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How Can Structure-Based Computational Methods Support Antibiotic Drug Discovery in Addressing Antimicrobial Resistance?

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Abstract

Antimicrobial resistance (AMR) has emerged as a major global health challenge, necessitating the development of innovative strategies to accelerate antibiotic drug discovery. Traditional drug development approaches are often time-consuming, costly, and resource-intensive, creating a growing need for computational methods that can improve research efficiency and therapeutic candidate identification. This study investigates the role of computational protein structure prediction in advancing antibiotic drug discovery through a conceptual literature review of recent research published between 2022 and 2026. The review examines the application of protein structure prediction techniques, including deep learning, machine learning, molecular simulations, and AlphaFold-based approaches, in supporting structure-based drug design. Particular attention is given to their contributions in drug target identification, binding site prediction, protein–ligand interaction analysis, virtual screening, and candidate prioritization. The findings indicate that computational approaches significantly enhance the efficiency of early-stage drug discovery by enabling accurate structural modeling, rapid screening of large compound libraries, and improved identification of promising antibacterial targets. Furthermore, the integration of artificial intelligence with molecular modeling techniques has strengthened prediction accuracy and facilitated the discovery of novel therapeutic candidates against drug-resistant pathogens. Despite these advancements, challenges related to prediction reliability, biological complexity, computational resource requirements, and dependence on high-quality datasets continue to affect the robustness of current approaches. Additionally, the reviewed studies emphasize the necessity of experimental validation to confirm computational findings and ensure clinical applicability. Overall, the study concludes that computational protein structure prediction plays a critical role in accelerating antibiotic drug discovery and offers substantial potential for addressing antimicrobial resistance through more efficient and data-driven therapeutic development strategies.

Keywords

AlphaFold2, Antibiotic Drug Discovery, Drug Target Identification, Molecular Dynamics Simulation, Virtual Screening.

INTRODUCTION & LITERATURE REVIEW

Antimicrobial resistance (AMR) is now one of the most important health threats worldwide and is making current antibiotic treatment of infectious diseases less effective [1]. With the growing occurrence of antibiotic resistant bacterial pathogens, the effectiveness of routine treatment has diminished, causing extended illnesses, increased mortality, and cost of healthcare [2]. The development of new antimicrobial drugs is a pressing need in the field of medicine, as bacteria have developed various mechanisms to resist the effects of antibiotics [3]. The discovery of conventional antibiotic drugs is a complicated, lengthy and costly process however, that frequently involves a lot of laboratory experimentation, target validation and clinical assessment before a possible drug is available for sale [4], [5]. These hurdles have created an urgent need for new methods that will enable identification of new therapeutic targets as soon as possible and increase the efficiency of drug development pipelines. Thus, computational methods are being increasingly used to assist and improve all stages of the discovery process for antibiotics.

With recent developments in computational biology, it has become possible to predict the three-dimensional shapes of bacterial survival and resistance mechanisms proteins [6], [7] which are crucial to greatly speed up the process of drug discovery. The prediction of protein structure is an important tool in understanding the functional properties of biological molecules and identifying possible drug targets for structure-based drug design [8], [9]. Researchers can also study protein interactions, pinpoint binding sites, and virtually test vast compound libraries using techniques like homology modelling, molecular simulations, and machine-learning predict methods, before sending compounds to the lab for testing [10]. Moreover, the development of artificial intelligence (AI) based methods has greatly enhanced the accuracy and speed of protein structure prediction, which has streamlined the selection of potential candidates and drug optimization [11], [12]. These computational techniques are capable of cost reduction, speed up research and development time and increase the chances of identifying a successful antibacterial agent [13]. However, computational protein structure prediction has become an interesting approach to speed up the discovery of antibiotics and solve the problem of antibiotic resistance around the world.

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A recent study designed a molecular docking framework based on AlphaFold2 to predict protein–ligand interactions for antibiotic discovery in the essential proteome of Escherichia coli. The strategy was to combine predicted protein structures with docking and machine learning-based protein rescoring to generate a list of potential antibacterial targets. Experimental benchmarking confirmed the promiscuity of many compounds and proteins, and rescoring strategies were used to boost prediction accuracy with auROC up to 0.63. Overall docking was, however, not very accurate and the overall docking performance showed poor predictive ability to ensure a reliable identification of the target [14]. In another study proposed a machine learning framework that combines structural information from the protein and its corresponding ligand to AlphaFold2-predicted structures. The approach employs 3D protein fingerprints and integrates them with the information on ligands to acquire protein–ligand interaction pattern in one model for prediction. The model improved the ability to predict inhibition potencies and was made more broadly applicable. But the accuracy of the prediction is still dependent on the accuracy of the AlphaFold-generated structures, and on the quality of the training data [15].

Furthermore, an artificial intelligence approach for the discovery and optimization of antimicrobial peptides against ESKAPE pathogens and multidrug-resistant fungi. The strategy combined cutting-edge machine learning methods such as reinforcement learning, transformer embeddings, and variational autoencoder latent representations to create and improve peptide candidates for improved antimicrobial activity. The framework helped to optimize peptide candidates and enhance the efficiency of peptide design. But there is still a large amount of experimental confirmation and evaluation of peptide stability, toxicity and clinical effectiveness to be done before they can be used clinically [16]. In a related investigation, a structure–activity relationship-based target prediction approach to study clindamycin variants having broad-spectrum bacteriostatic antibacterial activity. The study used molecular docking and molecular dynamics simulations to investigate the interactions between three clindamycin derivatives and 300 bacterial target proteins with the objective of discovering new targets and resistance mitigating mechanisms for antibacterial activity. Twenty-six protein targets with potential for improved antibacterial activity were identified by the approach. The results obtained, however, were mainly computational and need to be thoroughly validated in experiments to support the engagement of the targets and therapeutic efficacy [17].

In a similar study, developed structure-aware machine learning approaches for APs discovery and the method used the structural and sequence-based representations to enhance the identification and optimization of antimicrobial bioactive peptides. The incorporation of structure awareness facilitated peptide characterization and informed drug candidate selection for therapeutic development. The performance of the models, however, still relied on the availability and accuracy of structural data on the proteins, and this could reduce the generalizability of the models to other targets in the biological realm [18]. In a related study, an informatics approach based on artificial intelligence and AlphaFold that leverages the power of machine learning to predict protein structures, with a particular focus on its role in target discovery and therapeutic design. The method was based on the protein structure predictions made by AlphaFold2, which were used to aid biological research and speed up the drug discovery process. The framework proved to be very useful for enhancing the structural understanding of a variety of proteins such as GPCRs. However, there were some limitations, such as AlphaFold2 not being able to accurately model dynamic conformational changes and protein flexibility during molecular interactions, which hindered the reliability of the predictions [19].

Another study proposed a framework of machine learning based on perturbation theory for multi-objective antibacterial discovery, which aims to discover compounds with activity against multiple targets and bacterial strains at once. The method combined chemical structural data with perturbation-theory descriptors, creating a model to describe complex relationships between the structures and antibacterial properties of molecules and selecting promising compounds for further development. The framework improved the efficiency of multi-target and multi-strain antibacterial screening, and was useful for rational drug design. Nevertheless, the predictive power was greatly influenced by the diversity of the data set and the quality of the data and experimental validation was required to ensure that the predicted antibacterial activity is biologically relevant [20]. Although great progress has been made in computational protein structure prediction research, the studies mostly cover one aspect, such as molecular docking, inhibition potency prediction, antimicrobial peptide discovery, target identification and structure-aware machine learning. Most rely on the static AlphaFold-predicted structures and computational validation, and do not take protein dynamics, prediction reliability, and experimental validation into account. Moreover, the potential of collective acceleration in target identification, binding site prediction and virtual screening in the antibiotic drug discovery process through comprehensive evaluation of the ability of protein structure prediction is still under explored.

A systematic review approach was employed to identify and analyze recent original research studies related to computational protein structure prediction and antibiotic drug discovery. The review included peer-reviewed articles published between 2022 and 2026 from reputable publishers, namely IEEE, Springer, and MDPI. Studies focusing on AlphaFold-based modeling, structure-based drug design, molecular docking, target identification, binding site prediction, virtual screening, antimicrobial peptide discovery, and machine learning applications in drug development were considered. Review papers, survey

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articles, editorials, book chapters, conference summaries, non-English publications, duplicate studies, and articles published before 2022 were excluded to ensure the inclusion of high-quality and relevant primary research contributions.

COMPUTATIONAL APPROACHES IN ANTIBIOTIC DRUG DISCOVERY

In this section, the computational methods that have been used to help speed the process of drug discovery for antibiotics are discussed, including protein structure prediction, target identification and structure-based drug design. The examined research papers feature the application of AI, machine learning, molecular simulation, virtual screening, and protein–ligand docking, demonstrating their role in enhancing the efficiency of therapeutic development. Computational methods have improved the prediction of protein structure, identification of potential drug targets and prioritization of promising candidate compounds. Although considerable progress has been made on increasing the accuracy of predictions and the efficiency of screening, issues of data quality, computational complexity, model interpretability, and experimental validation remain to impact prediction reliability and its translation to the clinic.

Computational Protein Structure Prediction Methods

The reviewed studies highlight the increasing relevance of artificial intelligence, machine learning, and molecular simulation methods in the field of protein structure prediction, as well as other bioinformatics applications. The protein folding analysis has been greatly enhanced by deep learning-based protein structure prediction methods, which have shown great potential in gaining a more comprehensive understanding and extracting more information from the complex sequence–structure relationships, to realize efficient structural modeling and mass-scale biological data utilization [21]. By combining machine learning with molecular dynamics simulations, this approach has allowed the exploration of protein conformational ensembles to include more than just static structures, as well. The applications of machine learning have been further expanded to predict protein function, where better annotations and machine learning methods are used to enhance the accuracy and automation of the prediction of protein function by analysis of sequence, structure and interactions [22]. Moreover, the application of experimental methods like Cryo-EM and NMR spectrography, combined with computational methods has boosted the prediction and validation of protein dynamics, leading to a better understanding of the mechanisms that biomolecules employ. In the field of pharmaceuticals, computational modeling has also found applications in drug formulation optimization and prediction of intermolecular interactions, demonstrating its effectiveness in drug development [23].

The reviewed studies provide a clear illustration that the application of computational biology, artificial intelligence, and molecular modeling methods are increasingly playing an important role in speeding up the discovery of new antimicrobial drugs. In order to find pathogen-specific therapeutic targets and assess potential inhibitory compounds, subtractive genome analysis, virtual screening, molecular docking and molecular dynamics simulations have been successfully applied [24]. They have aided in identifying novel drug candidates for bacteria like Vibrio vulnificus, Mycobacterium tuberculosis and Pseudomonas aeruginosa, and drug repurposing and target prioritization strategies. Additionally, machine learning and AI-driven methodologies have led to more efficient target identification, lead optimization, and prediction of ligand–target interactions, which has helped improve the screening process, decreased development costs, and accelerated the selection of new candidates [25]. The combination of bioinformatics, computational modelling and structure-based drug design has greatly enhanced the ability to analyse complex biological systems and to find new therapeutic targets to fight antimicrobial resistance [26].

Although all these developments have been achieved there are certain drawbacks in the studies. The majority use large computational resources and also rely on high-quality datasets to be readily available for model training and validation. The reliability of predictions can get limited for rare proteins, highly dynamic biomolecular systems, or in the case of complex long-timescale conformational transitions [27]. Furthermore, limitations in data scalability, data heterogeneity and model interpretability still remain a hurdle to wider application. Many of these frameworks also depend on reliable initial structural predictions, so that errors made during the initial predictions could cascade through the analysis procedure [28]. Despite the tremendous advances in protein modeling and computational biology, there is still a need for further studies to increase robustness of prediction, decrease computational complexity, make it more biologically interpretable, and develop more general frameworks that can be used in the context of reliable structure-based drug discovery and antibiotic development.

Applications in Antibiotic Drug Discovery

The reviewed studies provide a clear illustration that the application of computational biology, artificial intelligence, and molecular modeling methods are increasingly playing an important role in speeding up the discovery of new antimicrobial drugs. In order to find pathogen-specific therapeutic targets and assess potential inhibitory compounds, subtractive genome analysis, virtual screening, molecular docking and molecular dynamics simulations have been successfully applied [24]. They have aided in identifying novel drug candidates for bacteria like Vibrio vulnificus, Mycobacterium tuberculosis and Pseudomonas aeruginosa, and drug repurposing and target prioritization strategies. Additionally, machine learning and AI-driven methodologies have led to more efficient target identification, lead optimization, and prediction of ligand–target interactions, which has helped improve the screening

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Although all the above mentioned developments were accomplished, there are some general drawbacks found in these studies. Results obtained are mostly based on computations and are highly dependent on molecular docking scores, computer simulations, and models that do not necessarily mimic real biological behaviour under actual conditions [29]. The accuracy of the predictions still depends on the quality of the structural, genomic and biochemical data that have been used to build up the model. Moreover, limitations associated with target validation, the evolution of resistance, model interpretability, and computation remain a significant issue affecting the reliability and the generalizability of the approaches. Numerous drugs currently being developed and targets for therapeutic intervention have not been fully validated in experiments, preclinical, or clinical studies and thus have low immediate translation value [30]. Overall, while computational approaches have shown significant potential for speeding up the discovery of antibiotic drugs, there remains a need for additional advances in experimental validation, high quality biological data, and reliable predictive tools to enhance the reliability of computational methods and contribute to the development of clinically effective antimicrobial drugs.

Structure-Based Drug Design

The analyzed research papers underline the trend towards the use of structure-based drug discovery, machine learning and artificial intelligence approaches in drug discovery and optimization of therapeutic candidates [31]. Several tools have been used in the past for evaluating protein–ligand interactions, prioritising candidate compounds and speeding up the drug discovery process, such as virtual screening, molecular docking, molecular dynamics simulations, and drug–target interaction prediction [32]. Machine learning is also integrated into computational drug design, enhancing the efficiency of screening, the accuracy of prediction and candidate selection in different therapeutic areas like WEE2 inhibitors, ALK inhibitors, antiviral drugs, nanobiology -driven drug development, etc. [33]. In addition, sophisticated DTI prediction algorithms and analytical models with the help of artificial intelligence have proven to be effective tools in identifying new therapeutic potential by analyzing vast amounts of biological and structural data, as well as in shortening and cost-saving the traditional drug development process.

A number of key challenges which are not yet addressed. The majority of studies are based on computational prediction and/or in silico validation which often does not provide trustworthy results in physiological conditions [34]. Quality, completeness and diversity of datasets play an important role in the effectiveness of virtual screening and interaction prediction methods. Further, some of the difficulties, like lack of interpretability in the models, data heterogeneity, inaccuracies in screening, and limited generalizability, persist and negatively impact the robustness of computational frameworks. The lack of experimental, pharmacological and clinical data to assess the efficacy of drugs in humans results in the fact that many potential drug candidates exhibit good binding properties and are structurally stable in simulated environments, but have not been shown to be effective in humans. Moreover, current methods usually fail to integrate multimodal biological data and dynamics of molecular behavior very effectively [35]. Thus, although AI and structure-based computational methods have provided great benefit in improving the efficiency of the drug discovery process, there is still a need for even more reliably predictive models, more interpretable models, more diverse sources of biological data, and greater experimental validation of computational findings to ensure successful translation of these models.

FINDINGS AND ANALYSIS

Overview of Selected Studies

The chosen studies are examples of the increasing use of computational approaches in understanding protein structure and discovery of antibiotics. The research published in the years 2022-2026 mainly dealt with artificial intelligence, machine learning, molecular docking, molecular dynamics simulations, and structure based drug design. The studies looked at different steps in the process of developing an antibacterial drug, such as protein modeling, target identification, virtual screening, and ligand–protein interaction analysis. A few studies applied AlphaFold based framework and machine learning algorithms to enhance prediction accuracy and screening efficiency. The literature reviewed together gives a thorough knowledge of the latest developments and trends in computational antibiotic discovery.

Table 1. Comparative Analysis of Computational Approaches Applied in Antibiotic Drug Discovery

Antibiotic Discovery Task	Year	Computational Technique	Application Domain
Protein–Ligand Interaction Prediction	2024	AlphaFold2, Molecular Docking, Machine Learning Rescoring	Antibiotic Discovery
Inhibition Potency Prediction	2024	Machine Learning, AlphaFold2 Protein Fingerprints	Drug–Target Interaction Analysis

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Antibiotic Discovery Task	Year	Computational Technique	Application Domain
Antimicrobial Peptide Discovery	2024	Reinforcement Learning, Transformer Embeddings, Variational Autoencoders	Antimicrobial Therapeutics
Drug Target Identification	2023	Molecular Docking, Molecular Dynamics Simulation	Antibacterial Target Discovery
Antimicrobial Peptide Optimization	2024	Structure-Aware Machine Learning	Peptide Engineering
Protein Structure Prediction	2024	Artificial Intelligence, AlphaFold2	Structural Biology
Multi-Target Antibacterial Screening	2024	Perturbation-Theory Machine Learning	Antibacterial Drug Discovery
Protein Folding Prediction	2024	Deep Neural Networks	Protein Structure Modeling
Protein Conformational Analysis	2024	Machine Learning, Molecular Dynamics	Structural Dynamics
Protein Function Prediction	2023	Machine Learning, Deep Learning	Functional Annotation
Protein Dynamics Validation	2024	Molecular Dynamics, Cryo-EM, NMR, AI	Structural Validation
Antimicrobial Candidate Discovery	2024	Molecular Docking, Virtual Screening	Antimicrobial Drug Discovery
Anti-Tuberculosis Target Identification	2023	Genomic and Computational Analysis	Tuberculosis Drug Discovery
Drug Repurposing	2024	Virtual Screening, Docking, Molecular Dynamics	Therapeutic Repositioning
Drug Design Optimization	2024	Artificial Intelligence, Bioinformatics	Drug Development
Inhibitor Discovery	2024	Virtual Screening, Molecular Dynamics	Structure-Based Drug Design
Drug–Target Interaction Prediction	2024	Machine Learning, Deep Learning, Network Analysis	Interaction Modeling
Protein Corona Analysis	2024	Artificial Intelligence, Machine Learning	Nanobiology and Drug Discovery
Protease Inhibitor Discovery	2023	Structure-Based Virtual Screening	Antiviral Drug Discovery
Lead Compound Identification	2024	Machine Learning, Virtual Screening, Molecular Dynamics	Lead Optimization

Table 1. shows a comparison of computational methods used in the discovery of antibiotic drugs. The studies chosen illustrate the use of artificial intelligence, machine learning, molecular docking, molecular dynamics simulation and virtual screening in the different phases of discovery. The results show the growing importance of computational methods for assisting in the identification of therapeutic targets, screening of therapeutic candidates and structure-based drug development.

Findings on Protein Structure Prediction Performance

The studies reviewed suggest that the use of deep learning, machine learning and molecular simulation approaches can significantly enhance the prediction of protein structures. AlphaFold-based models showed superior prediction accuracy of proteins in terms of structures, successfully leveraging the sequence–structure relationships to produce high-quality 3D protein models. Combined with the molecular dynamics simulations, the characterization of protein flexibility and conformational behavior was further enhanced. These improvements enabled more accurate structures to be provided for downstream drug discovery applications. The accuracy, however, depended on the quality of training data and computational resources and on the accurate modeling of dynamic protein behavior under complex biological conditions.

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Table 2. Critical Comparison of Protein Structure Prediction Methods

Method	Principle	Advantages	Limitations	Application in Drug Discovery
Homology Modelling	Template-based structure prediction	Fast and cost-effective	Depends on template availability	Target structure generation
Molecular Simulations	Physics-based protein modeling	Captures protein dynamics	Computationally expensive	Binding interaction analysis
Machine Learning-Based Prediction	Learns sequence–structure relationships	High prediction accuracy	Requires large datasets	Structure prediction and target identification
AlphaFold-Based Prediction	Deep learning protein folding prediction	Highly accurate structures	Limited dynamic information	Structure-based drug design

The production of widely used protein structure prediction methods found in the reviewed articles is presented here in Table 2. where a critical comparison is made. They are compared on the basis of their principles, their benefits, their drawbacks and their use in drug discovery for example. The results show that the AI models are more accurate at predicting the results, and the molecular simulations give more detailed information about the structure, but at higher computational cost.

Findings on Drug Target Identification

The reviewed studies showed that computational protein modeling is a crucial method for identification and prioritization of potential antibacterial drug targets. Predicted protein structures provided the researchers with the ability to study key biological pathways, isolated proteins unique to pathogens and explored the mechanisms of bacterial survival and resistance. The use of artificial intelligence and machine learning techniques further enhanced the target selection processes, based on the analysis of large-scale biological datasets and prediction of functional relationships. Such computational methods shortened the time and effort needed in the process of target discovery. However, validity of identified targets needs to be fully confirmed through a large amount of experiments before their potential therapeutic applicability can be fully confirmed.

Table 3. Comparison of Computational Tools Used in Literature

Tool	Purpose	Strength	Limitation
AlphaFold2	Protein structure prediction	High structural accuracy	Static structure prediction
RoseTTAFold	Protein modeling	Fast prediction	Lower accuracy for some proteins
AutoDock Vina	Molecular docking	Efficient virtual screening	Sensitive to docking parameters
GROMACS	Molecular dynamics simulation	Detailed dynamic analysis	High computational cost
PyMOL	Structure visualization	Easy structural interpretation	Not predictive
Deep Learning Models	Protein analysis and prediction	Learns complex patterns	Data dependency

Table 3. shows a comparison of the computational tools used in the studies selected for protein structure prediction, molecular docking, simulation and structural analysis. The comparison emphasizes the purpose, advantages and disadvantages of each tool. The results illustrate that the combination of multiple computational platforms can bring benefits in terms of efficiency and reliability to the structure-based drug discovery workflow.

Findings on Binding Site and Protein–Ligand Interaction Analysis

The selected studies, it can be seen that computational methods play an important role in the identification of protein binding sites and the study of protein–ligand interactions. Molecular docking and molecular dynamics simulations are extensively used for exploring binding affinity, interaction stability and molecular recognition mechanisms. The active sites were predicted to identify potential targets for antibacterial compound using the predicted protein structure. In addition, the use of machine learning techniques enhanced the prediction of interactions and prioritization of candidates. These approaches improved the knowledge of molecular binding properties, and provided assistance in rational drug design. But the predictive power was still affected by the quality of the structure, the ability of the algorithm and the biological complexity.

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Findings on Virtual Screening and Candidate Prioritization

Virtual screening proved to be a key tool in the computational antibiotic drug discovery process in all the reviewed studies. Large compound libraries were rapidly screened using structure-based approaches to generate a number of potentially therapeutic compounds. Molecular docking, machine learning algorithms, and prioritizing using artificial intelligence enhanced the efficiency of screening and decreased the number of compounds that needed experimental testing. Based on several studies a number of candidate molecules were identified that possess good binding properties and therapeutic potential. The use of computational screening methods helped shorten the lead discovery and optimization processes. The results of screening, however, still relied on the reliability of the predictive model and the quality of the structural data available.

Table 4. Comparative Analysis of Drug Discovery Applications

Application Area	Computational Approach	Contribution
Target Identification	Protein Structure Prediction	Identification of essential proteins
Binding Site Prediction	Docking and Structural Analysis	Detection of active sites
Virtual Screening	Molecular Docking	Compound prioritization
Lead Optimization	Molecular Dynamics	Stability assessment
Drug Repurposing	AI and Machine Learning	Candidate selection

The computational prediction of the protein structure has some important applications in the field of antibiotic drug discovery, which are summarized in Table 4. The comparison shows the contribution of various computational methods to target identification, prediction of binding sites, virtual screening, lead optimization and drug repurposing. The results highlight the critical role of computational approaches in speeding up the therapeutic development process in the early stages.

Findings on Research Efficiency

The literature reviewed showed that computational methods can enhance the efficiency of the total antibiotic drug discovery process. The protein structure prediction, molecular modelling and artificial intelligence methods shortened the time and expense of the traditional experimental process. Automated target identification and virtual screening and interaction analysis helped inform quicker decision-making and better candidate selection. Research productivity was greatly boosted by the use of computational frameworks for investigating many proteins and compounds at once. In addition, sophisticated predictive models were incorporated to improve the early discovery techniques. While these benefits are significant, large computing capacity and special skills are still required for successful implementation.

Key Challenges Identified

Even though there have been substantial technological advances, several common challenges have been found in the studies reviewed. Most computational methods require high-quality biological, structural and interaction data to accurately predict. Reliability is still not satisfactory due to restrictions in model interpretability, prediction uncertainty, computational complexity, and scalability. Furthermore, most of the studies were predominantly in silico based, which raises concerns about how well this would work in vivo. A proper modeling of protein flexibility, conformational dynamics, and complex cellular interactions still remains a challenge. Therefore, experimental validation is still necessary to validate computational results and to provide the clinical proof of successful translation of predicted candidates into clinically viable antibacterial therapies.

DISCUSSION

Results of this research show that computational biology is a fundamental requirement in the process of discovery of new antibiotics. Increased understanding of protein structure prediction, such as AI and machine learning, molecular docking, and molecular dynamics simulations, have enhanced the capacity to identify potential drug targets and prioritize promising therapeutic candidates. These strategies allow biologists to study complex systems more efficiently and at a fraction of the time and expense of conventional experimental drug discovery processes. Moreover, computational methods can aid in quick hypothesis generation, binding site identification and virtual screening, which expedites pharmaceutical research efforts at the early stages. While these benefits are apparent, there are still a few obstacles that hinder the complete potentiality of computational drug discovery. The accuracy of the predictions remains to depend on the biological datasets and computational models. The dynamic processes of protein flexibility and the complex nature of biological systems can be hard to accurately represent with current computation. Furthermore, the majority of the findings have to be further investigated in the lab to prove their biological activity, therapeutic use, and clinical relevance as well, indicating the need for the combination of computational and experimental approaches.

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CONCLUSION

This study aimed to assess the contribution of computational protein structure prediction to speed up the drug discovery process for fighting antimicrobial resistance. The collected literature shows that in the field of drug target identification and prediction of protein–ligand interactions, as well as screening potential therapeutic compounds, advances in AI, machine learning, molecular docking, molecular dynamics simulations and structure-based drug design have significantly improved efficiency. Computational techniques give valuable structural information, which can be used in rational drug design, and can also be used to examine a large number of proteins and compounds in a shorter amount of time than traditional experimental methods. These features can help lower development expenses, speed up candidate prioritization and help with decision making in early drug discovery.

The study also identified that computational prediction of protein structure has turned into an effective tool for the development of antibiotics against resistant bacterial pathogens. There are however, certain constraints: reliance on good quality data, complexity of the problem, uncertainty of prediction, and challenges of adequately describing biological dynamics. Most of the computational results also need to be validated experimentally before they can be applied clinically. However, continued development of AI and computational biology is likely to further improve the accuracy of prediction and efficiency of drug discovery. Hence, computational protein structure prediction is an important area that could help significantly speed antibiotic discovery efforts and has great promise in the potential to aid future drug discovery efforts to combat the worldwide problem of antimicrobial resistance.

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