimensional Structure Prediction, Editor(s): Shoba Ranganathan, Michael Gribskov, Kenta Nakai, Christian Schönbach, Encyclopedia of Bioinformatics and Computational Biology, Academic Press, 2019, Pages 497-511, ISBN 9780128114322
14. Li H., Wei X. A Concise Review of Biomolecule Visualization. Curr Issues Mol Biol. 2024 Feb 2; 46(2): 1318-1334. doi: 10.3390/cimb46020084. PMID: 38392202; PMCID: PMC10887528.
15. Iqbal, Muhammad & Shahab, Muhammad & Zheng, Guojun& Sun, Xinxiao& Yuan, Qipeng. (2025). 41598 2024 Article 78232.
16. Couch G.S., Hendrix D.K., Ferrin T.E. Nucleic acid visualization with UCSF Chimera. Nucleic Acids Res. 2006 Feb 14; 34(4): e29. doi: 10.1093/nar/gnj031. PMID: 16478715; PMCID: PMC1368656.
17. Henrik Land, Maria Svedendahl Humble Series**:** Methods In Molecular Biology >, Book**:** Protein Engineering Protocol | DOI: 10.1007/978-1-4939-7366-8_4
18. Torres, P.H.M., Sodero, A.C.R., Jofily, P., & Silva-Jr, F.P. (2019). Key Topics in Molecular Docking for Drug Design. International journal of molecular sciences, 20(18), 4574. https://

doi.org/10.3390/ijms20184574

19. Agu, P.C., Afiukwa, C.A., Orji, O.U. *et al.* Molecular docking as a tool for the discovery of molecular targets of nutraceuticals in diseases management. Sci Rep 13, 13398 (2023).

20. Hollingsworth S.A., Dror R.O. Molecular Dynamics Simulation for All. Neuron. 2018 Sep 19; 99(6): 1129-1143. doi: 10.1016/j. neuron.2018.08.011. PMID: 30236283; PMCID: PMC6209097.

21. Super User. "Detailed Comparison: Gromacs vs. Amber for Molecular Dynamics Simulations." Parssilico.com, 2025, parssilico.com/blogs/85-gromacs-vs-amber-md-software. Accessed 1 Feb. 2025.

22. Pratibha Chaurasia, Anasuya Bhargav, Srinivasan Ramachandran, Chapter 28 - Free tools and databases in ligand and structure-based drug design, Editor(s): Kunal Roy, Cheminformatics, QSAR and Machine Learning Applications for Novel Drug Development, Academic Press, 2023, Pages 701-727, ISBN 9780443186387.

23. Verma, J., Khedkar, V.M., & Coutinho, E.C. (2010). 3D-QSAR in drug design-a review. Current topics in medicinal chemistry, 10(1), 95-115.

24. Oliveira TAd, Silva MPd, Maia EHB, Silva AMd, Taranto AG. Virtual Screening Algorithms in Drug Discovery: A Review Focused on Machine and Deep Learning Methods. Drugs and Drug Candidates. 2023; 2(2):311-334.

25. Hemant Arya, Mohane Selvaraj Coumar, Chapter 4 - Lead identification and optimization, Editor(s): Tarun Kumar Bhatt, Surendra Nimesh, The Design & Development of Novel Drugs and Vaccines, Academic Press, 2021, Pages 31-63, ISBN 9780128214718

26. author = "J. Bienstock, Rachelle", title = "Computational Drug Design Targeting Protein-Protein Interactions", journal= "Current Pharmaceutical Design", year = "2012", volume = "18", number = "9", pages = "1240-1254", doi = "https://doi.org/10.2174/138920012799362891", publisher = "Bentham Science Publishers", issn = "1873-4286", type = "Journal Article"

27. Dong Zou, Lina Ma, Jun Yu, Zhang Zhang, Biological Databases for Human Research, Genomics, Proteomics & Bioinformatics, Volume 13, Issue 1, 2015, Pages 55-63, ISSN 1672-0229.

28. Paolini G.V., Shapland R.H.B., van Hoorn W.P., Mason J.S., Hopkins A.L. Global mapping of pharmacological space. Nat. Biotechnol. 2006; 24: 805–815. doi: 10.1038/nbt1228

29. David S. Wishart, Yannick D. Feunang, An C. Guo, Elvis J. Lo, Ana Marcu, Jason R. Grant, Tanvir Sajed, Daniel Johnson, Carin Li, ZinatSayeeda, Nazanin Assempour, IthayavaniIynkkaran, Yifeng Liu, Adam Maciejewski, Nicola Gale, Alex Wilson, Lucy Chin, Ryan Cummings, Diana Le, Allison Pon, Craig Knox, Michael Wilson, DrugBank 5.0: a major update to the DrugBank database for 2018, Nucleic Acids Research, Volume 46, Issue D1, 4 January 2018, Pages D1074–D1082

30. Bassani, D., & Moro, S. (2023). Past, Present, and Future Perspectives on Computer-Aided Drug Design Methodologies. Molecules, 28(9),3906. https://doi.org/10.3390/molecules28093906

31. Baig, M.H., Ahmad, K., Rabbani, G., Danishuddin, M., & Choi, I. (2018). Computer Aided Drug Design and its Application to the Development of Potential Drugs for Neurodegenerative Disorders. Current neuropharmacology, 16(6), 740–748. https://doi.org/10.2174/1570159X15666171016163510