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AI-Assisted Drug Discovery Against Multidrug-Resistant Bacteria

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Abstract: The increasing occurrence of multidrug-resistant (MDR) bacteria, commonly known as superbugs. It is a leading global health threat. The antibiotic discovery pipeline is effectively stagnant due to excessive costs, a long lead time for drug development, and decreased profits for pharmaceutical companies. Artificial intelligence (AI) and machine learning (ML) have proven to be thriving zeitgeists for advancing antimicrobial research through the rapid evaluations of large biological and chemical datasets, predicting antimicrobial activity, identifying novel drug targets, and optimizing pharmacokinetics. This review outlines the various applications of AI-based endeavours in solving the issue of MDR pathogens. These include target identification, virtual screenings, de novo drug design, drug repurposing, optimizing pharmacokinetics, and integrating with experimental systems biology. We will discuss significant discoveries such as halicin and abaucin, as well as limitations including data availability and interpretability. We will explore regulatory aspects and ethical aspects of AI and ML applications, and we will propose future directions for integrating AI and ML in clinical microbiology and personalized medicine to subsume the global antimicrobial resistance (AMR) crisis.

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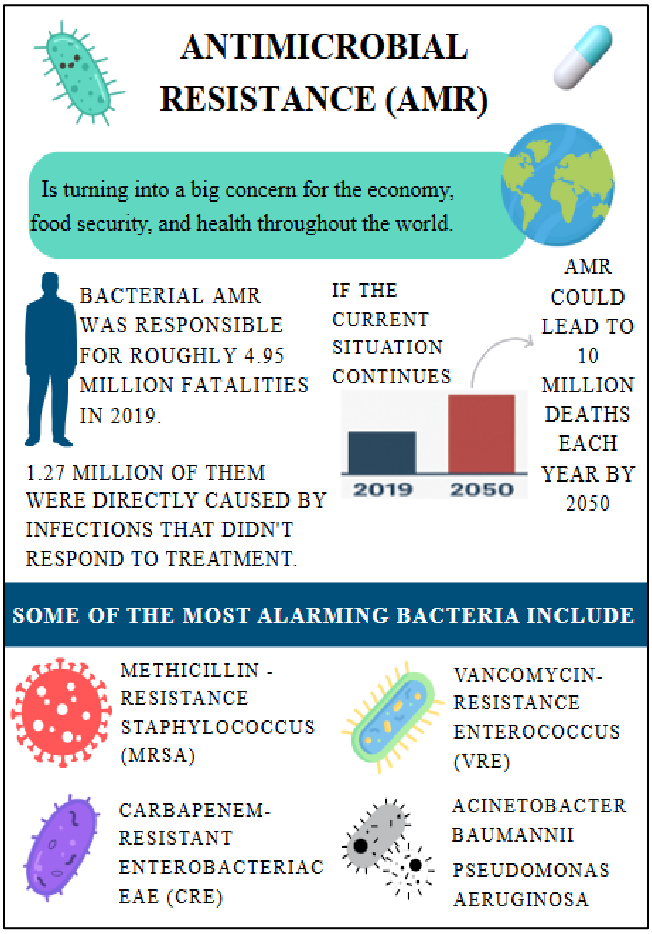
I. INTRODUCTION

Antimicrobial resistance (AMR) is becoming a serious problem for global health, food security, and the economy. In 2019, about 4.95 million deaths were linked to bacterial AMR, and 1.27 million of these were directly caused by resistant infections (Tang et al., 2023). If the current situation continues, AMR could lead to 10 million deaths each year by 2050 (Price, 2016).Some of the most alarming bacteria include methicillin-resistant Staphylococcus aureus (MRSA), carbapenem-resistant enterobacteriaceae (CRE), vancomycin-resistant Enterococcus (VRE), Acinetobacter baumannii and Pseudomonas aeruginosa in shown (figure 1) (Brown & Wright, 2016; Stokes et al., 2020). Antibiotic resistance is growing, but the development of new antibiotics has slowed considerably. Making a new antibiotic takes a long time about 10–15 years and costs over US$1 billion (DiMasi et al., 2016). Throughout the drug discovery process, candidates fail during development, while antibiotics typically return less revenue than medicines for long-term diseases. Consequently, large pharmaceutical companies have shifted their R&D focus away from antibiotics and towards drug development for long-term diseases (Payne et al., 2007). Since the 1980s, there have been few new classes of antibiotics developed, which shows that we need new ways to find drugs (Preuer et al., 2018).



ANTIMICROBIAL RESISTANCE (AMR)

Is turning into a big concern for the economy, food security, and health throughout the world.

BACTERIAL AMR WAS RESPONSIBLE FOR ROUGHLY 4.95 MILLION FATALITIES IN 2019.

1.27 MILLION OF THEM WERE DIRECTLY CAUSED BY INFECTIONS THAT DIDN'T RESPOND TO TREATMENT.

IF THE CURRENT SITUATION CONTINUES

AMR COULD LEAD TO 10 MILLION DEATHS EACH YEAR BY 2050

SOME OF THE MOST ALARMING BACTERIA INCLUDE

METHICILLIN - RESISTANCE STAPHYLOCOCCUS (MRSA)

VANCOMYCIN-RESISTANCE ENTEROCOCCUS (VRE)

CARBAPENEM-RESISTANT ENTEROBACTERIACEAE (CRE)

ACINETOBACTER BAUMANNII

PSEUDOMONAS AERUGINOSA

Fig 1 Antimicrobial Resistance (AMR)

II. ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY

Artificial intelligence comprises a variety of computing approaches that mimic human learning and decision-making. The typical methods for drug discovery include machine learning has been used to predict bioactivity and toxicity through techniques such as random forests, support vector machines, and gradient boosting (Vamathevan et al., 2019). Deep Learning (DL) employs convolutional and recurrent neural networks to learn complex molecular interactions from extensive datasets (H. Chen et al., 2018a).Generative models, such as generative adversarial networks (GANs) and variation auto encoders (VAEs), are able to create new ant bacterially active compounds (Sanchez-Lengeling & Aspuru-Guzik, 2018). NLP mining of biological literature, clinical notes, and patents to discover new compounds and processes (Wei et al., 2016). RL is an iterative optimization method for molecular design that enables exploration of a wide range of chemical spaces (Popova et al., 2018). AI provides numerous distinct benefits in combating MDR pathogens: Efficiently explores over 10^{60} drug-like compounds (Polishchuk et al., 2013).Used virtual screening to prioritize compounds for wet-lab validation (Rifaioglu et al., 2019). Discovered novel drug targets through genomic & proteomic databases (Ahn & Wang, 2008). Use of existing non-antibiotic medicines to treat bacterial infections (Opal, 2016). Predicting effective antibiotic combinations to combat resistance (17). Optimizing pharmacokinetics (ADMET) early in the discovery process in shown (Table 1) (Eddershaw et al., 2000).

Table 1 Applications of Artificial Intelligence in Drug Discovery

AI Technique / Approach	Application in Drug Discovery	Examples / Methods	Key Benefits / Outcomes
Machine Learning (ML)	Predicts bioactivity, toxicity, and target interactions	Random Forests, Support Vector Machines (SVM), Gradient Boosting	Enhances accuracy in compound screening and toxicity prediction (J. Zhang et al., 2025).
Deep Learning (DL)	Learns complex molecular interactions from large datasets	Convolutional Neural Networks (CNNs), Recurrent Neural Networks (RNNs)	Identifies novel molecular patterns and relationships (H. Chen et al., 2018b).
Generative Models	Designs new drug-like molecules with desired properties	Generative Adversarial Networks (GANs), Variational Autoencoders (VAEs)	Generates novel antibacterially active compounds (Gangwal et al., 2024).
Natural Language Processing (NLP)	Extracts knowledge from scientific texts, patents, and clinical data	Text mining, entity recognition, semantic analysis	Identifies new drug targets and compound interactions (Withers et al., 2025).
Reinforcement Learning (RL)	Optimizes molecular design iteratively	Policy gradient algorithms, reward-based learning	Explores vast chemical spaces and refines lead compounds (Jarallah et al., 2025).
Virtual Screening	Prioritizes promising compounds for experimental testing	Docking simulations, ML-based scoring	Reduces time and cost in wet-lab screening (Cosconati et al., 2010).
Genomic & Proteomic AI Analysis	Discovers novel drug targets from biological databases	Omics data mining, network-based learning	Enables target-specific antibiotic discovery (Liu et al., 2019).
Drug Repurposing with AI	Identifies new antibacterial uses for existing drugs	Predictive modeling, molecular similarity analysis	Saves cost and accelerates development timeline (A. Singh, 2024).

AI for Drug Combination Prediction	Suggests synergistic antibiotic combinations	Deep learning, Bayesian optimization	Combats multi-drug resistance (MDR) effectively (Elalouf et al., 2025).
AI in ADMET Prediction	Optimizes pharmacokinetics and toxicity early in discovery	QSAR modeling, deep neural networks	Improves drug safety and efficacy profiles (Pathan et al., 2025).

III. AI-ASSISTED TARGET IDENTIFICATION

The growing availability of bacterial genome sequences makes it easier to identify key genes and proteins. AI tools like PATRIC and the Comprehensive Antibiotic Resistance Database (CARD) combine genomic, proteomic, and phenotypic data to pinpoint vulnerabilities in multidrug-resistant (MDR) pathogens (McArthur et al., 2013). Machine learning is used to rank potential drug targets by their essentiality, conservation, and role in virulence (Bi et al., 2025). Some essential bacterial proteins cannot be targeted by drugs. AI models help find druggable proteins by analyzing their structures, binding sites, and similarity to known targets (Kandoi et al., 2015). AlphaFold, a deep learning system, can predict protein structures with near-experimental accuracy, making it a major advancement (Jumper et al., 2021). This enables the discovery of hitherto unidentified binding sites in proteins. Rational drug design is accelerated by combining molecular docking simulations with AlphaFold prediction.

IV. FINDING LEADS AND SCREENING VIRTUALLY

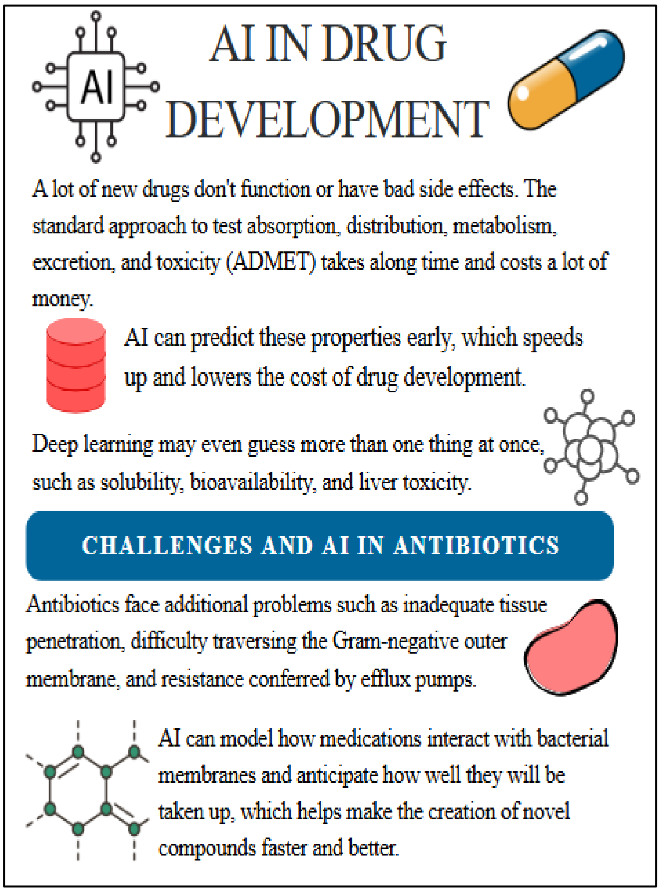
Conventional high-throughput screening (HTS) screens thousands to millions of different chemicals in vitro, a lengthy and costly process. AI makes this task much easier with the use of virtual screening with extensive chemical libraries. For example, deep neural networks developed and trained with ChEMBL datasets predict antimicrobial activity among biochemically diverse set of drugs. Support vector machines and random forests have been used to sort antibiotics and non-antibiotics (S. Singh et al., 2024). The ability to design de novo therapeutics is among the most revolutionary capabilities of artificial intelligence. Generative adversarial networks (GANs) and reinforcement learning algorithms have the ability to identify new scaffolds that are not available in chemical libraries (Gangwal & Lavecchia, 2024a). Identifying Halcion by MIT researchers in 2020 was a landmark achievement in the field since it utilized a deep learning system to screen over 100 million molecules. Halcion performed quite favourably against MDR Acinetobacter baumannii, among other infections. Another AI platform recently discovered abaucin, a narrow-spectrum antibiotic that targets A. baumannii, demonstrating that AI can create pathogen-specific drugs (Awan et al., 2024).

V. THE USE OF AI IN REGARDS TO DRUG REPURPOSING

Drug repurposing is one of the most commonly employed method for finding new indications for a drug due to their already characterized pharmacokinetics and safety. AI algorithms have the potential to identify non-antibiotic medications that possess antibacterial properties. For example, machine learning approaches discovered that mitoxantrone, a cancer drug, is an efflux pump inhibitor that also kills bacteria (Kulkarni et al., 2023). An NLP-driven analysis of academic databases has identified some psychiatric and cardiovascular medications with unexpected antibacterial properties (Wang et al., 2009). AI can figure out which combinations of medicines work best against resistance, which will help humans utilize them better. Deep learning frameworks like Deep Synergy use transcriptomic and chemo genomic data to create models of synergistic interactions. AI-guided screening, for example, found that combinations of β-lactams and β-lactamase inhibitors worked against Enterobacteriaceae that were resistant to carbapenems (Yu et al., 2022). Such methods help make current types of antibiotics last longer.

VI. AI IN DRUG OPTIMIZATION AND PHARMACOKINETICS

Many new medications fail because they either cause harmful side effects or do not work effectively in the body. Testing Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) the usual way takes a long time and costs a lot. AI can predict these properties early, making drug development quicker and cheaper. AI models using large datasets such as ADMET lab and PubChem can predict these properties early in the drug development process (Li et al., 2019). Deep learning can even predict several features at the same time, such as solubility, bioavailability, and liver toxicity (Mostafa & Chen, 2024). For antibiotics, there are extra challenges like poor tissue penetration, trouble crossing the Gram-negative outer membrane, and resistance from efflux pumps. AI can simulate how drugs interact with bacterial membranes and predict their uptake, helping to improve and speed up the design of new compounds in shown (figure 2) (Popa et al., 2022). In addition to ADMET, reinforcement learning (RL) can help optimize drug candidates by gradually modifying structures to improve efficacy and reduce toxicity. RL operates on the principle of feedback via scoring mechanisms that take into account multiple factors, that is, potency, selectivity, and molecules' "drug-likeness" (Gangwal & Lavecchia, 2024b). An example of RL is the application of riboswitch-binding molecules for antibacterial potential, which yielded modifications that offered increased stability and less side effect availability (Machtel et al., 2016). Generative chemistry platforms (e.g., Insilico Medicine's Chemistry42 and BenevolentAI's molecular design tools) have also been used to optimize antibiotic leads (Ivanenkov et al., 2023). These platforms afford researchers the ability to vary structures to enhance activity against Gram-negative bacteria, which has been a challenge for those developing antibiotics for decades (Rossiter et al., 2017).



AI IN DRUG DEVELOPMENT

A lot of new drugs don't function or have bad side effects. The standard approach to test absorption, distribution, metabolism, excretion, and toxicity (ADMET) takes along time and costs a lot of money.

AI can predict these properties early, which speeds up and lowers the cost of drug development.

Deep learning may even guess more than one thing at once, such as solubility, bioavailability, and liver toxicity.

CHALLENGES AND AI IN ANTIBIOTICS

Antibiotics face additional problems such as inadequate tissue penetration, difficulty traversing the Gram-negative outer membrane, and resistance conferred by efflux pumps.

AI can model how medications interact with bacterial membranes and anticipate how well they will be taken up, which helps make the creation of novel compounds faster and better.

Fig 2 AI in Drug Development

VII. EXPERIMENTAL METHODS WITH AI INTEGRATION

AI technologies in microfluidics make it possible to do drug screening at a high-throughput level with very little amounts of microorganisms (Qiao et al., 2025). After some drugs, machine vision and ML algorithms have measured morphological measurements, growth curves, and survival/mortality rates of bacteria (Navarro-López et al., 2024). In the laboratory, this expedited our validation of the in silico predictions, giving provide real time feedback on phenotypes. Robotic platforms utilizing supervised learning, for example the Eve robot scientist, design screening experimental protocols with AI that remove manual labor process, as well as speeding the identification of novel antimicrobials (Serrano et al., 2024a). The discipline of systems biology integrates genomes, transcriptomics, proteomics, and metabolomics to offer a comprehensive analysis of bacterial physiology under pharmacological influence.. Artificial Intelligence (AI) models such as multi-omics deep neural networks reveal relationships among gene expression, metabolic fluxes, and phenotypes of antibiotic resistance (Pinu et al., 2019). For instance, one research project successfully combined transcriptomic and metabolomic information to identify new metabolism bottlenecks in E. coli resistant strains for downstream therapeutic applications (Kim et al., 2019). Network-based machine learning (ML) algorithms can also assess cellular networks of bacterial protein-protein interaction and reveal synergistic vulnerabilities (James & Muñoz-Muñoz, n.d.).

VIII. PROBLEMS AND LIMITATIONS

AI models are only as strong as the data they are trained on. Unfortunately, antimicrobial datasets are often fragmented, inconsistent, or biased toward compounds that have more study (Pennisi et al., 2025). The primary problem with current antibiotic treatments is that antimicrobial resistance is rapidly spreading in hospitals and communities (Kushwaha et al., 2025). While rare pathogens, such as Acinetobacter baumannii may lack sufficient data to generalize the model findings, under-reporting of negative results leads to the training data being biased toward false positives (Peleg et al., 2008). Publicly available datasets (e.g. ChEMBL, PubChem Bioassay, CARDS) may be informative, but require curation and standardization to overcome these deficiencies to include in the training of AI models. Therefore, a collaborative effort to share datasets of the highest quality and rigor is needed across academia, industry and government agencies (Wilkinson et al., 2016).Deep learning models are often treated as "black boxes," so being able to ascertain what led to the model predicting activity in a certain compound is complicated. Never the less, regulatory agencies like the FDA and European Medicines Agency (EMA) require mechanistic insight to approve drug candidates, and therefore prohibit translation of models. To help mitigate this issue, explainable Ai (XAI) techniques are being developed to increase interpretability of predictions, with methods ranging from attention maps to Shapley additive explanations (SHAP) (Serrano et al., 2024b). However, just as important as accuracy and explain ability, is experimental validation. Any prediction made proving a new compound interacts with a target protein can only be valuable once demonstrated an accurate prediction and/or validated by use of wet-lab based assays in vitro, in vivo models, and eventually human clinical trial testing (Y. Zhang et al., 2024).

IX. ETHICAL, REGULATORY, AND ECONOMIC PERSPECTIVES

The quick adoption of AI in health care raises ethical challenges, including data privacy, and algorithmic discrimination and equitable access. Many AI models are trained on very big datasets from high income countries, leading to what might be a lack of relevance for low- and middle-income countries, where AMR burden is highest. Fairness and transparency in AI-driven antibiotic discovery is essential (Weiner et al., 2025). Another moral dilemma has to do with how to take care of newly found antibiotics. Even if AI accelerates discovery, improper use could accelerate resistance emergence. Responsible deployment frameworks are necessary to prevent overuse of novel antibiotics (Cesaro et al., 2025). Regulatory pathways for pharmaceuticals identified using artificial intelligence (AI) are still in their infancy. Agencies such as the FDA and EMA have insisted on strict validation of their computational predictions, which attended to slow the rate of translation (Derraz et al., 2024). Antibiotics are still considered economically unattractive due to short treatments durations and restricted use. In response, policymakers are trailing interventions, such as pull incentives (subscription models, market entry rewards) to encourage antibiotic products into development (So & Shah, 2014). AI may help reduce their costs for R&D activities, but will still need to figure out the market reform to enable sustainable innovation (L. Chen et al., 2025).

X. FUTURE PERSPECTIVES

The future of antimicrobial discovery will be in hybrid models that marry computational horsepower with humans. The choice for antimicrobial therapy is usually straight forward when the etiologic agents and their susceptibility patterns are known (A. Singh & Kumar, 2025). That means rather than AI completely autonomous, it serves as a partner that generates hypotheses, and microbiologists and chemists provide context and experimental verification, adding to our confidence (Arnold et al., 2025). This combination can shorten cycles of discovery overall and reduce attrition rates. AI has the ability to further precision medicine in infectious disease beyond drug development. AI could allow patient-specific data about microbiome, resistance profiles, and pharmacogenomics to inform personalized antibiotic prescribing (Serrano et al., 2024c). It would be the best option in regards to treatment and destruction of the microbiome and resistance profiles. Developing technologies, especially AI-based rapid diagnostics and precision therapeutic suggestions, are poised to transform the clinical landscape of infections in the next decade (McCoubrey et al., n.d.). Environmental sequencing has been used to identify dark taxa, or fungi with no cultivated examples (e.g., the Illumina, PacBio, or Nanopore) and programs like NCBI GenBank, MycoBank, and UNITE facilitate the identification of species and the updating of taxonomy (Dubey, n.d.). It is important to know commonly involved pathogens and current antibiotic sensitivity patterns to treat respiratory infections. Knowledge of current patterns of pathogens involved in respiratory infection and antibiotic sensitivity patterns may help greatly in treating infections, avoiding complications, and reducing mortality as well as in making antibiotic policy at departmental, institutional, or regional level (A. Singh & Kumar, 2025).

XI. CONCLUSION

AI has changed the process for antibiotic discovery at a moment when multidrug-resistant bacteria are causing increasing concern for global health security. AI accelerates each stage of the process from target identification to compound screening to drug optimization and ultimately drug repurposing. Landmark discoveries such as halicin and abaucin show the disruptive potential of computational models to discover entirely new classes of antibiotics. Nonetheless, challenges still exist, such as limited data availability, model interpretability and regulatory uncertainty. Addressing these obstacles requires an interdisciplinary strategy among computer scientists, microbiologists, pharmacologists and policy makers. In addition, the pathways must be economically viable so that antibiotics discovered using AI will eventually reach the market and be responsibly utilized. If these technologies can be incorporated with systems biology and precision medicine, AI can help to replenish the antibiotic pipeline; it may also improve how we think about personalized antimicrobial treatment; thus, beginning a new era of personalized medicine. By utilizing the synergies between human knowledge and machine intelligence, we could shift the balance against the worldwide AMR crisis.

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