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Review Article

Applications of Artificial Intelligence in Computer-Aided Drug Discovery Against Infectious Microorganisms

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Abstract

The emergence of antimicrobial resistance and infectious disease outbreaks represents an escalating global health crisis demanding innovative therapeutic strategies. Artificial intelligence has revolutionised computer-aided drug discovery by accelerating the identification of novel antimicrobial agents, predicting resistance patterns, and optimising drug design processes. Recent breakthroughs include the discovery of halicin and other structurally novel antibiotics through deep learning algorithms, the development of generative AI frameworks for de novo antibiotic design yielding compounds with selective activity against multidrug-resistant pathogens, and AI-powered antimicrobial peptide discovery platforms that have identified nearly one million candidate peptides from global microbiome data. This review examines these applications of machine learning and deep learning approaches in discovering therapeutics against infectious microorganisms, including bacteria, viruses, fungi, and parasites. Key areas explored include virtual screening platforms, de novo drug design using generative models, antimicrobial peptide discovery,

structure-based drug design leveraging AlphaFold predictions, and resistance prediction algorithms. Despite significant advances, including the discovery of halicin through deep learning algorithms showing broad-spectrum activity against drug-resistant bacteria, the development of generative models capable of designing novel antimicrobial scaffolds with distinct mechanisms of action, and the deployment of AlphaFold for structure-based drug design against previously intractable pathogen targets, challenges persist regarding data quality, model interpretability, and translational validation. This review highlights both the transformative potential and current limitations of AI-driven approaches in addressing the antimicrobial resistance crisis and emerging infectious diseases.

Keywords: Artificial Intelligence; Machine Learning; Drug Discovery; Antimicrobial Resistance; Infectious Diseases; Virtual Screening; Deep Learning

Introduction

Infectious diseases remain among the leading causes of mortality worldwide, with antimicrobial resistance emerging as one of the most pressing public health threats of the 21st century [1]. The World Health Organisation estimates that drug-resistant infections could cause 10 million deaths annually by 2050 if current trends continue. Traditional antibiotic discovery methods have proven increasingly inadequate, with the pharmaceutical industry experiencing a discovery void over the past three decades [2]. The time required to develop new antimicrobial agents through conventional approaches typically spans 10-15 years with estimated costs ranging from $161 million to $4.5 billion, while success rates remain discouragingly low [3].

Artificial intelligence, particularly machine learning and deep learning methodologies, has emerged as a transformative tool capable of addressing these challenges. AI-driven approaches can analyse vast chemical libraries, predict molecular properties, identify novel drug targets, and optimize lead compounds with unprecedented speed and efficiency [4,5]. Recent breakthroughs, such as the discovery of halicin and other novel antibiotics through deep learning algorithms, demonstrate the practical potential of these technologies [6].

This review examines the current landscape of AI applications in computer-aided drug discovery against infectious microorganisms, focusing on developments from 2020 to 2025. We explore various AI methodologies, their specific applications across different pathogen types, and discuss both achievements and remaining challenges in translating computational predictions to clinical therapeutics.

AI technologies in drug discovery

Machine learning fundamentals

Machine learning encompasses algorithms that enable computers to learn patterns from data without explicit programming. In drug discovery, supervised learning approaches train models on labelled datasets containing known drug-target interactions, molecular properties, or biological activities. Random forests, support vector machines, and gradient boosting algorithms have demonstrated success in quantitative structure-activity relationship modelling and classification tasks [7].

Deep learning architectures

Deep neural networks employ multiple layers of interconnected nodes to extract hierarchical features from complex datasets. Convolutional neural networks excel at analysing molecular structures represented as graphs or images, while recurrent neural networks process sequential data such as protein or nucleic acid sequences [8]. Recent architectures including transformers and graph neural networks have shown particular promise for molecular property prediction and generation [9].

Generative models

Generative adversarial networks and variational autoencoders enable de novo molecular design by learning to generate novel chemical structures with desired properties. These models can explore vast regions of chemical space beyond enumerated libraries, potentially discovering structurally distinct antimicrobial scaffolds [10]. Junction tree variational autoencoders and molecular graph generation methods have been specifically adapted for antibiotic discovery applications [11]. Table 1 shows the comparison of AI methologies in drug discovery.

AI Method	Applications	Advantages	Limitations	Representative Tools
Random Forest	QSAR modelling, property prediction	High interpretability, robust to overfitting	Limited performance on complex data	Scikit-learn, WEKA
Support Vector Machines	Classification, activity prediction	Effective in high-dimensional spaces	Computationally intensive for large datasets	LIBSVM, Scikit-learn
Deep Neural Networks	Molecular property prediction, toxicity	Handles complex patterns, high accuracy	Requires large datasets, low interpretability	TensorFlow, PyTorch
Graph Neural Networks	Molecular generation, interaction prediction	Captures molecular topology	Computationally demanding	DeepChem, DGL
Generative Adversarial Networks	De novo drug design	Generates novel structures	Training instability, validation challenges	RDKit, Moses
Variational Autoencoders	Molecular optimization	Continuous latent space	May generate invalid structures	ChemVAE, JTVAE
Transformers	Sequence analysis, protein modelling	Attention mechanism, scalability	High computational cost	AlphaFold, ESM

Table 1: Comparison of AI Methodologies in Drug Discovery.

Source: Authors' compilation based on references [5,7,8].

Virtual screening and hit identification

AI-accelerated virtual screening platforms

Structure-based virtual screening has been revolutionized by AI-powered platforms that can efficiently screen multi-billion compound libraries. Zhou., *et al*. developed RosettaVS, an open-source AI-accelerated platform that outperforms traditional docking methods, successfully identifying novel hits against challenging targets including those relevant to infectious diseases [12]. The integration of active learning strategies allows iterative refinement of predictions, substantially reducing computational costs while maintaining accuracy.

Deep docking approaches employ neural networks to guide the exploration of ultra-large chemical libraries, achieving orders of magnitude acceleration compared to conventional molecular docking [13]. These platforms have demonstrated particular utility in identifying inhibitors for viral targets, including SARS-CoV-2 protease and RNA-dependent RNA polymerase [14]. Figure 1 presents the AI-Accelerated Virtual Screening Workflow.

AI has enhanced ligand-based approaches through sophisticated similarity searching and pharmacophore modelling. Machine learning models trained on known active compounds can identify structurally diverse molecules with similar biological activities. Consensus approaches combining multiple algorithms have shown improved hit rates compared to individual methods [15].

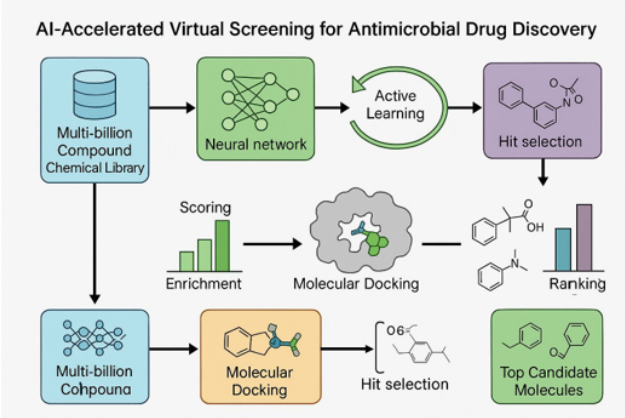

Figure 1: AI-Accelerated Virtual Screening Workflow.

Source: Original schematic based on workflows described in references [9,12-14].

De Novo antibiotic design

Generative deep learning for novel scaffolds

A landmark study by researchers at MIT and the Broad Institute demonstrated the power of generative AI for de novo antibiotic

design. Using genetic algorithms coupled with variational autoencoders, they screened over 10^7 chemical fragments in silico against bacterial pathogens, subsequently synthesizing 24 compounds of which seven exhibited selective antibacterial activity [16]. Two lead compounds demonstrated bactericidal efficacy against multidrug-resistant *Neisseria gonorrhoeae* and *Staphylococcus aureus* in mouse models with distinct mechanisms of action.

This fragment-based approach comprehensively explores chemical space by first identifying promising molecular fragments, then expanding them into complete drug-like molecules. The unconstrained de novo generation mode enables discovery of compounds beyond the boundaries of existing chemical databases [17].

Target-specific design optimization

Graph neural networks trained to predict antibacterial activity enable rapid evaluation of synthetic compounds. These models integrate structural features, physicochemical properties, and predicted biological activities to guide molecular optimization. Recent work has demonstrated the successful application of reinforcement learning to optimize multiple drug properties simultaneously, including antimicrobial potency, selectivity, and pharmacokinetic profiles [18]. Table 2 presents recent AI-discovered antimicrobial compounds with experimental validation.

Compound	AI Method	Target Organism	Validation Stage	Key Features	Reference
Halicin	Graph Neural Network	*E. coli, A. baumannii, C. difficile*	*In vivo* (mouse models)	Broad-spectrum, structurally distinct	Stokes., *et al*. 2020
Compound 1 (De novo)	GAN + VAE	*N. gonorrhoeae*	*In vivo* (mouse models)	Novel mechanism of action	Wan., *et al*. 2025
Compound 2 (De novo)	GAN + VAE	*S. aureus (MRSA)*	*In vivo* (mouse models)	Bactericidal, low resistance	Wan., *et al*. 2025
Mammuthusin	Deep Learning (APEX)	Multiple bacteria	Preclinical	Mined from extinct organisms	Torres., *et al*. 2024
Elephasin	Deep Learning (APEX)	Multiple bacteria	Preclinical	Peptide antibiotic	Torres., *et al*. 2024
Baricitinib	Knowledge Graph Mining	SARS-CoV-2	Clinical trials	Repurposed JAK inhibitor	Richardson., *et al*. 2020

Table 2: Recent AI-Discovered Antimicrobial Compounds with Experimental Validation.

Sources: Data compiled from references [6,16,19,32].

Antimicrobial peptide discovery

Mining natural sources

Antimicrobial peptides represent a promising therapeutic class due to their broad-spectrum activity and lower propensity for resistance development. Deep learning models have been successfully applied to mine vast biological databases for novel AMP candidates. Santos-Junior., *et al*. developed machine learning algorithms to discover antimicrobial peptides in the global microbiome, identifying nearly one million candidate peptides [19].

The APEX model mines extinct organisms as sources of antibiotic molecules, leading to identification of preclinical candidates including mammuthusin and elephasin [20]. This approach expands the searchable biological space beyond extant organisms, potentially uncovering unique antimicrobial mechanisms.

Predictive models and design

Deep neural networks trained on physicochemical parameters of peptides have achieved over 90% accuracy in predicting antimicrobial activity against specific pathogens. Conversion

of peptide sequences into signal images enables extraction of complex features through convolutional architectures [21]. These models can predict Gram-positive versus Gram-negative selectivity, minimum inhibitory concentrations, and potential cytotoxicity.

Machine learning approaches also accelerate rational peptide design by predicting structure-function relationships. Models incorporating sequence, secondary structure, amphipathicity, and charge distribution enable systematic optimization of AMP properties [22]. Figure 2 Presents the deep learning pipeline for AMP discovery.

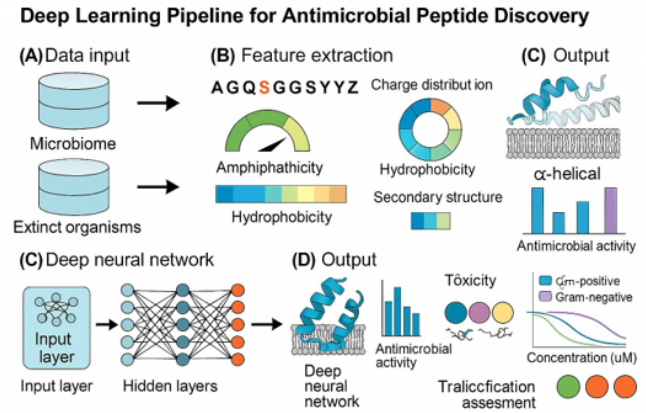

Figure 2: Deep Learning Pipeline for AMP Discovery.

Source: Original schematic based on methodologies in references [17,19,20].

Structure-Based Drug Design with AlphaFold

Protein structure prediction

AlphaFold2 and its successor AlphaFold3 have revolutionised structural biology by predicting protein structures with near-experimental accuracy. For drug discovery against infectious diseases, this technology enables structure-based design for pathogen targets lacking experimental structures. The AlphaFold Protein Structure Database now contains over 200 million predicted structures, providing unprecedented coverage of potential antimicrobial targets [23,24].

AlphaFold3 extends capabilities to predict protein-ligand complexes, protein-nucleic acid interactions, and modified residues, showing at least 50% improvement over previous methods for molecular interactions [25]. This advance facilitates more accurate virtual screening and structure-based optimisation.

Applications and limitations

While AlphaFold models provide valuable starting points for drug design, several limitations affect their utility for ligand docking. Studies demonstrate that AlphaFold predictions typically represent apo (ligand-free) conformations, which may differ substantially from ligand-bound states [26]. The models cannot capture protein flexibility or conformational changes induced by ligand binding, potentially reducing docking accuracy compared to experimental structures.

Nevertheless, AlphaFold models have proven particularly valuable for novel targets in understudied pathogens where no experimental structures exist. Combined with molecular dynamics simulations to sample conformational ensembles, these predictions enhance structure-based drug discovery efforts [27]. Figure 3 shows the AlphaFold in Antimicrobial Drug Discovery

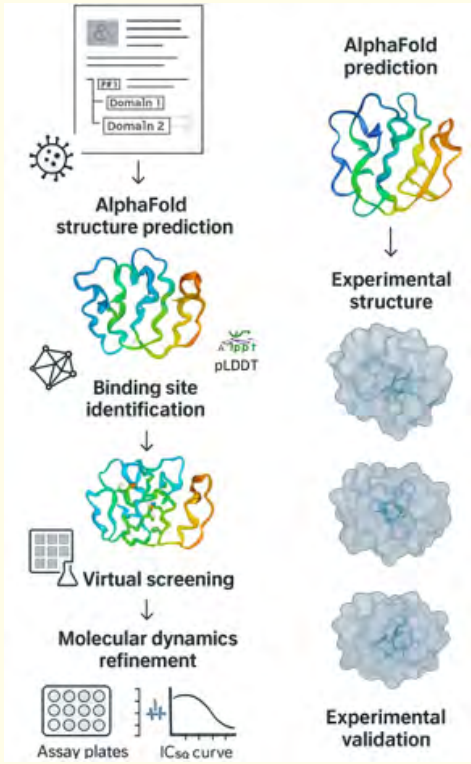

Figure 3: AlphaFold in Antimicrobial Drug Discovery.

Source: Original schematic based on AlphaFold applications described in references [23-27].

Resistance prediction and surveillance

Machine learning for resistance detection

AI algorithms trained on genomic and phenotypic data enable rapid prediction of antimicrobial resistance patterns. These models analyse genetic markers, mutations in resistance genes, and gene expression profiles to forecast resistance phenotypes with high accuracy [28]. Integration with clinical data allows real-time surveillance and early warning systems for emerging resistant strains.

Deep learning approaches can identify novel resistance mechanisms by detecting subtle patterns in genome sequences that elude conventional analysis. Convolutional neural networks trained on bacterial genome assemblies successfully classify resistant versus susceptible isolates across multiple antibiotic classes [29].

Predicting resistance evolution

Computational models simulate the evolution of resistance under drug selection pressure, informing combination therapy design and treatment strategies. Machine learning algorithms analyse thousands of potential drug combinations to identify synergistic interactions that suppress resistance development [30]. These approaches consider pharmacokinetic-pharmacodynamic parameters, resistance mutation rates, and bacterial growth dynamics. Table 3 shows the AI Applications in Antimicrobial Resistance Prediction.

Application Area	AI Approach	Data Sources	Prediction Target	Accuracy	Clinical Impact
Genomic resistance prediction	CNN, Random Forest	Whole genome sequences	Resistance phenotype across antibiotic classes	85-95%	Rapid susceptibility testing
Mutation effect prediction	Deep Learning	Protein sequences, structural data	Impact of mutations on resistance	80-90%	Targeted therapy selection
Resistance surveillance	Machine Learning	Clinical isolate data, genomic databases	Emerging resistance patterns	75-85%	Early warning systems
Combination therapy design	Reinforcement Learning	Drug interaction data, PK/PD models	Synergistic combinations	Variable	Resistance suppression
Evolution prediction	Agent-based models	Evolutionary data, fitness landscapes	Resistance trajectory	70-80%	Treatment strategy optimisation

Table 3: AI Applications in Antimicrobial Resistance Prediction.

Source: Authors' synthesis based on references [28-30].

Applications across pathogen types

Antibacterial discovery

AI has demonstrated particular success in antibacterial drug discovery, with multiple compounds advancing to preclinical and clinical evaluation. Beyond halicin, other notable examples include AI-designed molecules targeting *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, and methicillin-resistant *Staphylococcus aureus* [31]. Graph neural networks enable the identification of compounds with activity against antibiotic-resistant strains while maintaining low toxicity profiles.

Machine learning models also facilitate antibiotic repurposing by identifying existing drugs with previously unrecognised antibacterial properties. Natural language processing approaches mine scientific literature and clinical databases to uncover hidden connections between compounds and bacterial targets [32].

Antiviral drug development

The COVID-19 pandemic accelerated AI applications in antiviral discovery. Virtual screening campaigns identified potential inhibitors of SARS-CoV-2 proteins, including main protease, spike protein, and RNA polymerase [33]. Generative models designed novel protease inhibitors within weeks of viral genome sequencing, demonstrating rapid response capabilities.

AI platforms now support antiviral development against diverse viral families including influenza, HIV, hepatitis viruses, and emerging pathogens. Models trained on viral protein structures and known inhibitors can rapidly propose candidates for new viral threats [34]. Figure 4 gives the AI-Driven Antiviral Discovery Timeline.

Figure 4: AI-Driven Antiviral Discovery Timeline.

Source: Authors' compilation based on references [32-34].

Antifungal and antiparasitic applications

While less extensively studied, AI approaches show promise for antifungal drug discovery. Machine learning models predict inhibitors of fungal-specific targets, including CYP51, β-1,3-glucan synthase, and chitin synthase [35]. The limited number of antifungal drug classes makes AI-enabled discovery particularly valuable for addressing resistant Candida and Aspergillus infections.

For antiparasitic applications, AI facilitates the identification of compounds against neglected tropical diseases. Virtual screening against parasitic enzymes and computational prediction of compound selectivity accelerate lead discovery for malaria, leishmaniasis, and trypanosomiasis [36].

Integration with experimental workflows

Automated screening platforms

The true potential of AI in drug discovery emerges when integrated with automated experimental validation. High-throughput screening robotics coupled with machine learning create closed-loop systems where computational predictions guide synthesis and testing, while experimental results refine models [37]. Active learning frameworks minimise the number of compounds requiring synthesis while maximising information gain.

ZairaChem exemplifies the successful implementation of end-to-end AI/ML workflows in resource-limited settings. This platform enables fully automated QSAR modelling for malaria and tuberculosis drug discovery, demonstrating that AI tools can be effectively deployed beyond well-resourced institutions [38].

Challenges in translation

Despite computational successes, significant gaps persist between in silico predictions and clinical therapeutics. Models trained on limited datasets may not generalize to structurally novel compounds or complex biological systems. *In vitro* activity does not guarantee *in vivo* efficacy, and computational predictions of pharmacokinetics, toxicity, and formulation properties require extensive experimental validation [39].

Bridging this gap requires integration of diverse data types including transcriptomics, proteomics, and clinical outcomes. Multi-task learning approaches that simultaneously predict multiple relevant properties show promise for improving translational success rates. Figure 5 presents the Integrated AI-Experimental Drug Discovery.

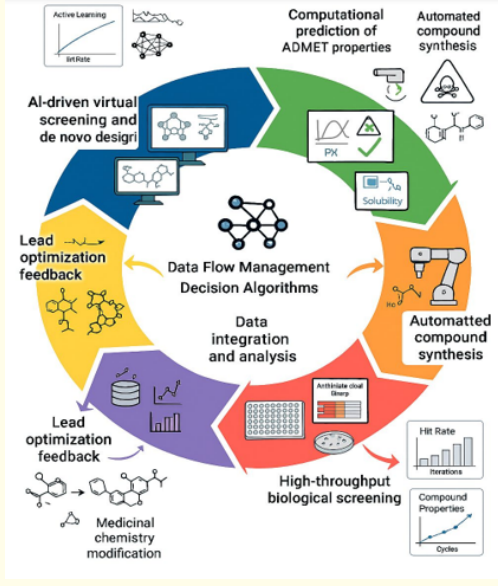

Figure 5: Integrated AI-Experimental Drug Discovery

Source: Original schematic based on integrated workflows described in references [1,3,43].

Challenges and future directions

Data quality and availability

AI model performance depends critically on training data quality. Inconsistent experimental protocols, reporting bias toward positive results, and limited data for certain pathogen-drug combinations constrain model development. Efforts to create standardised, curated datasets for antimicrobial research remain essential [40]. The establishment of benchmark datasets and the sharing of negative results would substantially improve model robustness.

Model interpretability

Deep learning models often function as "black boxes," providing limited insight into underlying mechanisms. Explainable AI approaches that elucidate feature importance and decision pathways can build confidence in predictions and guide medicinal chemistry optimisation [41]. Integration of chemical and biological knowledge into model architectures may enhance both interpretability and generalisation.

Regulatory considerations

As AI-discovered compounds advance toward clinical development, regulatory frameworks must evolve to accommodate these technologies. The FDA and other agencies are developing guidance for AI/ML applications in drug development, addressing issues of validation, transparency, and reproducibility [42]. Clear standards for computational model validation and documentation will facilitate regulatory acceptance.

Future prospects

Emerging directions include integration of multi-omics data, development of foundation models trained on diverse biological data, and application of reinforcement learning for sequential decision-making in drug optimisation. Quantum computing may eventually enable more accurate molecular simulations, while improved natural language processing could better leverage scientific literature [43].

The combination of AI with other technologies such as CRISPR-based target validation, organ-on-chip models, and advanced imaging creates powerful synergies. These integrated approaches promise to accelerate the discovery of next-generation antimicrobials capable of combating resistant pathogens and emerging infectious diseases.

Conclusion

Artificial intelligence has fundamentally transformed computer-aided drug discovery against infectious microorganisms, providing tools to address the antimicrobial resistance crisis and respond rapidly to emerging pathogens. From virtual screening of billion-compound libraries to de novo generation of novel antimicrobial scaffolds, AI technologies demonstrate both remarkable successes and ongoing challenges. While computational predictions have led to experimentally validated hits and preclinical candidates, substantial work remains to consistently translate these advances into approved therapeutics.

Success requires continued investment in high-quality datasets, interdisciplinary collaboration between computational scientists and medicinal chemists, and integration with automated experimental platforms. As AI methodologies mature and regulatory frameworks adapt, these technologies will increasingly become standard components of antimicrobial drug discovery pipelines, ultimately delivering novel therapeutics to patients facing life-threatening infections.

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Conflict of Interest

The authors declare no conflicts of interest.

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