Indian Journal of Pharmaceutical Chemistry and Analytical Techniques (IJPCAT)
ISSN: 3049-3765 | Vol. 02, Issue-03, May-June, 2026, pp. 64-76
https://ijpcat.com/1

A Review on Structure-Based Drug Design and Its Role in Modern Medicinal Chemistry

Urmila Raghuvanshi[1*], Nitish Gupta[1], Aishwarya Jhala[1], Nisha Patidar[2], Prateek Gavande[1]

[1]Department of Applied Chemistry, Shri Govindram Seksaria Institute of Technology and Science, 23, Park Road, Indore, MP, Pin 452003

[2]Department of Engineering Science and Humanities, Chameli Devi Group of Institutions, Khandwa Road, Village Umrikheda, Near Toll booth, Indore, Madhya Pradesh, Pin -452020

***Corresponding Author E-mail: uraghuvanshi@sgsits.ac.in**

Abstract:

The Structure-Based Drug Design (SBDD) has become one of the most sophisticated and rational methods of modern medicinal chemistry, profoundly changing the conventional process of drug discovery by applying the detailed 3D structural knowledge of biological targets, enzymes, receptors and ion channels. This review gives an in-depth review of the principles, methodologies and preclinical applications of SBDD with special interest in animals. It also emphasizes the combination of major computational methodologies, such as molecular docking, virtual screening, and molecular dynamics simulations, and experimental methods, such as X-ray crystallography and cryo-electron microscopy that, together, provide efficient prediction and analysis of drug-target interactions on a molecular scale. The animal models are considered vital in verifying the pharmacokinetics, pharmacodynamics, efficacy, and safety of SBDD-derived compounds, thus sealing the gap between the theoretical design and biological systems. Moreover, the review covers key drug development milestones, such as target identification, lead compound discovery, and optimization, and successful uses of SBDD in disease models, such as cancer, neurological disorders, infectious diseases, and inflammatory diseases. Although its benefits are significant (greater drug specificity, decreased development time, and higher success rates), SBDD has several issues connected with relying on high-resolution structural data, high implementation costs, and difficulties in the translation of computational predictions into in vivo results.

Keywords: Structure-Based Drug Design (SBDD), Molecular Docking, Preclinical Studies, Animal Models, Drug Discovery, Lead Optimization, Computational Biology, Medicinal Chemistry

Received: March 01, 2026 **Revised: April 12, 2026** **Accepted: May 28, 2026** **Published: June 5, 2026**

DOI: https://doi.org/10.64062/IJPCAT.Vol2.Issue3.5

https://ijpcat.com/index.php/1/issue/archive

1. INTRODUCTION

Structure-Based Drug Design (SBDD) has become a pillar of contemporary medicinal chemistry, providing a target-oriented and rational strategy to drug discovery based on three-dimensional structure of biological targets including enzymes, receptors and ion channels. In contrast to the conventional approaches that use empirical screening extensively, SBDD combines high-tech computational, e.g. molecular docking, virtual screening, and molecular dynamics simulations, with experimental, e.g. X-ray crystallography and cryo-electron microscopy, to gain insights into the nature of molecular interactions in a more atomic manner[1]. The methodology allows the design of drug candidates with increased specificity, better binding affinity, and decreased off-target effects. During the preclinical phase, animal models are essential in confirming these computational predictions by evaluating pharmacokinetics, pharmacodynamics and toxicity to ensure the biological relevancy and efficacy of the compounds designed.

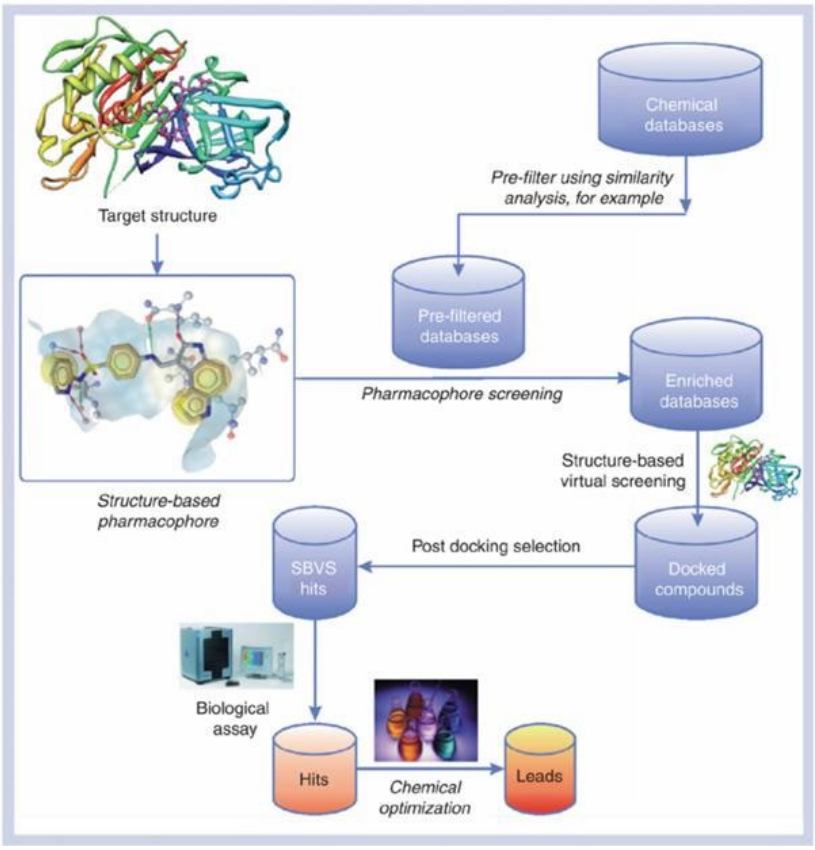

Figure 1: Workflow of Structure-Based Drug Design (SBDD)[2]

The rising significance of SBDD is due to its capability to speed up the drug development process and enhance the overall success rate of therapeutic discovery. SBDD enables the production of highly selective and efficient drugs to a broad array of diseases, including cancer, neurological disorders, infectious diseases and inflammatory conditions by systematically stepping through processes such as the identification of targets, the discovery of lead compounds, and the optimization of these lead compounds. Additionally, its use in animal models offers essential information on drug dynamics in multifaceted biological models, enhancing the translation of preclinical results[3]. As new technologies are developed, such as

artificial intelligence, structural analysis and computational biology are continually improved, SBDD is developing as a powerful and essential tool in the future of developing innovative and effective drugs.

1.1 Background and Context

The Structure-Based Drug Design (SBDD) has become a revolutionary and highly advanced technology in the field of medicinal chemistry, representing a considerable breakthrough of approaches rooted in the tradition of trial and error to a more rational, target and efficient approach to drug discovery. SBDD allows the design and optimization of drug molecules with increased specificity, binding affinity and selectivity by using detailed three-dimensional structural information of biological targets like enzymes, receptors and ion channels[4]. Quick development of computational methods such as molecular docking, virtual screening, and molecular dynamics simulations has played a key role in the prediction of ligand-target interactions. Simultaneously, experimental methods, including X-ray crystallography and cryo-electron microscopy, have also given high-resolution structural data on an atomic scale. In the preclinical field, animal models are necessary to verify these computational predictions through testing of pharmacokinetics, pharmacodynamics, and toxicity thus closing the divide between theory design and the actual biological system.

1.2 Objectives of the Review

The primary objective of this review is to:

- To examine the principles and methods of Structure-Based Drug Design (SBDD) in contemporary medicinal chemistry.
- To determine the efficacy of SBDD-derived drug candidates in animal-based preclinical models.
- To discuss major phases of drug development in SBDD such as identification of a target, lead discovery, and optimization.
- To determine the therapeutic use of SBDD in different disease models in animals including cancer, neurological, infectious, and inflammatory diseases.
- To determine the strengths, weaknesses, and future research opportunities of SBDD in enhancing the efficiency and translational performance of drug discovery.

1.3 Importance of the Topic

SBDD is of great significance in modern drug discovery, because it can greatly increase the specificity of the drug, the time and cost of development can be reduced, and the overall success rate of preclinical investigations can be increased. Its use in animal models has shown promising results in the treatment of a large scale of diseases such as cancer, neurodegenerative disorders, infectious diseases and inflammatory and metabolic diseases[5]. SBDD reduces off-target effects and improves safety profiles by facilitating the rational development of highly selective and potent therapeutic agents. Moreover, the possibilities of SBDD are still growing as new technologies like artificial intelligence, machine learning, or advanced structural biology methods are being integrated. It is therefore a vital and developing field of study that plays a very important role in the development of effective, specific and novel therapeutic approaches in contemporary medicinal chemistry[6].

2. PRECLINICAL APPLICATIONS AND THERAPEUTIC POTENTIAL OF STRUCTURE-BASED DRUG DESIGN IN ANIMAL MODELS

SBDD has been successfully used in animal models to generate highly specific drug candidates that enhance animal outcomes, including tumor reduction, viral suppression, and neuroprotection. It combines both computational and experimental techniques to aid in efficient drug discovery yet is limited through reliance on structural information, expensive computation, and discrepancies between predicted and in vivo animal outcomes[7].

2.1 Key Research Studies and Findings

The Structure-Based Drug Design (SBDD) has been shown to be effective in many animal-based studies in order to expedite the process of creating targeted and effective therapeutics. An example of this is the tumor reduction of the murine cancer models with kinase inhibitors that were engineered using SBDD techniques to specifically target the aberrant signaling pathways that led to cell proliferation and cell survival[8]. They are frequently highly specific to specific kinase domains, and reduce off-target effects and enhances therapy. On the same note, the antiviral agents that are directed by their structure have been shown to have a better viral suppression effect on the infected animal system since they specifically bind to viral enzymes or proteins which are vital in the viral lifecycle, and thus inhibit the development of the viral lifecycle leading to reduced severity of the disease.

Moreover, the research on enzyme inhibitors has shown that the rationally designed ligands have the best binding affinity and molecular specificity because of optimized interactions in the active site of the target enzymes. This has resulted in improved therapeutic responses in rodent model which has enhanced efficacy and diminished side effects[9]. Moreover, neuroprotective agents produced by SBDD have demonstrated encouraging effects in animal models of neurodegenerative diseases where they lead to less neuronal damage, oxidative stress, and cognitive performance. These results underscore the possibility of developing highly selective and potent drug candidates with enhanced safety and efficacy profile in preclinical studies using SBDD.

2.2 Methodologies Used in SBDD

Structure-Based Drug Design (SBDD) is a hybrid approach in computational and experimental methods used to design and optimize drug candidates with high accuracy. The methodologies enable scientists to know the structural features of biological targets and how the potential drug molecules will react with the targets[10]. A combination of in silico modeling and experimental validation will guarantee a comprehensive and effective flow of work between the target identification and therapeutic assessment. Key methodologies include:

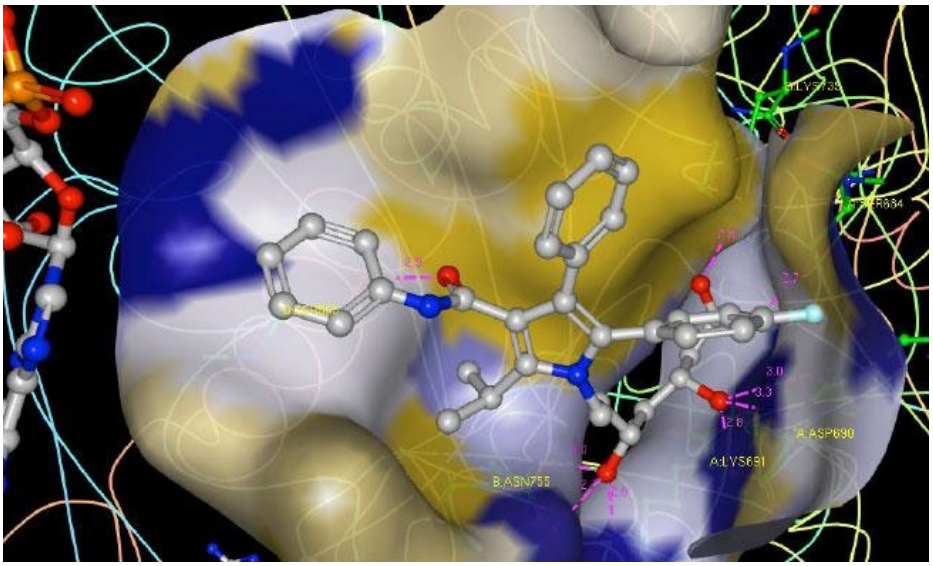

Figure 2: Molecular Docking and Protein–Ligand Interaction Mechanism[11]

- **Molecular Docking:** It is a computational method used to predict the optimal orientation of a ligand binding to a target protein and is used to estimate binding affinity and strength of interaction. Hydrogen bonds, hydrophobic contacts and electrostatic forces are also identified as important interactions in docking studies, allowing promising drug candidates to be selected and optimized prior to experimental testing.
- **Molecular Dynamics Simulations:** These simulations offer valuable information on how ligand-target complexes, in physiological settings, behave and how they remain stable over time. Studying parameters like conformational changes, flexibility and interaction stability can help the researchers to understand the dynamic character of binding and optimize drug molecules to perform better.
- **X-ray Crystallography & Cryo-EM:** These experimental techniques offer high-resolution structural information about protein–ligand complexes. X-ray crystallography is a technique that gives very accurate atomic-level information on binding sites and cryo-electron microscopy (cryo-EM) allows one to visualize large and complex structures of biomolecules that might not be easy to crystallize. These structural clues are critical in designing and optimization of drugs rationally[12].
- **In Vivo Animal Testing:** Computational and structural validation is followed by testing drug candidates in animal models to assess the pharmacokinetics (absorption, distribution, metabolism, and excretion), pharmacodynamics (biological effects), and toxicity. This is an essential step to ensure the effectivity and safety of compounds in a live system and to determine the possible adverse effects before undertaking the clinical trials.

The combination of these methodologies forms a comprehensive and systematic framework that bridges the gap of theoretical predictions and biological validation, greatly improving the effectiveness and success rate of drug discovery by using SBDD.

2.3 Critical Evaluation

Strengths

Structure-Based Drug Design (SBDD) offers a number of valuable benefits to drug discovery. It increases the specificity and binding ability of drugs by allowing specific reactions between the drug molecules and their biological targets, which leads to a reduced likelihood of off-target effects[13]. The SBDD is also useful to save time and cost during the early drug discovery process, where computational techniques are used to sift and refine compounds prior to experimental testing. It is also able to provide mechanistic information about the drug action, which enables the researcher to know the atomic interaction between molecules, which is useful in optimizing drugs rationally. In addition, SBDD leads to better success rates in animal model validation, with compounds in preclinical studies often already optimized in efficacy and selectivity.

Weakness

SBDD has a number of limitations even though it has its strengths. It is also very reliant on the availability of high-resolution target structures, which not all proteins can have, particularly flexible or hard-to-crystallize proteins. In addition, computational predictions do not always scale well to the real life, since biological systems are more complicated than the simulated ones. The second limitation is the variable in species using animal models which may influence the extrapolation of preclinical results to the animal condition[14]. Also, the structural determination methods, including X-ray crystallography and cryo-electron microscopy, are costly making them less accessible and scalable especially in resource-constrained environments[15].

3. KEY STAGES AND PRECLINICAL VALIDATION OF STRUCTURE-BASED DRUG DESIGN IN ANIMAL MODELS

Structure-Based Drug Design (SBDD) is whereby biological targets are identified and validated, then computational screening and optimization of lead compounds are performed, followed by efficacy and safety testing in animal models. The case studies conducted using animals show that SBDD can be used to design therapeutics with better effects like tumor regression, less inflammation, and better antimicrobial effect[16].

3.1 Target Identification and Validation

Structure-Based Drug Design (SBDD) involves the initial process of identifying biologically relevant targets like enzymes, receptors, or ion channels that are important factors in disease development. Advanced techniques like genomics, proteomics, and bioinformatics are often used to identify these targets[17]. The functional role of these targets in certain disease pathways is then validated using animal models. Through the physiological and pathological observations of the changes following the modulation of the target, researchers have the opportunity to ascertain its therapeutic significance and determine whether it is worth developing a drug. This is a very important step in determining translational potential of preclinical results to human uses[18].

3.2 Lead Compound Identification

After identifying a validated target, computational methods are employed to determine potential lead compounds capable of effectively binding to the target site (e.g., virtual screening and molecular docking). In silico screening is done on large chemical libraries to identify

molecules with desirable binding affinity and interaction profiles[19]. These chosen lead compounds are then subjected to animal models to determine their biological performance, efficacy and initial safety. Such a combination of computational prediction and biological validation is used to reduce potential candidates to be developed.

3.3 Lead Optimization

Once first lead compounds are identified, structural changes are made with the aim of improving their pharmacological properties. This is done by enhancing efficacy, selectivity against the target, minimizing toxicity, and maximizing pharmacokinetic properties including absorption, distribution, metabolism and excretion (ADME)[20]. Such modifications are often directed by techniques like structure activity relationship (SAR) analysis. Animal research is crucial at this phase as it can evaluate dose-response, efficacy, and adverse effects, and thus has the ability to ensure that optimised compounds are safe and effective enough to meet the necessary safety and efficacy criteria.

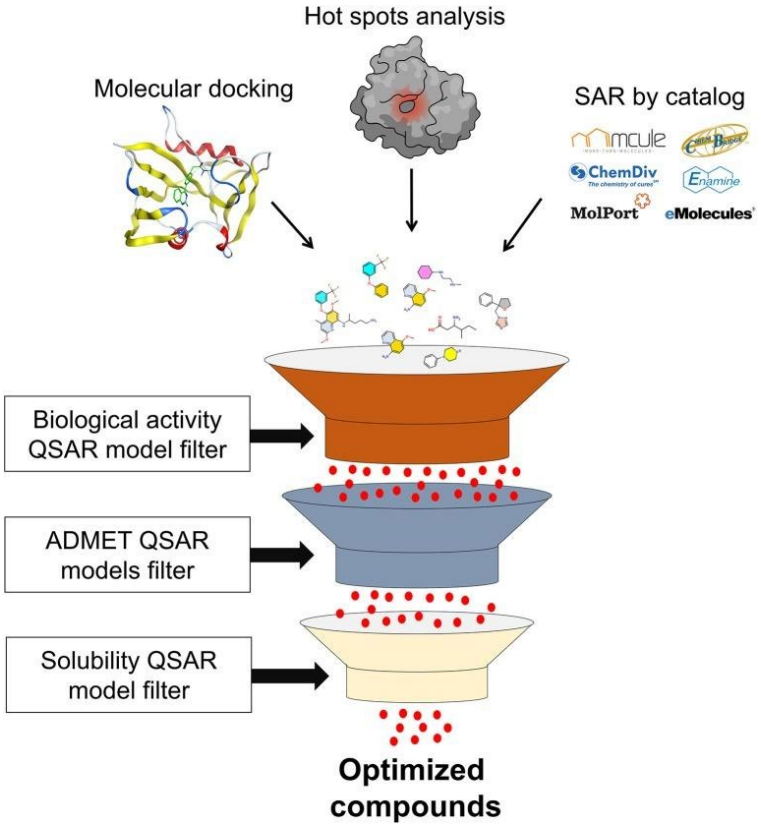

Figure 3: Lead Optimization and Structure–Activity Relationship (SAR) in Drug Design[21]

3.4 Case Studies in Animal Models

A number of animal studies emphasize the usefulness of SBDD during drug discovery. In anticancer agents, structure-guided inhibitors have proven to be effective in tumor regression in mice by selectively modulating important signaling pathways of cancer progression. In the case of anti-inflammatory drugs, optimized ligands generated by SBDD have demonstrated decreased inflammatory reactions in rat models by suppressing inflammatory mediators and enzymes. Equally, antimicrobial agents designed by structure-based systems have been shown to display better bacterial clearance in infected animals system, and in many cases with increased specificity and reduced resistance emergence[22].

All these examples demonstrate how SBDD combines computational design with experimental validation to eventually lead to the creation of useful and specific therapeutic agents in preclinical studies.

4. APPLICATIONS OF STRUCTURE-BASED DRUG DESIGN IN ANIMAL DISEASE MODELS

Structure-Based Drug Design (SBDD) has already been shown to be of great usefulness in a variety of animal disease models, especially including oncology, which has seen the creation of highly targetable anticancer drugs like kinase inhibitors and pro-apoptotic compounds[23]. These structure-guided drugs have demonstrated significant tumor regression and survival in murine tumor models through selective targeting of dysregulated signaling pathways that contribute to cancer progression[24]. Likewise, in models of neurological disorders, SBDD has been used to design neuroprotective agents to inhibit important enzymes such as acetylcholinesterase and amyloid-associated proteins. Rat models of neurodegeneration have reported a reduction in neuronal damage, oxidative stress, and cognitive functions, which show that rational drug design is effective in the treatment of complex neurological disorders[25].

SBDD has been instrumental in the discovery and optimization of antimicrobial and antiviral agents that act on key microbial enzymes and viral proteins in the context of infectious diseases[26]. In models of animal infection, the use of these structure-guided therapeutics showed enhanced clearance of pathogens, less disease severity, and improved surviva[27]. Moreover, SBDD has also demonstrated potential in the context of inflammatory and metabolic disorder models, with inhibitors to inflammatory mediators and metabolic enzymes resulting in a decrease in inflammatory reactions and enhancement of metabolic regulation in animal systems[28].

These applications highlight the usefulness and applicability of SBDD in preclinical research. SBDD facilitates the generation of targeted, efficient, and safer therapeutic agents in a broad range of diseases with a combination of computational design and in vivo validation, which is why it is so important in the evolution of modern medicinal chemistry[29].

Table 1: Summary of Literature on Structure-Based Drug Design (SBDD)[30]

Author(s) & Year	Study Focus	Methodology Used	Key Findings	Relevance to SBDD
Saur et al. (2020)[31]	Fragment-based drug discovery using cryo-EM	Cryo-electron microscopy (cryo-EM)	Enabled high-resolution identification of ligand-binding sites and visualization of small molecular fragments	Enhanced lead identification and expanded SBDD application to complex targets
Goebel et al. (2021)[32]	Multidrug resistance in cancer via ABC transporters	Structure-based inhibitor design	Identified inhibitors targeting P-glycoprotein and ABCG2 to overcome drug resistance	Demonstrated SBDD potential in designing selective anticancer inhibitors

Tripathi et al. (2022)[33]	COVID-19 inflammatory response and therapeutics	Structure-based drug design approaches	Identified compounds with strong binding affinity to SARS-CoV-2 proteins	Highlighted SBDD role in rapid therapeutic development for infectious diseases
Maurya et al. (2020)[34]	Natural compounds against SARS-CoV-2	Molecular docking	Found phytochemicals with strong binding to viral spike protein and receptor	Showed potential of natural products as leads in SBDD-based antiviral development
Naqvi et al. (2018)[35]	Ligand–receptor interactions and simulations	Molecular docking & molecular dynamics simulations	Improved prediction of binding affinity, stability, and molecular interactions	Reinforced importance of computational tools in accurate and efficient SBDD

5. DISCUSSION

Structure-Based Drug Design (SBDD) is a powerful and logical method that enhances specificity and therapeutic efficacy of drugs in animal models via a combination of computational design and in vivo testing. It is, however, limited by structural data availability, prediction differences between simulations and real biology, and species differences, indicating the need of advanced technologies and improved animal models[36].

5.1 Interpretation and Analysis of Findings

The animal studies reviewed clearly suggest that Structure-Based Drug Design (SBDD) is a highly efficient and logical way of drug discovery because it allows the specific targeting of biological molecules and enhances therapeutic effects of reducing tumors, antiviral effects, and neuroprotection. SBDD to design ligands according to the structural configuration of the target protein not only increases binding affinity and selectivity but also results in a better efficacy profile in animal models. Moreover, the combination of computational modeling and in vivo validation makes sure that there is a systematic and reliable workflow, and that the researchers refine drug candidates before moving them further. The overall effectiveness and predictability of preclinical drug development is greatly enhanced with this combined approach[37].

5.2 Implications and Significance

The results indicate that SBDD plays an important role in contemporary medicinal chemistry because it saves time and money used in the traditional drug discovery process and increases drug specificity and safety profiles. Its use in a variety of disease models, such as cancer, neurological diseases, infectious diseases, and inflammatory diseases, shows its versatility and wide therapeutic potential. Moreover, animal models are important to offer biological validation so that researchers can determine pharmacokinetics, pharmacodynamics, and toxicity in more complex living systems. This enhances the predictability of translation of

SBDD-derived compounds and promotes their advancement towards higher levels of drug development[38].

5.3 Research Gaps and Future Directions

SBDD has several limitations including a great reliance on high-resolution structural data that might not be accessible to all biological targets, especially flexible or membrane-bound proteins. Further, the weaknesses of computational simulations to predict in vivo outcomes are further evidenced by the inability to predict them with the accuracy of biologic complexity[29]. The fact that animal models have species differences also makes it difficult to extrapolate the findings to larger biological contexts. In the future, research ought to aim at refining the methods of structural analysis, including the development of cryo-electron microscopy and hybrid modeling methods and the incorporation of artificial intelligence and machine learning to increase the predictive accuracy. Also, more realistic and standard animal models will be necessary to enhance the reliability and translational capabilities of SBDD in drug discovery[40].

6. CONCLUSION

Structure-Based Drug Design (SBDD) has proven itself to be a very potent and logical method in contemporary medicinal chemistry transforming the drug discovery environment greatly with its accuracy, efficiency and scientific. SBDD can be used to design and optimize drug candidates with increased specificity, binding affinity, and decreased off-target effects by taking advantage of structural information of biological targets, which is highly detailed and three-dimensional. The application of the modern computational methods with experimental validation has developed a powerful and systematic framework that enhances the overall success of the preclinical drug development. Animal research has been important in proving the efficacy of SBDD, offering the necessary information on pharmacokinetics, pharmacodynamics, efficacy, and safety, and thus closing the gap between theoretical forecasts and actual biological systems. A wide range of disease models such as cancer, neurological diseases, infectious diseases and inflammatory diseases have been successfully treated with SBDD, which reflects its versatility and further therapeutic potential. Irrespective of its many merits, issues like reliance on high-resolution structural information, high operational expenses, and the inability to translate computational results to in vivo systems still exist. However, it is hoped that since the field of structural biology, computational tools, and new technologies (artificial intelligence and machine learning) are constantly developing, these weaknesses will be resolved, and the possibilities of SBDD will only increase. SBDD is an exciting and progressive paradigm which could have a huge potential to develop safer, more effective and targeted therapeutic agents, and thus be one of the most important factors in the future of innovative drug discovery.

REFERENCES

1. Batool, M., Ahmad, B., & Choi, S. (2019). A structure-based drug discovery paradigm. International journal of molecular sciences, 20(11), 2783.
2. Wang, X., Song, K., Li, L., & Chen, L. (2018). Structure-based drug design strategies and challenges. Current Topics in Medicinal Chemistry, 18(12), 998-1006.

3. Pant, S., Verma, S., Pathak, R. K., & Singh, D. B. (2022). Structure-based drug designing. In Bioinformatics (pp. 219-231). Academic Press.
4. Ejalonibu, M. A., Ogundare, S. A., Elrashedy, A. A., Ejalonibu, M. A., Lawal, M. M., Mhlongo, N. N., & Kumalo, H. M. (2021). Drug discovery for Mycobacterium tuberculosis using structure-based computer-aided drug design approach. International Journal of Molecular Sciences, 22(24), 13259.
5. Isert, C., Atz, K., & Schneider, G. (2023). Structure-based drug design with geometric deep learning. Current Opinion in Structural Biology, 79, 102548.
6. Fischer, A., Smiesko, M., Sellner, M., & Lill, M. A. (2021). Decision making in structure-based drug discovery: visual inspection of docking results. Journal of Medicinal Chemistry, 64(5), 2489-2500.
7. Bera, I., & Payghan, P. V. (2019). Use of molecular dynamics simulations in structure-based drug discovery. Current pharmaceutical design, 25(31), 3339-3349.
8. Lee, Y., Basith, S., & Choi, S. (2018). Recent advances in structure-based drug design targeting class AG protein-coupled receptors utilizing crystal structures and computational simulations. Journal of Medicinal Chemistry, 61(1), 1-46.
9. Śledź, P., & Caflisch, A. (2018). Protein structure-based drug design: from docking to molecular dynamics. Current opinion in structural biology, 48, 93-102.
10. Kaczor, A. A., Zięba, A., & Matosiuk, D. (2024). The application of WaterMap-guided structure-based virtual screening in novel drug discovery. Expert Opinion on Drug Discovery, 19(1), 73-83.
11. Kulkarni, P. U., Shah, H., & Vyas, V. K. (2022). Hybrid quantum mechanics/molecular mechanics (QM/MM) simulation: a tool for structure-based drug design and discovery. Mini reviews in medicinal chemistry, 22(8), 1096-1107.
12. Tang, Y., Moretti, R., & Meiler, J. (2024). Recent advances in automated structure-based de novo drug design. Journal of Chemical Information and Modeling, 64(6), 1794-1805.
13. Cummings, M. D., & Sekharan, S. (2019). Structure-based macrocycle design in small-molecule drug discovery and simple metrics to identify opportunities for macrocyclization of small-molecule ligands. Journal of Medicinal Chemistry, 62(15), 6843-6853.
14. Özçelik, R., van Tilborg, D., Jiménez-Luna, J., & Grisoni, F. (2023). Structure-based drug discovery with deep learning. ChemBioChem, 24(13), e202200776.
15. Ferraro, M., D'Annessa, I., Moroni, E., Morra, G., Paladino, A., Rinaldi, S., ... & Colombo, G. (2018). Allosteric modulators of HSP90 and HSP70: dynamics meets function through structure-based drug design. Journal of medicinal chemistry, 62(1), 60-87.
16. Velmurugan, D., Pachaiappan, R., & Ramakrishnan, C. (2020). Recent trends in drug design and discovery. Current Topics in Medicinal Chemistry, 20(19), 1761-1770.
17. Aplin, C., Milano, S. K., Zielinski, K. A., Pollack, L., & Cerione, R. A. (2022). Evolving experimental techniques for structure-based drug design. The Journal of Physical Chemistry B, 126(35), 6599-6607.
18. Wu, K., Karapetyan, E., Schloss, J., Vadgama, J., & Wu, Y. (2023). Advancements in small molecule drug design: A structural perspective. Drug Discovery Today, 28(10), 103730.

19. Zhang, Z., Yan, J., Liu, Q., Chen, E., & Zitnik, M. (2023). A systematic survey in geometric deep learning for structure-based drug design. arXiv preprint arXiv:2306.11768.

20. Lee, Y., Lazim, R., Macalino, S. J. Y., & Choi, S. (2019). Importance of protein dynamics in the structure-based drug discovery of class AG protein-coupled receptors (GPCRs). Current opinion in structural biology, 55, 147-153.

21. Sanyal, S., Amin, S. A., Banerjee, P., Gayen, S., & Jha, T. (2022). A review of MMP-2 structures and binding mode analysis of its inhibitors to strategize structure-based drug design. Bioorganic & Medicinal Chemistry, 74, 117044.

22. Dutkiewicz, Z., & Mikstacka, R. (2018). Structure-based drug design for cytochrome P450 family 1 inhibitors. Bioinorganic chemistry and applications, 2018(1), 3924608.

23. Cons, B. D., Twigg, D. G., Kumar, R., & Chessari, G. (2022). Electrostatic complementarity in structure-based drug design: miniperspective. Journal of Medicinal Chemistry, 65(11), 7476-7488.

24. Sugiki, T., Furuita, K., Fujiwara, T., & Kojima, C. (2018). Current NMR techniques for structure-based drug discovery. Molecules, 23(1), 148.

25. Ouma, R. B., Ngari, S. M., & Kibet, J. K. (2024). A review of the current trends in computational approaches in drug design and metabolism. Discover Public Health, 21(1), 108.

26. Zhang, S., Krumberger, M., Morris, M. A., Parrocha, C. M. T., Kreutzer, A. G., & Nowick, J. S. (2021). Structure-based drug design of an inhibitor of the SARS-CoV-2 (COVID-19) main protease using free software: A tutorial for students and scientists. European journal of medicinal chemistry, 218, 113390.

27. Picarazzi, F., Vicenti, I., Saladini, F., Zazzi, M., & Mori, M. (2020). Targeting the RdRp of emerging RNA viruses: the structure-based drug design challenge. Molecules, 25(23), 5695.

28. Bianco, G., Goodsell, D. S., & Forli, S. (2020). Selective and effective: current progress in computational structure-based drug discovery of targeted covalent inhibitors. Trends in pharmacological sciences, 41(12), 1038-1049.

29. Mustafa, M., & Winum, J. Y. (2022). The importance of sulfur-containing motifs in drug design and discovery. Expert opinion on drug discovery, 17(5), 501-512.

30. Powers, A. S., Yu, H. H., Suriana, P., Koodli, R. V., Lu, T., Paggi, J. M., & Dror, R. O. (2023). Geometric deep learning for structure-based ligand design. ACS Central Science, 9(12), 2257-2267.

31. Saur, M., Hartshorn, M. J., Dong, J., Reeks, J., Bunkoczi, G., Jhoti, H., & Williams, P. A. (2020). Fragment-based drug discovery using cryo-EM. Drug Discovery Today, 25(3), 485-490.

32. Goebel, J., Chmielewski, J., & Hrycyna, C. A. (2021). The roles of the human ATP-binding cassette transporters P-glycoprotein and ABCG2 in multidrug resistance in cancer and at endogenous sites: Future opportunities for structure-based drug design of inhibitors. Cancer Drug Resistance, 4(4), 784.

33. Tripathi, N., Tripathi, N., & Goshisht, M. K. (2022). COVID-19: inflammatory responses, structure-based drug design and potential therapeutics. Molecular Diversity, 26(1), 629-645.

34. Maurya, V. K., Kumar, S., Prasad, A. K., Bhatt, M. L., & Saxena, S. K. (2020). Structure-based drug designing for potential antiviral activity of selected natural products from Ayurveda against SARS-CoV-2 spike glycoprotein and its cellular receptor. Virusdisease, 31(2), 179-193.

35. Naqvi, A. A., Mohammad, T., Hasan, G. M., & Hassan, M. I. (2018). Advancements in docking and molecular dynamics simulations towards ligand-receptor interactions and structure-function relationships. Current topics in medicinal chemistry, 18(20), 1755-1768.

36. Gurung, A. B., Ali, M. A., Lee, J., Farah, M. A., & Al-Anazi, K. M. (2021). An updated review of computer-aided drug design and its application to COVID-19. BioMed research international, 2021(1), 8853056.

37. Halder, S. K., Ahmad, I., Shathi, J. F., Mim, M. M., Hassan, M. R., Jewel, M. J. I., ... & Hossen, M. S. (2024). A comprehensive study to unleash the putative inhibitors of serotype2 of dengue virus: insights from an in silico structure-based drug discovery. Molecular biotechnology, 66(4), 612-625.

38. Siebenmorgen, T., Menezes, F., Benassou, S., Merdivan, E., Didi, K., Mourão, A. S. D., ... & Popowicz, G. M. (2024). MISATO: machine learning dataset of protein–ligand complexes for structure-based drug discovery. Nature computational science, 4(5), 367-378.

39. Cheng, H., Orr, S. T., Bailey, S., Brooun, A., Chen, P., Deal, J. G., ... & Kath, J. C. (2020). Structure-based drug design and synthesis of PI3Kα-selective inhibitor (PF-06843195). Journal of medicinal chemistry, 64(1), 644-661.

40. Naithani, U., & Guleria, V. (2024). Integrative computational approaches for discovery and evaluation of lead compound for drug design. Frontiers in Drug Discovery, 4, 1362456.