IJPSR (2024), Volume 15, Issue 1 **(Review Article)**

INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES AND RESEARCH

Received on 25 May 2023; received in revised form, 29 July 2023; accepted, 21 November 2023; published 01 January 2024

CADD: AN ABSOLUTE REPLACEMENT FOR TRADITIONAL DRUG DISCOVERY

Vaishali Pardeshi, Bhagyashree Pawar Gaikwad, Anuja Uday Vaidya, Khushal Madanlal Ghanchi *, Rohan Sunil Kengarkar and Tarun Singh Rajput

Abhinav Education Society College of Pharmacy, Narhe, Pune - 411041, Maharashtra, India.

Keywords:

Drug design, Drug discovery, Molecules, CADD, Lead optimization, Lead discovery

Correspondence to Author:
Khushal Madanlal Ghanchi

Pharm D Student,
Abhinav Education Society College of Pharmacy, Narhe, Pune - 411041, Maharashtra, India.

E-mail: khushalghanchi0987@gmail.com

ABSTRACT: CADD is a powerful method to discover possible therapeutic compounds in conventional drug discovery. It has now surpassed all other high-throughput screening options, commonly used in drug discovery and development. The creation and optimization of several clinically utilized medications have significantly advanced thanks to CADD, or computer-aided drug design. Computer-aided drug design can take one of two methods: (1) Ligand-based (Analogue based) or (2) Structure-based (Target Based). All of these methods rely on MM force fields to represent atomic-level interactions and define molecular shapes, energy, and motion. The two most common approaches to drug design are structure-based drug design and ligand-based drug design. We can learn about drug-receptor interactions from it. Structure-based drug design includes the discovery of binding sites as well as docking and stocking, virtual screening, compound selection, and lead optimization. Quantitative structure-activity relationships (QSAR), pharmacologic modeling and other processes are aspects of the structure-based drug design process. As can be seen, CADD assists in recognizing appropriate pharmacological properties and compatibility to get an advantage in pre-clinical trials.

INTRODUCTION: Computer-aided drug design (CADD) provides a variety of tools and methods to help with drug design at different phases, minimizing overall research expenditure and shortening the time it takes to develop a medication. The process of discovering new drugs and developing them is a lengthy, expensive, hazardous, and complex one with few counterparts in the business world. The pharmaceutical industry commonly uses computer-aided drug design (CADD) techniques to improve the process of drug discovery [1, 2].

QUICK RESPONSE CODE

DOI: 10.13040/IJPSR.0975-8232.15(1).12-19

This article can be accessed online on www.ijpsr.com

DOI link: https://doi.org/10.13040/IJPSR.0975-8232.15(1).12-19

During the lead optimization phase of drug development, using computational methods offers a sizable economical advantage. Pharmacological research laboratories dedicate a great deal of time and resources to the various stages of drug discovery, beginning with the identification of therapeutic targets, candidate drug discovery, and drug optimization through pre-clinical and extensive clinical experiments to assess the efficacy and safety of newly developed drugs.

The largest pharma companies have made significant investments in the regular Ultra-High Throughput Screening (u-HTS) of several drug-like candidates [3]. In contrast, drug design and optimization progressively use computer-based virtual screening. Technological breakthroughs in DNA microarray research analyze hundreds of genes linked to disease and can be used to learn more in-depth information about the disease

targets, metabolic pathways, and pharmacological toxicity. Empirical quantum mechanics, statistical mechanics and molecular mechanics are some of the theoretical methods available. This most recent development has inspired to integrate explicit solvent effects. All of this work is based on high-end computer graphics, which are mostly supported by workstations.

Drug Discovery Process: Drug discovery is a set of procedures that, identify the drug molecules for the effective management or control of disease causes. To begin, many chemical compounds are screened to find the best disease targets. Understanding the structure of the drug receptor is required to modify the drug molecules to the binding site [4].

The drug discovery process starts with understanding the therapeutic index for which the drug to be designed. It consists of the following steps

Lead Drug Discovery:

- Target Drug Discovery
- Lead Identification
- Lead Optimization [5]

Pre-clinical and Clinical trials to confirm the drug's safety, efficacy and side effects [6].

- Animal trials
- Clinical trials

The steps involved in getting FDA clearance for a newly discovered drug and releasing it onto the market so that the general public may utilize it [7].

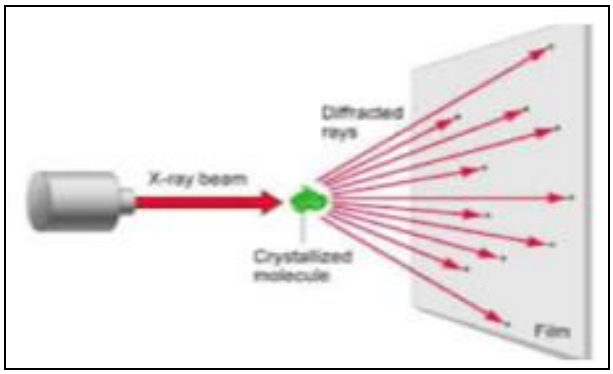
- Additional research after commercialization
- Development of the medication

Pre-clinical development and the discovery of novel drugs often take 3-6 years. Before a product is sold on the market, it may take up to 10 years for the clinical trials to be completed. A successful drug's market entry typically takes 10–15 years and more than $1.2 billion. About 250 of the 5000–10000 evaluated compounds on average are chosen for preclinical studies. Only one of the five is authorized by the FDA after a thorough analysis of the newly found medicine. Only five of them enter clinical trials.

Major Types of Approaches in CADD:

- Direct approach / Structure-based Drug Design
- Indirect approach / Ligand-based Drug Design

Direct Approach / Structure-Based Drug Design: Structure-based drug design, often referred to as direct drug design, is based on the three-dimensional structure of the biological target, which may be established using methods like X-ray crystallography or NMR spectroscopy. It could be feasible to anticipate the experimental structure of a target if the experimental structure of a protein that is similar to the target is known. Potential drugs that are predicted to connect to the biological target with high affinity and selectivity can be developed using interactive visualizations and a medicinal chemist's intuition. Structure-based design is one of the oldest techniques for producing drugs. A tool that has benefited in the quest for new medications is structure-based drug design. We investigate the structural dynamics and electrical properties of ligands using parallel simulations [8]. This has aided in the quick advancement of structure-based medication creation. Structure-based drug design may be loosely categorized into two groups 1. Database searches or Ligand-based Drug Design 2. Receptor-Based Drug Design.



X-ray Crystallography: A method of extremely high-resolution microscopy that improves our

understanding of how proteins work by allowing us to see protein structures at the atomic level. An X-ray beam is fired at a crystal, scattering the light in many different directions. This procedure, called X-ray crystallography, is used to ascertain how atoms are arranged within a crystal. The angles and intensities of these diffracted beams may be used by a crystallographer to provide a three-dimensional picture of the density of electrons within the crystal [9].

X-rays are useful for studying within crystals because their wavelengths are comparable to the size of atoms. X-Ray Crystallography utilizes the regularity of a crystal's light diffraction to determine the structure of a molecule or an atom. After that, they "strike" the crystallized molecule with an X-ray beam. As the X-rays strike them, the electrons around the molecule diffract [10].

NMR Spectroscopy: Since clinically used drugs are usually natural or synthetic compounds, a quantitative approach by solution-state NMR is quite useful in determining the contamination profile of the drugs, outlining the makeup of drug products, and examining drug metabolites in bodily fluids. It is also useful in studying the trends and kinetics of proteins on solid surfaces and enzyme allostery [11].

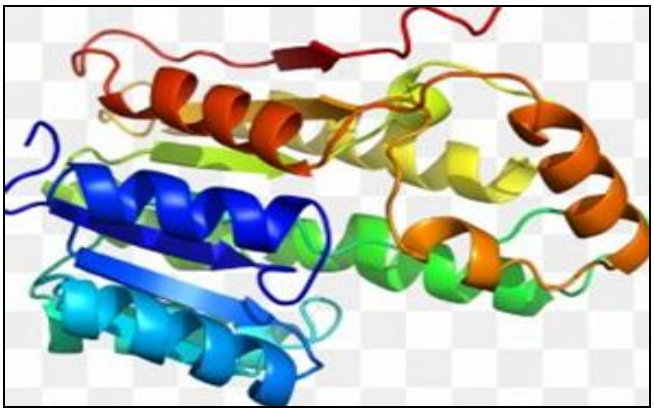
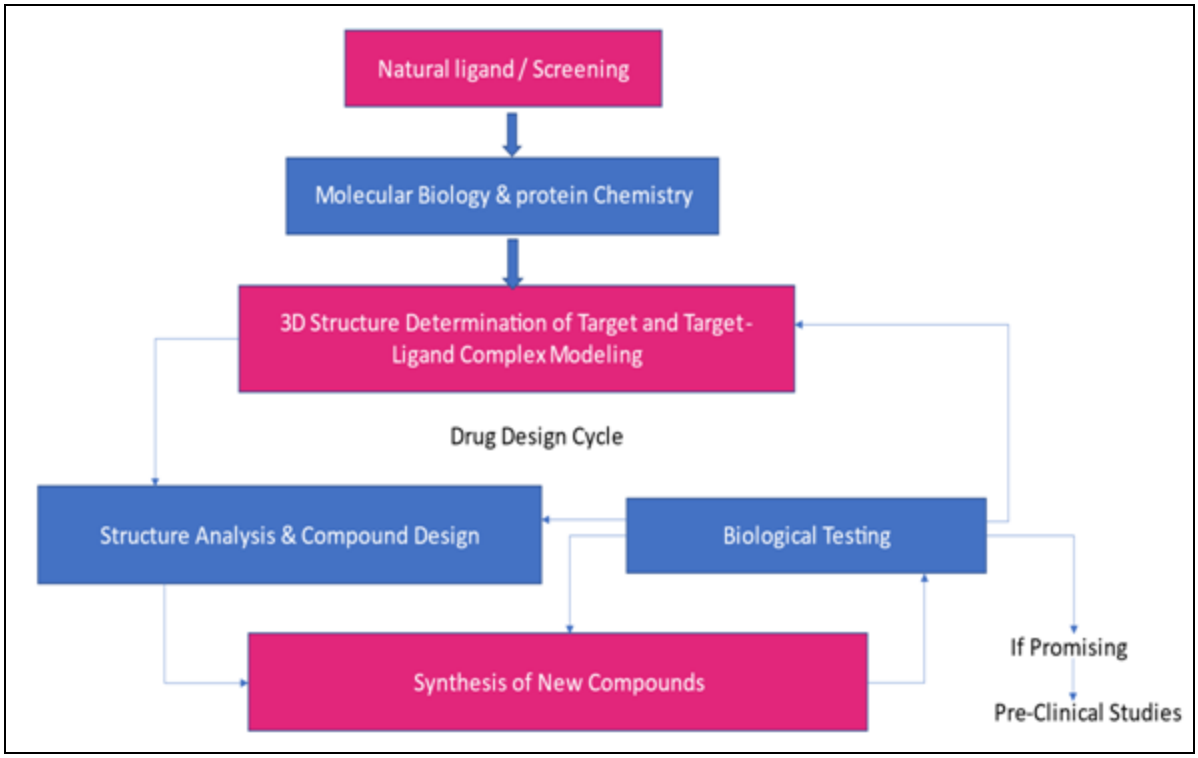


FIG. 1: TPR-LIKE FOLDING & PROTEIN FIS1 MEDIATES MITOCHONDRIAL FISSION

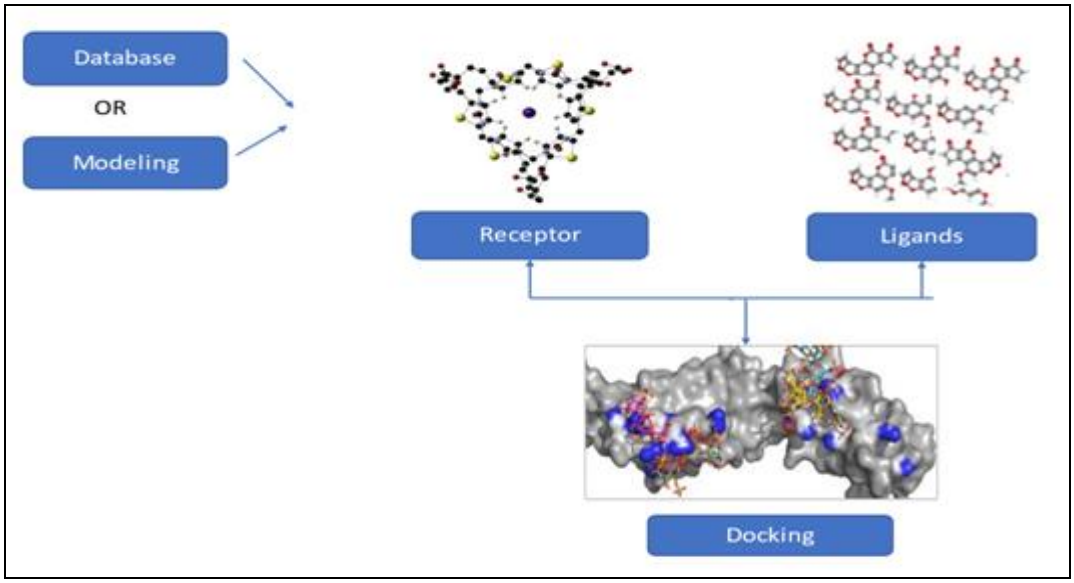
Homology Modelling: Any SBDD approach must have the target's 3D structure as a prerequisite. To identify the three-dimensional (3D) structure of molecules, a variety of integrated structural biology methods are available, such as single-particle cryo-electron microscopy, NMR spectroscopy, and X-ray crystallography. However, because it is technically challenging to generate, purify, or characterize proteins, it is challenging to determine the structure of a therapeutic protein. *In-silico* methods like homology modeling, threading, or ab initio modeling are used to approximate the three-dimensional structure of a target in the absence of any experimental structures [12]. The most reliable of the three computer methods for predicting the 3D structure of a target is homology modeling, which uses the structural features of a protein that is identical to the target in question by more than 40%. (Known as template structure). Homology modeling is based on the idea that two extremely

similar sequences have equivalent structural traits. When there isn't a template structure (>40% sequence similarity) available in the protein structure database but the target sequences have the same protein fold as those of known structures, threading or fold recognition is the method of choice [13].

Structure-Based Drug Design:



Indirect Approach / Ligand Based Drug Design: Drug Design Based on Ligands An strategy called ligand-based drug design, which focuses on understanding of compounds that bind to the desired biological target, is employed in the lack of 3D information about the receptor.



The alternate strategy is LBDD if no structural data for the therapeutic target is available. LBDD just needs structural data and data on the bioactivity of small molecules, unlike SBDD, which also requires a previous understanding of mechanisms of action. The LBDD hypothesis states that molecules with

comparable structural characteristics are likely to have related properties. A critical stage in LBDD is acquiring and preparing small molecule libraries. Chemical structures are frequently created, processed, and dealt with using molecular graphs. Atoms and bonds are represented in a molecular graph as nodes and edges, respectively, or as a combination of nodes and edges [14].

Two common methods of interacting with molecular graphs are linear notations and connection tables. A connection table has sections with details on the types of atoms, connections, and coordinates. Mol2, SDF, pdb and other file formats are examples of connection tables. Combinations of alphanumeric characters make up linear notation. The Wiswesser line notation and the SMILE (simplified molecular input line entry specification) are two examples of linear notations. When storing or sending millions of tiny molecules, linear notations are preferred to connection tables because they are more compact [15]. The most popular LBDD methods are pharmacophore modeling, quantitative structure-activity relationships (QSAR) and molecular similarity-based search. Pharmacophore modeling and 3D quantitative structural activity interactions are the most significant and often utilized techniques in ligand-based drug design (3D QSAR). For lead optimization and lead discovery, they can provide suitable prediction models. Search for molecular fingerprints and structures QSAR for pharmacophore [14].

Molecular Similarity-based Search: Molecular similarity-based search is the LBDD strategy that is easiest to use to find attractive small molecules. LBDD and SBDD techniques both independently employ and include molecular similarity-based search when exploring small chemical libraries utilizing molecular descriptors. Molecular descriptors include, among many others, molecular weight, atom types, bond lengths, surface area, electro negativities, atom distributions, aromaticity indices, solvent properties, and many others. It requires experiments, the application of quantum mechanical tools, or previous knowledge to create molecular descriptors. Molecular descriptors are classified as 1D, 2D, or 3D descriptors based on their "dimensionality". One-dimensional descriptors include scalar properties of molecules such as molecular weight, logP values, and molar refractivity. 2D descriptors derived from chemical composition or configuration include topological indices and 2D fingerprints, for instance. A molecule's conformation is where 3D properties originate. Examples of 3D descriptors include electrostatic potentials, dipole moments, the highest occupied/lowest empty molecular orbital energies, and others [16].

Common Software to Predict Molecular Descriptors

- ADAPT >260 (topological, geometrical, electronic, physicochemical) [17].
- ADMET Predictor>290 (constitutional, functional group counts, topological, E-state [18].
- CODESSA >1500 (constitutional, topological, geometrical, charge related, semiempirical, thermodynamical) [19].
- DRAGON >5200 (constitutional, geometrical, topological, 2D autocorrelations, WHIM, GETAWAY, RDF, functional groups, properties, 2D binary, and 2Dfrequency fingerprints, *etc*.) [15].
- Pre-ADMET >955 (constitutional, geometrical, topological, physicochemical, *etc*.) [15].

Quantitative Structure Activity Relationship (QSAR): The link between chemical structures and biological activity may be determined using a computer technique called QSAR, as the term suggests. The quantitative structural property relationship (QSAR) technique is frequently employed in the rational drug design process, but it is also frequently used to forecast other physicochemical properties and is known as such. The underlying principle of QSAR is the possibility of linked biological activity between compounds with similar structural characteristics [20].

Commonly used QSAR Methods ad descriptions are given below:

HQSAR Descriptor type: 2D

Description: Hologram by combining binary patterns with biologically relevant fingerprints, QSAR is a technique that leverages molecular substructures to produce molecular holograms [22].

CoMFA Descriptor type: 3D

Description: The steric and electrostatic properties of molecules are associated to their biological activities by comparative molecular field analysis [23].

CoMSIA Descriptor type: 3D

Description: In addition to the parameters for steric and electrostatic contribution, comparative molecular similarity indexes also include terms for hydrophobicity, H-bond donor/acceptor, and hydrophobicity [24].

Pharmacophore Modelling: A pharmacophore is a combination of "steric" and "electronic" properties that must be assembled in a three-dimensional (3D) configuration in order to interact with a certain biological target structure optimally and trigger or inhibit its biological response. The creation of ligand-based pharmacophore models is predicated on data that is currently accessible on the biological functions of drugs and ligands. Instead of representing a real molecule, ligand, or link between functional groups, a pharmacophore offers an abstract description of the properties of molecules that are important for molecular interactions with macromolecular ligands [21].

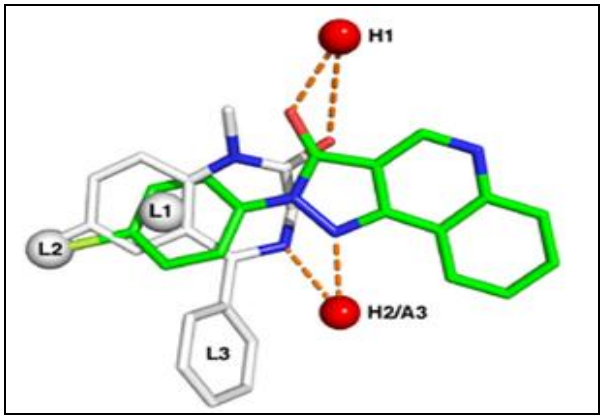


FIG. 2: PHARMACOPHORE

Virtual Screening: A computational approach used in drug design is virtual screening. This technique includes associating extensive chemical libraries to specific locations on target molecules, such as proteins and the substances being tested. Similar to physical screening, virtual screening aids in finding or identifying the structures most likely to bind to a pharmaceutical target (protein receptors or enzymes). The process of finding new drugs and therapeutic targets, which are generally protein receptors or enzymes, now includes virtual screening. Virtual screening scenarios prioritize improving targeted combinational libraries of accessible compounds from internal compound repositories, even though filtering the entire universe may be more feasible. Virtual screening is more efficient than traditional screening in terms of cost, time, quantity of possible substances scanned, and speed [25].

Application of Computer-Aided Drug Discovery: Moving the drugs from concept to clinic: Improvements in computational technique and parallel hardware support have made it possible for *in-silico* methods, particularly the structure-based drug design method, to speed up the selection of new targets in the drug discovery process from the identification of hits to the optimization of the lead compound [26]. Through the application of this technique, certain small compounds were developed that are now in clinical trials or have received approval for medicinal use [27].

CADD for Development of Potential Drugs for Neurodegenerative Disorders (NDs): The development of possible treatments for NDs provides a significant challenge because current therapies are ineffective and frequently unable to prevent neuro-degeneration. CADD has shown to be a successful method for creating medication candidates to treat neurodegenerative disorders [28]. It produces the most promising therapeutic candidate by removing molecules with undesirable characteristics. Drug development for Alzheimer's based on computer-aided drug design [29].

New Advancement in CADD: The availability of data affects a drug discovery and development effort's efficiency. Scientific literature and case reports include a significant quantity of knowledge about chemical compounds, biological sequences, and relevant fields. These data are collected and grouped in the databases that are shown below. Numerous biological databases are described each year. In order to assist in the development of combinatorial algorithms, computational libraries are actively being created at the same time. These are the main areas where computer-aided drug design is focused [31, 32].

Some small molecule databases:

1. http**:**//pubchem**.** ncbi**.** nlm**.** nih**.** gov/ http**:**//pubchem**.** ncbi**.** nlm**.** nih**.** gov [33]
2. ACD http://www.mdli.com [34]
3. https://pubs.acs.org/doi/abs/10.1021/ci049714 [35]
4. Ligand: https://onlinelibrary.wiley.com/doi/abs/10.1002/jcc.21467#pane-pcw-references [36]
5. Drug Bank Database: https://link.springer.com/article/10.1186/s13321-016-0138-2 [37]
6. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3918487 [38]

CONCLUSION: The field of drug discovery and development benefits greatly from the use of computer-based drug design since it allows for the rapid and cost-effective identification of the most promising therapeutic candidates. Always encouraging for the future of drug discovery. Computer-aided medication design has helped scientists conduct a number of spectacular experiments in recent years, and it will be crucial in the coming years. Given the progress made to date, computer-aided drug design holds great promise for assisting in the search for further therapies in the future. The recent history of CADD's effectiveness in drug discovery has shown how valuable it is to the process of developing new drugs. Target molecules, lead compounds, screening, and optimization are all topics that CADD offers useful information on. QSAR and combinatorial chemistry are recent innovations. Various databases and new software tools available provide the basis for the design of ligands and inhibitors that require specificity. The CADD method is based on several techniques, design phases, docking, pharmacophore modeling, and homology modeling. Understanding the three-dimensional features of drug-molecule-based receptor interaction is another benefit of computational chemistry.

ACKNOWLEDGMENT: The authors would like to formally thank everyone who contributed to rendering this article possible. The HOD and faculty of the Abhinav Education Society's College of Pharmacy in Narhe, Pune, are also acknowledged by the authors for their valuable inputs and discussion that significantly improved the quality of this review article.

CONFLICTS OF INTEREST: The Authors declare no conflict of interest.

REFERENCES:

1. Yu W and MacKerell AD: Computer-Aided Drug Design Methods. Methods Mol Biol 2017; 1520: 85-106. doi: 10.1007/978-1-4939-6634-9_5. PMID: 27873247; PMCID: PMC5248982.
2. Daina A, Blatter MC, Baillie Gerritsen V, Palagi PM, Marek D and Xenarios I: Drug Design Workshop: A web based Educational Tool To Introduce Computer-Aided Drug Design to the General Public. Journal of Chemical Education 2017; 94(3): 335-44.
3. Parker CN and Bajorath J: Towards unified compound screening strategies: a critical evaluation of error sources in experimental and virtual high-throughput screening. QSAR Comb Sci 2006; 12: 1153–1161.
4. Hoque I, Chatterjee A, Bhattacharya S & Biswas R: An approach of computer-aided drug design (CADD) tools for *in-silico* pharmaceutical drug design and development. Int J Adv Res Biol Sci 2017; 4(2): 60-71.
5. Dubey RD: Computer-aided drug design: A review. Research Journal of Engineering and Technology 2(3): 104-108.
6. Thomsen GM, Gowing G, Svendsen S & Svendsen CN: The past, present, and future of stem cell clinical trials for ALS. Experimental Neurology 2014; 262: 127-137.
7. Van Norman GA: Drugs, devices, and the FDA: part 1: an overview of approval processes for drugs. JACC: Basic to Translational Science 2016; 1(3): 170-179.
8. Batool M, Ahmad B and Choi S: A Structure-Based Drug Discovery Paradigm. International Journal of Molecular Sciences 2019; 20(11): 2783. https://doi.org/10.3390/ijms20112
9. Carvalho AL, Trincão J & Romão MJ: X-ray crystallography in drug discovery. Ligand-macromolecular interactions in drug discovery. Methods and Protocols 2010; 31-56.
10. Drenth J: Principles of protein X-ray crystallography. Springer Science & Business Media 2007.
11. Singh MK & Singh A: Characterization of Polymers and Fibers. Woodhead Publishing 2021.
12. Muhammed MT and Aki-Yalcin E: Homology modeling in drug discovery: Overview, current applications, and future perspectives. Chem Biol Drug Des 2019; 93(1): 12-20. doi 10.1111/cbdd.13388. Epub 2018 Oct 8. PMID: 30187647.
13. Geethu S & Vimina ER: (Improved 3-D protein structure predictions using deep Res Net model. The Protein Journal 2021; 40: 669-681.
14. Bacilieri M & Moro S: Ligand-based drug design methodologies in drug discovery process: an overview. Current Drug Discovery Technologies 2006; 3(3): 155-165.
15. Sharma V, Wakode S & Kumar H: Structure-and ligand-based drug design: Concepts, approaches, and challenges. Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences 2021; 27-53.

16. Jenkins JL: A 3D similarity method for scaffold hopping from known drugs or natural ligands to new chemotypes. J Med Chem 2004; 47: 6144–6159.
17. Mezzasalma SA, Grassi L & Grassi M: Physical and chemical properties of carbon nanotubes given mechanistic neuroscience investigations. Some outlooksare from condensed matter, materials science, and physical chemistry. Materials Science and Engineering: C, 2021; 131: 112480.
18. Katritzky AR, Kuanar M, Slavov S, Hall CD, Karelson M., Kahn I & Dobchev DA: Quantitative correlation of physical and chemical properties with chemical structure: utility for prediction. Chemical Reviews 2010; 110(10): 5714-5789.
19. Dixit VA, Lal LA & Agrawal SR: Recent advances in the prediction of non-CYP450-mediated drug metabolism. Wiley Interdisciplinary Reviews: Computational Molecular Science 2017; 7(6): 1323.
20. Zhong F, Xing J, Li X, Liu X, Fu Z, Xiong Z, Lu D, Wu X, Zhao J, Tan X, Li F, Luo X, Li Z, Chen K, Zheng M, Jiang H. Artificial intelligence in drug design. Sci China Life Sci 2018; 61(10): 1191-1204. doi 10.1007/s11427-018-9342-2. Epub 2018 Jul 18. PMID: 30054833.
21. Arooj M, Thangapandian S, John S, Hwang S, Park JK and Lee KW: 3D QSAR pharmacophore modeling, *in-silico* screening, and density functional theory (DFT) approaches for identification of human chymase inhibitors. Int J Mol Sci 2011; 12(12): 9236-64. doi: 10.3390/ijms12129236. Epub 2011 Dec 12. PMID: 22272131; PMCID: PMC3257128.
22. Prabhakar YS & Gupta MK: Chemical structure indices *in-silico* molecular design. Scientia Pharmaceutica 2008; 76(2): 101-132.
23. Waller CL and Marshall GR: Three-dimensional quantitative structure-activity relationship of angiotensin-converting enzyme and thermolysin inhibitors. II. A comparison of CoMFA models incorporating molecular orbital fields and desolvation-free energies based on active-analog and complementary-receptor-field alignment rules. J Med Chem 1993; 36(16): 2390-403. doi: 10.1021/jm00068a017. PMID: 8360884
24. Klebe G, Abraham U and Mietzner T: Molecular similarity indices in a comparative analysis (CoMSIA) of drug molecules to correlate and predict their biological activity. J Med Chem 1994; 37(24): 4130-46. doi 10.1021/jm00050a010. PMID: 7990113.
25. Ozawa SI, Takahashi M, Yamaotsu N and Hirono S: Structure-based virtual screening for novel chymase inhibitors by *in-silico* fragment mapping. J Mol Graph Model 2019; 89: 102-108. doi 10.1016/j.jmgm.2019.03.011. Epub 2019 Mar 12. PMID: 30884446.
26. Briem H and Lessel U: *In-vitro* and *in-silico* affinity fingerprints: finding similarities beyond structural classes. Perspect. Drug Discov Des 2000; 20: 231–244.
27. da Silva TH, Hachigian TZ, Lee J & King MD: Using computers to ESKAPE the antibiotic resistance crisis. Drug Discovery Today 2022; 27(2): 456-470.
28. Baig MH, Ahmad K, Rabbani G, Danishuddin M & Choi I: Computer-aided drug design and its application to the development of potential drugs for neurodegenerative disorders. Current Neuropharmacology 2018; 16(6): 740-748.
29. de Sousa NF, Scotti L, de Moura ÉP, dos Santos Maia M, Rodrigues GCS, de Medeiros HIR & Scotti MT: Computer-aided drug design methodologies with natural products in the drug research against Alzheimer's Disease. Current Neuropharmacology 2022; 20(5): 857.
30. Bhaskar V, Namboori K & Pappachen LK: *In-silico* discovery of novel ligands for anti-tubercular targets using computer-aided drug design. Research Journal of Pharmacy and Technology 2019; 12(11): 5646-5650.
31. Pandey M, Fernandez M, Gentile F, Isayev O, Tropsha A, Stern AC & Cherkasov A: The transformational role of GPU computing and deep learning in drug discovery. Nature Machine Intelligence 2022; 4(3): 211-221.
32. Zhao L, Ciallella HL, Aleksunes LM & Zhu H: Advancing computer-aided drug discovery (CADD) by big data and data-driven machine learning modeling. Drug Discovery Today 2020; 25(9): 1624-1638.
33. Hidup DR & Kemoterapi EA: Sumber: http://pubchem. NCBI. NLM. NIH. gov/Sumber: http://pubchem. NCBI nlm. nih. gov.
34. Song CM, Lim SJ & Tong JC: Recent advances in computer-aided drug design. Briefings in Bioinformatics 2009; 10(5): 579-591.
35. Irwin JJ & Shoichet BK: ZINC− a free database of commercially available compounds for virtual screening. Journal of Chemical Information and Modeling 2005; 45(1): 177-182.
36. Chen L, Qian Z, Fen K & Cai Y: Prediction of interactiveness between small molecules and enzymes by combining gene ontology and compound similarity. Journal of Computational Chemistry 2010; 31(8): 1766-1776.
37. Awale M & Reymond JL: Web-based 3D visualization of the DrugBank chemical space. Journal of Cheminformatics 2016; 8: 1-8.
38. Sadowski P & Baldi P: Small-molecule 3D structure prediction using open crystallography data. Journal of Chemical Information and Mod 2013; 53(12): 3127-3130.
39. Liu B, He H, Luo H, Zhang T and Jiang J: Artificial intelligence and big data facilitated targeted drug discovery. Stroke Vasc Neurol 2019; 4(4): 206-213. doi 10.1136/svn-2019-000290. PMID: 32030204; PMCID: PMC6979871.
40. Abdulfatai U, Uzairu A and Uba S: Quantitative structure-activity relationship and molecular docking studies of a series of quinazolinonylanalogs as inhibitors of gamma amino butyric acid aminotransferase. J of Adv Res 2017; 8: 33- 43.
41. Lagorce D, Maupetit J, Baell J, Sperandio O, Tuffery P, Miteva MA, Galons H and Villoutreix BO: The FAFDrugs2 server: A multistep engine to prepare electronic chemical compound collections. Bioinformatics 2011; 27: 2018–2020.

How to cite this article:
Pardeshi V, Gaikwad BP, Vaidya AU, Ghanchi KM, Kengarkar RS and Rajput TS: CADD: an absolute replacement for traditional drug discovery. Int J Pharm Sci & Res 2024; 15(1): 12-19. doi: 10.13040/IJPSR.0975-8232.15(1).12-19.