ADVANCES IN DRUG DESIGN: A REVIEW OF RECENT TRENDS, CHALLENGES AND FUTURE SCOPE

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Abstract. Drug design, or ligand-based drug molecular design of new molecules to interact with a biological target for effective regulation of its activity has been an indispensable and ever-evolving discipline in pharmaceutical research. The addition of newer technologies like Computational Aided Drug Design (CADD) has enriched this process by using computational tools to screen and refine drug candidates, hence empowering for an easy parallel implementation which ultimately shortens the timeline and financial involvement in designing drugs. Artificial Intelligence (AI) and its subset Machine Learning (ML), have become increasingly prominent in recent years to facilitate better virtual screening, molecular docking, and predictive modeling which are crucial for the detection of novel therapies especially regarding the diseases with complex etiology like cancer. Nanotechnology-assisted targeted drug delivery systems have been successfully applied to the field, enabling site-specific release of drugs and reducing their side effects while improving therapeutic efficacy. Likewise, the advent of biologics, biosimilars and multitarget drug design has brought new directions to tackle diseases that have evolved from their relatively simple causative pathways. Nonetheless, the need to overcome drug resistance, with its accompanying toxicity and computational challenges remains a major hurdle. In short, the future of drug design is expected to be increasingly influenced through AI enabled platforms that will combine with our understanding from personalized medicines and nanotechnology. Such innovations are projected to realize more functional and specific treatments. On the other hand, AI-driven methods are likely to enhance accuracy in drug discovery, and nanotechnology-based delivery systems will give way to a number of new therapeutic opportunities. Maturing, these technologies are bound to make impactful changes in the development of safer, more efficient, and personalised healthcare solutions.
Keywords: *drug design, ligand-based drug molecular design, biological target, Computational Aided Drug Design (CADD)*

Introduction

Drug design is a process aimed at creating works of manpower in new molecules, brought into life only by their interaction with biological targets to adjust their activeness. It is essential in creating new medications that will be able to cure a lot of diseases. Drug design, otherwise referred to as rational drug design, is simply a process for creating new molecules that would interact with certain biological targets, modulating their activity either by inhibition or enhancement for therapeutic purposes (Yadav et al., 2024; Nimbalkar et al., 2023). This, therefore, implies knowledge of how molecules bind to cell receptors or other molecules to elicit some response with a view to coming up with effective and safe pharmaceutical products (Hardy et al., 1987). CADD is an important companion in this process, as it makes use of computer techniques on huge biological databases to identify possible drug candidates and reduces the chances of late failures (Yadav et al., 2024). These strategies of drug design also address the barriers of drug delivery by linking drugs to polymers or antibodies in order to enhance targeting and stability, thus improving their efficacy and bioavailability (Xu, 2022). The current evolution of drug design was fashioned by the

development of high throughput sequencing, proteomics, metabolomics, and in silico drug development. All these make up the complex yet imperative areas of modern pharmaceutical research (Nimbalkar et al., 2023; Hardy et al., 1987).

Drug discovery has changed significantly from the times when rather than macromolecules, active substances identified from natural products were utilized to generate drugs (Hardy et al., 1987). The idea of structure-activity relationships (SAR), followed by Quantitative SAR (QSAR) techniques that allowed high throughput screening and in silico drug development was developed during this time (Xu, 2022; Hardy et al., 1987) Computer-Aided Drug Designing (CADD) tools came into existence and helped make the process more efficient, thus reducing the costs and time required for drug discovery through approaches such as Structure-Based Drug Designing (SBDD) and Ligand-Based Drug Designing (LBDD) (Kaur et al., 2022). The integration of informatics with pharmaceutical sciences led to the emergence of Computer-Aided Drug Design(CADD), thus enhancing Rational Drug Design(RDD) through molecular modeling and simulations (Kumar, 2022). At present, drug design is a fine science that marries traditional knowledge with up-to-date artificial intelligence techniques in finding safe and effective medicines.

Being an advance trend in Drug design, this brings together latest technologies and new methodoligies to make pharma R&D more efficient. Among them, artificial intelligence has been a major factor in drug discovery; it uses virtual screening, de novo molecule design and toxicity prediction (Sarkar et al., 2023).Through these methodologies and others, computational drug design techniques, such as computer-aided drug design, molecular docking, and molecular dynamics simulations, have become indispensable in identifying new therapies, particularly in cancer research (Tur Razia et al., 2023). Advanced systems of drug delivery, based on nanoparticles, liposome, and micro needles, have therefore permitted a strict time and site control of the release of a medicament, making the medication administration much more effective and side effect-free (Prajapati et al., 2024). Cargo-based, such as liposomes and nanoemulsions, seem to be one of the most promising approaches in the formulations developed against atopic dermatitis (Amisha et al., 2024). These trends reflect a change in the current collaborations between disciplines and the implementation of AI-driven approaches to move drug discovery towards a new era of innovation and efficacy.

Discussion

Structure Based Drug Design (SBDD)

The main principles that structure based drug design identifies and uses includes target selection, determination of protein structure, identification of the active site,ligand docking and scoring algorithms.The key to successful SBDD lies in optimal interactions of the ligand with the target protein, while causing minimal strain on the ligand, and understanding how small changes in chemical structure modulate the conformational and interaction preferences of a ligand (Kuhn et al., 2023). The medicinal chemists need to possess sound knowledge in physical organic chemistry with respect to conformational analysis and intra- and intermolecular interactions in order to apply SBDD in any drug discovery project (Blaney and Davis, 2023). In addition, technology advancement, more specifically in the use of artificial intelligence and machine learning techniques, has pushed SBDD toward much faster sampling, enhanced diversity of generated molecules, and increased binding affinity to protein

pockets (Pinheiro et al., 2024). All these principles come together to drive the rational design of potential drug candidates with increased potency, selectivity, and lower off-target effects; hence, SBDD is critical in fast-tracking drug development against a myriad of diseases (*Figure 1*).

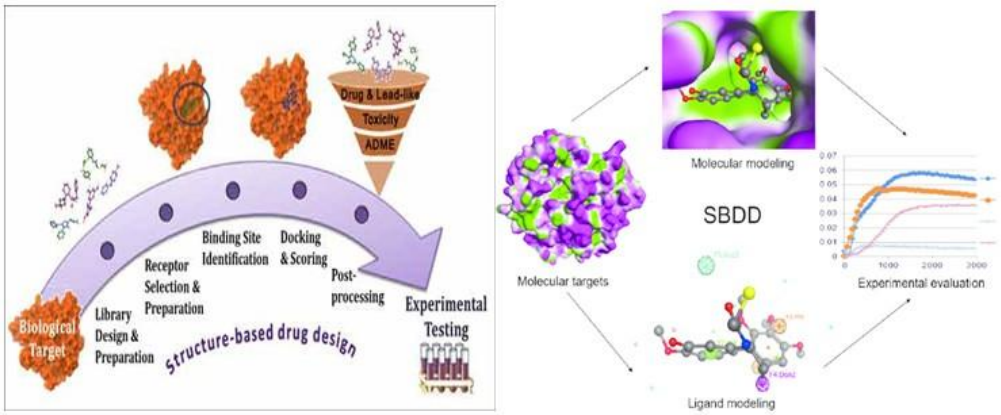

Figure 1. *SBDD drug development.*

Fragment Based Drug Design (FBDD)

FBDD is a method of drug design where fragments-low molecular weight compounds that weakly bind to a target-are identified and optimized for high binding affinity and selectivity. In FBDD, techniques such as NMR, X-ray crystallography, and surface plasmon resonance identify such weak binders with the critical interaction information required for their optimization. Although with issues like low throughput and associated high costs of experimental screening, computational methods have been developed that aid in fragment library design and optimization of the initial hits and are often used in conjunction with experimental approaches (Kryshchyshyn, 2017; Kumar et al., 2012). Due to its efficiency in covering chemical space and designing lead compounds effectively, it has become very popular and is a very promising hit-to-lead process in drug discovery (Feyfant et al., 2010; Bartoli et al., 2007) (*Figure 2*).

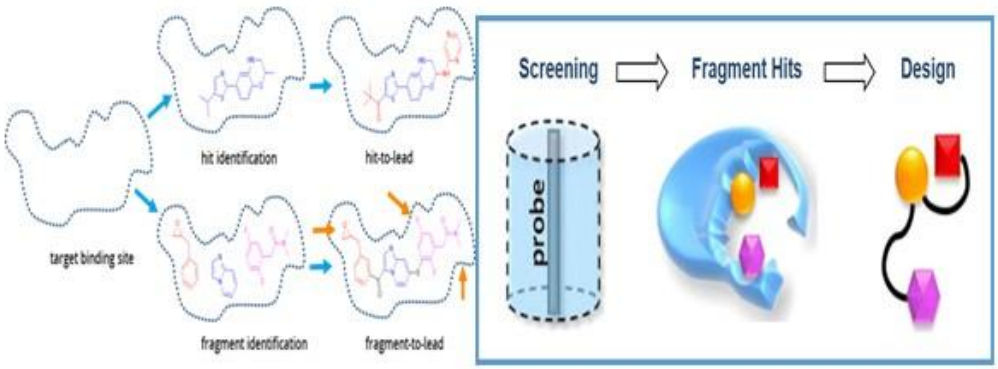

Figure 2. *Fragment Based Drug Design (FBDD).*

Computer Aided Drug Design

Here computational methods by employing Quantitative Structure Activity Relationship (QSAR), as well as machine-learning in vitro studies can play significant role to predict the biological activity of potential drug candidates, hence enhancing new

drugs discovery (Kumari and Wijesinghe, 2024). Moreover several techniques have been playing leading roles rationalizing and accelerating many aspects within context beside pharmaceutical research walls such as molecular docking,molecular dynamics simulation and high-throughput virtual screening with the aid its concepts from CADD (Wu et al., 2024; Niazi and Mariam, 2023). Although the method has really, in a way, advanced drug discovery by cutting the cost and time of discovery, some problems in algorithm optimization and privacy issues are still there (Niazi and Mariam, 2023). On top of the discussed details, integration of CADD with ML/deep learning technologies provides further potential and new vistas in the development of drugs through design and discovery (Liu et al., 2024). Although this method has had successful applications, it still uses an approximate force field, and high accuracy for the structure optimization of the auxiliary drug is not achieved. Therefore, there is a need to develop more accurate and efficient CADD models and algorithms (Shi, 2024). Basically, CADD improves drug design by computing a number of techniques that can be used in predicting ligand-receptor interactions, hence increasing the speed of drug discovery. For the purpose of improving efficiency in the discovery of new drugs, the CADD methods, such as homology modeling, molecular docking, and quantitative structure-activity relationships, rationalize the selection of compounds and optimize the structure of drugs. These approaches allow the rational design and optimization of target structures in a chemical entity, therefore making the drug development process focused and effective (Shi, 2024; Sing et al., 2024a; Wu et al., 2024). In general, CADD helps to accelerate drug discovery, reduce study costs, and increase the quality of data that will subsequently be developed into safer and more effective therapeutic solutions.

Artificial intelligence and machine learning in drug design

AI and ML has transformed drug discovery making it both faster and more effective with increased success rate in Pharmaceutical research (Aspatwar et al., 2024; Dey et al., 2024; Masoomkhah et al., 2024; Singh et al., 2024b; Sarkar et al., 2023). These models identify the drug properties, toxicity, bioactivity and its interaction with targets hence accelerating towards the identification of drugs.AI approaches like DL models have been essential for rational drug design by enabling identification of better therapeutic candidates with higher efficacy but lower side effects. Additionally, AI and ML techniques are increasingly used to optimize drug delivery systems such as controlled-release formulations and nano-scale delivery platforms which improve physicochemical characteristics of carriers.Although many obstacles like lack of data, while complying with regulations exists but current research and collaborations indicate the incorporation AI & ML in pharmaceutical formulation development will have an important role to play improving patient outcomes.

Current trends in drug design often rely heavily on artificial intelligence (AI) and machine learning applications in the pharmaceutical industry. AI and ML models are finding applications in shortening the time taken for drug development, increasing the probability of success of preclinical and clinical trials, anticipating the toxicity of drugs, improving the pharmacokinetics of drugs and supporting rationally designed drugs (Dey et al., 2024; Singh et al., 2024b; Sarkar et al., 2023). These technologies help in enumerating and filtering through the huge chemical space; in virtual screening for drug lead molecules, in designing novel small molecules from scratch, and in designing better and longer lasting drug delivery systems (Moingeon et al., 2024; Sarkar et al., 2023). Predictive models can be empowering new generations of personalized medicine

in drug discovery and development; therefore, they are enhancing the concept of computational precision medicine and influencing the pharmaceutical industry to adopt mixed-reality approaches (Moingeon et al., 2024). Thus, existing and future research and cooperation will contribute to the refinement and advancements of the application of AI and ML in the formulation design of pharmaceuticals with the ultimate goal of improving health and patients' lives (Dey et al., 2024).

Targeted drug delivery systems

The primarily targeted drug delivery systems are designed to send drugs right to the desired organs of the body, thus improving effectiveness while minimizing side effects (Russi et al., 2024; Caffrey and Borrelli, 2020). They employ different methods such as receptor-mediated interactions, delivery using nanotechnology and carriers like lipid-based, polymeric based and monoclonal antibody-based systems (Ani et al., 2024). Development of new nanoformulations like liposomes, dendrimers, micelles, and polymeric nanoparticles using nanotechnology has resulted in changing drug properties as well as enhancing their delivery to specific sites thus enabling controlled release of medicine (Garg et al., 2024). In addition to that, it seems that nanosponges have become an attractive colloid system which possesses a three dimensional porous structure so that they can hold both water-soluble and oil-soluble drugs hence solving problems such as toxicity of drugs, low bioavailability as well as releasing them at a defined rate; thus making these systems very important in targeting medicines directly to the right tissues (Wang and Strauss, 2023).

Biologicals and biosimilars in drug development

Biologicals and biosimilars are critical in drug development, offering novel treatment options for numerous disorders; however, their intricate manufacturing and subsequent high costs inhibit access (Wang and Strauss, 2023; Feng et al., 2022). Biosimilars are close replicas of approved biologicals; thus, they offer access to patient therapy considerably and safeguard patient safety and efficacy standards while doing so (Sheridan et al., 2024; Lakshmi and Rajakumari, 2022). Biosimilars are being developed swiftly in numerous nations, striving to ensure access for their own populations. Work is under the way in many nations to help biosimilar innovators through updated, scientist innovation, including fresh clinical pharmacology advances. This approach includes new pharmacodynamic biomarkers and modeling and simulation work employing newer and more innovative techniques, in addition to other prospects (Wang and Strauss, 2023; Dinh et al., 2022). The pharmaceutical business increasingly employs mathematical modeling and simulation in drug development throughout strands up preclinical development to clinical investigations to enhance efficiency, prioritize clinical research, and approve more medications with improved expense and difficulties (Dinh et al., 2022) (*Figure 3*).

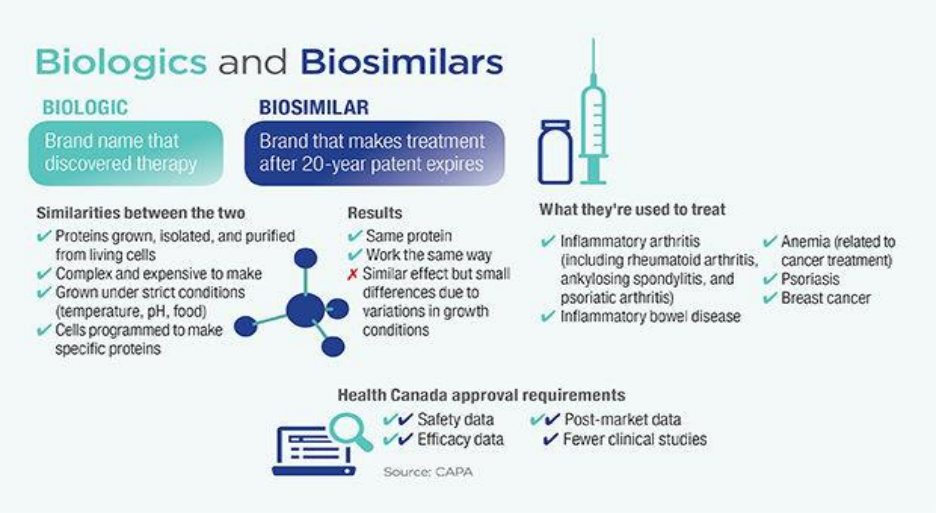

Figure 3. *Biologicals and biosimilars in drug development.*

Multi target drug design

As a result of the complexity seen in diseases like Alzheimer's, tuberculosis, major depressive disorders (MDD), cancer as well as cardiovascular and neurodegenerative pathologies research into multitarget drug design has blossomed due to targeting multiple mechanisms at once. Clinical observations have imperative the development of multi-target drugs (MTDs) combining multiple activities to synergy therapeutic effects (Turgutalp and Kizil, 2024; Maddeboina et al., 2024; Halder et al., 2023; Hazra et al., 2023; Mokrov, 2023). Through their use of novel approaches including structure-based in silico design of dual and triple-targeting ligands, systems biologically informed integrated analyses exploring intrinsic mechanisms that could be exploited to maximize efficacy, elucidation tenable synthetic lethal pathways triggered alongside drug resistance strategies/materializing at pre-defined settings/temperatures by translating the actual water bath system into a cold tub environment approach/path to new MTDs. Moving forward, further work in the overall field of multitarget drug design will necessitate the exploration and evaluation of new disease targets that also invokes some non-classical hallmarks or utilizes repurposing for chronic therapies such as these. LP-200 has only taken a first step to address other modern MT diseases with respect to this important aspect thereby showing strong consolidation across multimodal experiments using multiple coupled molecular dynamics simulations along virtual screening approaches - all combine towards enhancing current status quo-based development emerging multifactorial complexity which perhaps needs stability over time.

Challenges in drug deaign

Some of the challenges include dealing with the accuracy and computational cost trade-off in quantum mechanics (Ginex et al., 2024), complexity faced by computer-aided drug design scientists despite having access to experimental structures for their targets (Pala and Clark, 2024), supramolecular factor as a consideration when designing agents against drug-resistant fungi and bacteria (Regen, 2024), increasing need to employ Deep Learning in pharmaceutical research, development practices especially during companion work involved in improved Drug Discovery (Masoomkhah et al., 2024) or modelling native structure & ligand-binding behavior associated problems

about translocator protein 18 kDa (TSPO) (Shah and Jain, 2022). This showcases the multi-faceted form of drug designing, highlighting challenges that stand in our way and corresponding efforts being made to surmount these barriers which will help push forward new lines of proceses: more effective and efficient drugs discovery pipelines.

Drug resistance and pathogen evolution are two critical issues in pharmaceutical research; consequently, there is a lot of interest among developmental biologists to address them the examination relating areas. To combat these challenges, many computational methodologies like quantum mechanics (QM) methods (Ginex et al., 2024) artificial intelligence (AI), specifically machine learning(ML)/deep learning(DL) (Masoomkhah et al., 2024) and computer-aided drug design(CADD) (Shah and Jain, 2022) techniques have been utilized. They are intended to improve molecule screening, increase drug discovery power and compensate for deficiencies in the modeling of protein structures including those that pertain ligand-binding behavior specifically seen with the translocator protein 18 kDa (TSPO) (Giladi et al., 2024). Using advanced computational methods and coupling AI with quantum mechanics, researchers are striving to develop promising strategies in tackling drug resistance phenotypes and evolutionary insights into the pathogens so this would eventually allow for the identification of new therapeutic agents which will be potent.

One of the biggest challenges in drug design is reducing toxicity, side effects that result as additional complications and arise when drugs affect general metabolism pathways leading to reduced potential for new medications. The supramolecular facet, underrepresented in drug breakthrough segments regarding selectivity of medication applicants, has an essential position-including some situations where selective monomers display better pickiness than aggregated forms (Regen, 2024). Moreover, human biology is so complex that designing drug molecules with a desired specificity and suitable pharmacokinetic profile becomes an aggressive act without side effects (Bano et al., 2023). New drug compounds are now being designed using cheminformatics and machine learning techniques in a more efficient way that leverages these advanced chemical descriptors to expedite compound selection with reduced toxicity risks (Houssein et al., 2021). Tackling this challenge will need an integrated, multidisciplinary effort of computational methods overlaid with structural-based drug design combined with a comprehensive understanding of biological target to discovery safe and potent therapeutics.

Future scope and innovations

There is much greater scope for drug design in the future, fueled by state-of-art technologies such as Artificial Intelligence and Nanotechnology along with advanced Drug Delivery systems. The incorporation of AI into drug design has disrupted the field and facilitated effective virtual screening, de novo ligand synthesis as well as predict toxicologically effects (Prajapati et al., 2024; Sarkar et al., 2023). Utilization of Nanotechnology for Drug delivery some definition Nanotherapeutics (Multifunctional) and nanorobots, 3D printing applications in drug administrations; leading to new approaches on personalized medicine, propose innovative therapeutics against diseases such as cancer (Kumari and Wijesinghe, 2024; Weerasinghe et al., 2024). Moreover, evolution of targeted cancer therapies like antibody-drug conjugates (ADCs) has tailor-made next-generation ADC to have better therapeutic index resulting in improved clinical outcomes for patients (Prajapati et al., 2024; Gauzy-Lazo et al., 2020). This

confluence of technologies will define the future for drug design-effacious drugs, personalized treatments and patient centricity to improve human diseases.

In the coming years, there are going to be some major improvements in drug design owing to the integration of Computer-aided Drug Design (CADD), prodrugs and virtual screening technologies. These technologies have grown rapidly with Machine Learning and Artificial Intelligence being integrated rapidly into the CADD systems and hence becoming quite instrumental in rationalizing drug discovery processes while also enhancing their predictive capabilities (Niazi and Mariam, 2023). Special drugs also referred to as prodrugs can provide personalized therapeutic solutions through special delivery systems which allow for controlling the rate at which the active ingredient is released into circulation leading to personalized medicine (Swathi et al., 2024). Moreover, virtual screening technology has become an inexpensive yet effective way of enhancing new antiviral drug development especially when dealing with dangerous viruses that change so fast like COVID-19 (Weikang, 2023). The limelight is on these new methods of drug discovery that will optimize algorithms, tackle ethical issues and support sustainability measures for a healthier and more resilient future regarding pharmaceutical interventions.

Conclusion

Advanced technologies, more so CADD, AI, and nanotechnology, have bundled to make a very huge impact on the evolution of drug design. The innovations that have altered the pharmaceutical landscape not only accelerate the discovery process of drugs but also enhance their precision and efficacy in therapeutic interventions. Targeted drug delivery systems, as most recently developed, offer very bright prospects for treating complex diseases, beside the development of biologics, biosimilars and multitarget approaches. Certainly, however, despite all the successes of these developments, resistance to medicaments, their toxicity, and problems with computational models remain serious hurdles. Further interdisciplinary efforts will be required to channel the strength of AI, molecular modeling, and other emerging technologies in refinement and innovations in drug development processes. There is a significant future ahead in the area of drug design that delivers safer and more potent treatments tailored to any given patient. Such an intersection between AI-driven drug discovery, state-of-the-art delivery systems, and individualized medicine can only result in leading-edge therapies that drive better outcomes for patients and set a new benchmark for healthcare. Pushing the threshold of innovation further, the next generation of drug design will be at the forefront of addressing unmet medical needs and improving health across the world.

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Conflict of interest

The authors confirm that there is no conflict of interest involve with any parties in this research study.

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