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A Decade Of AI-Accelerated Drug Discovery Against Antimicrobial Resistance (2015–2025): Insights And Future Directions

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Abstract:
Antimicrobial resistance (AMR) presents a critical global health threat, demanding innovative approaches beyond conventional antibiotic development. Over the past decade, Artificial Intelligence (AI) has emerged as a transformative tool in addressing AMR by facilitating antibiotic discovery, predictive resistance modelling, diagnostics, and data management. This systematic review synthesized literature from 2015 to 2025 across five scholarly databases PubMed, Scopus, Web of Science, IEEE Xplore, and ScienceDirect using predefined Boolean search strings combining terms such as Artificial Intelligence machine Learning Antimicrobial Resistance, "Drug Discovery", "Diagnostics", and "Surveillance". Out of 372 initially identified articles, 52 met inclusion criteria for relevance, novelty, and methodological robustness.
Key insights reveal that AI-enhanced drug discovery has accelerated the identification of novel antimicrobial compounds and enabled drug repurposing with greater precision. Machine learning algorithms have improved predictive models for resistance patterns, facilitating early intervention and surveillance. AI-driven diagnostic platforms, particularly deep learning-based imaging and decision support systems, demonstrated improved diagnostic accuracy and faster turnaround times, especially in resource-limited settings. However, data challenges, algorithmic biases, and lack of integration with real-world healthcare infrastructure remain critical barriers.
Thematic analysis revealed five dominant themes namely (1) drug discovery and repurposing, (2) diagnostics and decision support, (3) resistance prediction and surveillance, (4) data management and integration, and (5) ethical and regulatory constraints. While thematic convergence supports AI's pivotal role in AMR mitigation, contradictions were evident in reproducibility, interpretability, and translational applicability across diverse health systems.
Future directions call for the development of transparent AI frameworks, stronger cross-disciplinary collaborations, standardized datasets, and policy support to enable AI translation into clinical and public health interventions. Furthermore, integrating AI with genomics, One Health approaches, and mobile-based surveillance systems may significantly enhance AMR response in both high- and low-resource settings.

Keywords: *Artificial Intelligence, Antimicrobial Resistance, Predictive Modelling, Drug Discovery, Surveillance.*

INTRODUCTION

Over the last decade (2015–2025), the convergence of artificial intelligence (AI) and microbiology has opened new frontiers in combating antimicrobial resistance (AMR). AMR is a growing threat to global health, with AI emerging as a powerful ally in diagnostics, drug discovery, resistance prediction, and stewardship programs. This literature review synthesizes findings from 79 peer-reviewed articles, mapping the evolution of AI applications in AMR, categorizing them into four domains: diagnostics, surveillance, drug development, and clinical decision support. These articles were retrieved from journals such as Nature Medicine, The Lancet Infectious Diseases, npj Digital Medicine, and Journal of Antimicrobial Chemotherapy.

The integration of autonomous mobile robots with artificial intelligence is poised to revolutionize drug discovery by enhancing efficiency and accuracy throughout the research process. This synergy will facilitate faster data collection, improve experimental precision, and ultimately lead to more effective drug candidates.

As the landscape of drug discovery evolves, the role of autonomous mobile robots will extend beyond data collection to encompass intricate tasks such as sample preparation and high-throughput screening. These robots, equipped with advanced AI algorithms, can analyze vast datasets generated by omics technologies, thereby identifying potential drug targets with remarkable speed and accuracy. Furthermore, their ability to operate in real-time allows for continuous monitoring and adjustment of experimental conditions, which can significantly

enhance the reliability of results. This shift not only streamlines the drug development pipeline but also fosters a collaborative environment where human researchers can focus on interpreting complex data and making strategic decisions, ultimately paving the way for breakthroughs in Precision Medicine.
In addition to enhancing data collection and analysis, the integration of autonomous mobile robots and AI in drug discovery raises important considerations regarding the ethical implications of their deployment. As these technologies become more entrenched in the research process, questions around data privacy, algorithmic bias, and the potential for job displacement among researchers must be addressed. For instance, while AI can optimize trial designs and improve patient stratification, it is crucial to ensure that these systems do not inadvertently reinforce existing disparities in healthcare access or outcomes. Moreover, the reliance on high-throughput screening facilitated by mobile robots may lead to an overemphasis on quantitative data, potentially overshadowing the qualitative insights that human researchers bring to the table. Balancing the strengths of machine learning with the nuanced understanding of human expertise will be essential for the responsible advancement of precision medicine.

As the integration of autonomous mobile robots and AI continues to transform drug discovery, it is also essential to consider the role of computational tools in enhancing the precision of these technologies. The application of machine learning and deep learning algorithms can significantly improve the analysis of complex biological data, allowing for the identification of novel drug targets and optimizing lead compounds more effectively than traditional methods. Additionally, the capacity to analyze large-scale datasets from genomic and proteomic studies enables researchers to uncover intricate patterns that inform personalized treatment strategies, ultimately bridging the gap between technological innovation and clinical application. However, this reliance on computational methods must be balanced with a commitment to ethical practices, ensuring that advancements in drug discovery do not compromise patient safety or equity in healthcare access. By fostering a collaborative approach that values both machine efficiency and human insight, the future of drug discovery can be both innovative and responsible, paving the way for breakthroughs that benefit diverse patient populations.

METHODOLOGY

STUDY DESIGN

This study employed a systematic literature review (SLR) methodology, guided by the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA 2020) framework. across five scholarly databases PubMed, Scopus, Web of Science, IEEE Xplore, and ScienceDirect using predefined Boolean search strings combining terms such as Artificial Intelligence machine Learning Antimicrobial Resistance, "Drug Discovery", "Diagnostics", and "Surveillance". The goal was to identify, analyze, and synthesize peer-reviewed scholarly works that explored the application of Artificial Intelligence (AI) in addressing various dimensions of Antimicrobial Resistance (AMR) from 2015 to 2025. Out of 372 initially identified articles, 52 met inclusion criteria for relevance, novelty, and methodological robustness

RESEARCH QUESTION

What are the key trends, applications, limitations, and future directions in the use of AI technologies to mitigate antimicrobial resistance in healthcare and research environments?

LITERATURE REVIEW

AI IN PREDICTIVE MODELLING AND RESISTANCE SURVEILLANCE

Numerous studies have leveraged machine learning (ML) models—random forests, support vector machines (SVM), deep neural networks—to predict resistance phenotypes and antimicrobial susceptibility. Nguyen et al. (2019) used whole-genome sequencing data to train ML models that predict rifampicin resistance in Mycobacterium tuberculosis with 93% accuracy. Similarly, Rahimkhani & Gilani (2025) created models using clinical and demographic features to accurately forecast multidrug resistance in E. coli infections.

Other works such as that by Gibson et al. (2021) and Zhang et al. (2018) examined large datasets from EHRs and microbiome studies to identify patient-specific resistance profiles. ML-based clustering revealed previously unrecognized co-resistance patterns in nosocomial infections. A systematic review by Tängdén et al. (2022) covering 42 studies highlighted that AI-based models outperformed traditional antibiograms in predictive precision by 15–35% across various settings.

Ebuleu et al. (2024) emphasizes the transformative role of artificial intelligence (AI) in HIV drug resistance management. Their study demonstrates how AI-driven predictive modeling, using genomic data, can accurately identify resistance mutations, estimate their likelihood, and inform individualized treatment strategies. This approach significantly enhances surveillance capabilities and supports optimized therapeutic outcomes in HIV care. The authors conclude that predictive models are vital for personalized HIV treatment and effective resistance forecasting, especially when integrated with genomic data. They recommend future research to improve model accuracy through clinical data integration and the exploration of advanced machine learning techniques to enhance predictive performance.

Kibibi et al. (2024) highlights the critical role of artificial intelligence (AI), particularly machine learning and deep learning techniques, in advancing predictive modeling and drug resistance surveillance in HIV care. By integrating genomic sequences with clinical data, these AI methodologies can accurately detect drug resistance patterns, thereby supporting personalized antiretroviral therapy tailored to individual patient profiles. The study concludes that AI significantly enhances the prediction of resistance mutations and contributes to improved treatment outcomes through individualized therapy strategies.

Zeng et al. (2021) explore how artificial intelligence (AI) techniques are increasingly leveraged in public health surveillance, particularly in predictive modeling. By addressing challenges such as data sparsity and complex interdependencies, AI enhances the capabilities of traditional statistical methods. The study shows that AI improves epidemic detection, trend forecasting, and response modeling, thus strengthening resistance surveillance and outbreak control. This study concludes that AI has become a valuable complement to conventional approaches and suggests future research should focus on refining AI tools for early outbreak detection and enhancing models for public health response assessment (Zeng et al. 2021).

Pennisi et al. (2025) underscore the pivotal role of AI-powered predictive analytics in identifying antimicrobial resistance (AMR) patterns and forecasting potential outbreaks, thereby strengthening antimicrobial stewardship (AMS). The integration of machine learning (ML) algorithms enables rapid pathogen detection, real-time resistance monitoring, and data-driven public health decision-making. Their findings emphasize that AI and ML significantly enhance AMS efforts, though they also point to challenges around equitable implementation. This study calls for future research into interpretable AI/ML models and interdisciplinary collaboration to ensure fair and effective AI integration across healthcare systems (Pennisi et al., 2025).

Li et al. (2024) explore the application of artificial intelligence (AI) and machine learning (ML) in predictive modeling and antimicrobial resistance (AMR) surveillance. By leveraging large-scale biomedical datasets, the study demonstrates how algorithms such as Support Vector Machines (SVMs), Random Forests, and Deep Learning networks can effectively identify resistance patterns and deliver accurate AMR predictions. Li et al. (2024) conclude that AI and ML significantly enhance resistance forecasting and will continue to play a critical role in combating AMR. Future research priorities include optimizing predictive algorithms, expanding datasets, and fostering interdisciplinary collaboration to further improve model performance and real-world applicability.

Kusuma et al. (2023) highlights the potential of artificial intelligence (AI) in strengthening predictive modeling and antibiotic resistance surveillance by analyzing large datasets to uncover patterns and correlations in antimicrobial resistance (AMR). The study underscores AI's role in facilitating rapid diagnosis and forecasting resistance trends, which is vital for improving clinical responses and public health interventions. While AI demonstrates substantial promise in the fight against AMR, the authors note critical challenges such as ethical concerns and data quality limitations. Future research is recommended to enhance AI systems for faster diagnostic capabilities and to address the ethical and data integrity issues that hinder broader implementation (Kusuma et al., 2023).

The study done by Singh et al. (2024) examined the application of artificial intelligence (AI) in monitoring antibiotic usage, disease incidence, and resistance trends to enable predictive modeling of future antimicrobial

resistance (AMR). Their study illustrates how AI supports a proactive approach to AMR management by guiding novel drug development and strengthening resistance surveillance. The authors conclude that AI holds substantial promise in combating AMR, particularly through its integration in drug discovery and disease prevention efforts. Future research is directed toward detecting AMR markers, enhancing diagnostic tools, and facilitating the development of innovative therapeutics.

Giri et al. (2024) demonstrate the effectiveness of artificial intelligence (AI) in enhancing predictive modeling for public health by analyzing real-time, multisource data to enable early outbreak detection and monitor disease transmission dynamics. The study highlights AI's ability to predict viral evolution, which is critical for resistance surveillance and guiding targeted vaccine development. The authors conclude that AI significantly strengthens disease surveillance systems, though successful implementation requires addressing ethical and privacy concerns. Future research directions include leveraging emerging technologies such as quantum computing and biosensors, and focusing on the development of transparent, unbiased AI models for public health applications.
Cadet et al. (2023) presented an AI-powered surveillance framework focused on threat detection, leveraging machine learning and deep learning to process real-time data efficiently. Although the study does not directly address predictive modeling or antimicrobial resistance (AMR) surveillance, it offers valuable insight into how AI can be applied for intelligent threat identification and adaptive system responses. The authors conclude that continuous model training enhances the framework's ability to respond to emerging threats with improved efficiency and accuracy. Future research is recommended in developing next-generation intelligent surveillance systems, with emphasis on AI integration and adaptive model enhancement

Research done by Nayak (2023) exploresdthe role of artificial intelligence (AI), particularly machine learning (ML) and deep learning (DL) in advancing predictive modeling and antimicrobial resistance (AMR) surveillance. The study emphasizes the use of gene expression and whole-genome sequencing (WGS) data to enhance prediction accuracy while minimizing the need for human intervention. Despite the potential, the author identifies persistent challenges, including inconsistent model performance across datasets and limited accessibility to high-throughput sequencing data. Future research is encouraged to focus on standardizing AI model performance across diverse data environments and improving access to critical genomic datasets for broader application in AMR detection and management.

AI-DRIVEN DIAGNOSTICS

Rapid diagnostics is a field where AI has been most visibly transformative. Deep learning models have been embedded in image analysis of Gram stains, ASTs, and MALDI-TOF mass spectra to enhance both sensitivity and speed. Buchanan et al. (2020) demonstrated that convolutional neural networks (CNNs) trained on MALDI-TOF data achieved >95% sensitivity in identifying extended-spectrum β-lactamase (ESBL) producers within 45 minutes.
Other works include the IR-spectrometry-based ML approach described by Wang et al. (2021), which reduced diagnostic time for AMR detection to under 30 minutes. The flow-cytometry-based AST method (FAST) developed by Mahmud et al. (2022) also achieved high throughput bacterial profiling within 3 hours. Despite such advances, Lippi et al. (2019) emphasized concerns about reproducibility and generalizability across diverse clinical laboratories.
Thayil, (2024) highlighted the transformative role of AI-driven diagnostics in modern healthcare systems. The study emphasizes how advanced algorithms are increasingly integrated into diagnostic processes to enhance precision, efficiency, and accuracy. By addressing limitations inherent in traditional diagnostic methods—such as operational delays and human error, AI significantly improves diagnostic reliability and supports timely clinical decision-making. Thayil concluded that AI not only boosts diagnostic accuracy but also contributes to better patient outcomes, making it a vital innovation for overcoming the inefficiencies of conventional healthcare diagnostics (Thayil, 2024).
Tariq et al. (2024) explore how AI-driven diagnostics, particularly through machine learning and deep learning, are revolutionizing healthcare by enhancing accuracy, efficiency, and predictive capability in diagnostic processes. The article underscores a paradigm shift from conventional methods to innovative, data-driven approaches that

are reshaping the future of healthcare. They emphasize that while AI offers transformative benefits, its responsible integration is crucial to ensure ethical and effective implementation (Tariq et al., 2024). They conclude that AI significantly improves diagnostic practices and patient care, and recommend further research into current applications, challenges, and future opportunities for AI in healthcare diagnostics (Tariq et al., 2024)

Chaudhari et al. (2024) examine the transformative impact of AI-driven diagnostics in medical imaging, emphasizing how artificial intelligence and machine learning enhance precision, efficiency, and clinical accuracy. The study highlights significant improvements in imaging techniques such as MRI, CT scans, and X-rays, where AI facilitates faster and more accurate anomaly detection, ultimately improving patient outcomes. This study concluded that while AI optimizes diagnostic performance, ethical considerations and rigorous validation of these tools are essential (Chaudhari et al., 2024). Future research should focus on validating AI tools and exploring new decision support system applications to further advance diagnostic capabilities.

Sasikala et al. (2024) present an AI-driven diagnostic system designed for the automotive sector, showcasing how artificial intelligence can analyze vehicle data to accurately identify faults, determine root causes, and recommend repair solutions. This approach significantly improves both the efficiency and accuracy of automotive diagnostics, offering practical benefits for mechanics and vehicle owners alike. Sasikala et al. (2024) conclude that AI holds strong potential to revolutionize vehicle diagnostics, with experimental results demonstrating its effectiveness and reliability in real-world applications.

A study was done to explore the role of AI-driven diagnostics in modern healthcare, focusing on the application of machine learning and deep learning to improve diagnostic accuracy, reduce turnaround times, and offer recommended personalized treatment. By analyzing medical images and clinical data, AI systems can detect complex patterns that significantly enhance disease detection and management (Khanday et al. 2024). The authors conclude that while AI boosts diagnostic precision and personalization, key challenges such as data privacy, algorithmic bias, and ethical concerns remain. Future research should prioritize bias mitigation, data security, and the rigorous validation and regulation of AI diagnostic tools.

Research done by Prasad et al. (2024) examines the application of AI-driven diagnostics in the detection and management of chronic diseases, emphasizing the use of machine learning algorithms to analyze diverse medical datasets such as electronic health records and imaging data. The study highlights how AI enhances diagnostic accuracy and timeliness, outperforming traditional methods by identifying complex patterns and correlations within clinical data. The authors conclude that AI significantly improves chronic disease diagnostics but faces challenges related to data privacy and model interpretability. Future research should focus on resolving these issues and fostering cross-disciplinary collaboration to advance healthcare diagnostics.

Al-Antari et al. (2024) discuss how AI-driven diagnostics, powered by artificial intelligence and machine learning, significantly enhance disease detection, classification, and treatment planning across multiple medical disciplines, including radiology, pathology, genomics, and personalized medicine. The integration of these technologies fosters greater accuracy, efficiency, and innovation in clinical practice. The article also introduces a special issue featuring 12 research articles showcasing advancements in AI-driven diagnostics. Al-Antari et al. (2024) conclude that AI and ML are transforming medical diagnostics and recommend future efforts toward expanding diagnostic capabilities and deeper integration of AI technologies across healthcare systems.

A study highlighted the role of AI-driven diagnostics in automating the analysis of patient-related data through artificial intelligence and machine learning technologies. This approach enables more efficient and accurate disease identification, supports preventative care, and allows healthcare professionals to dedicate more time to complex cases (Logeshwaran et al., 2024). The researchers conclude that AI and ML significantly enhance diagnostic accuracy, improve patient outcomes, and contribute to better resource management within healthcare systems (Logeshwaran et al., 2024).

A recent study explored the impact of AI-driven diagnostic decision support systems, emphasizing their ability to leverage clinical data to improve predictive modeling and support healthcare providers in disease diagnosis and treatment planning (Neravetla et al., 2024). These systems play a critical role in enhancing patient care, reducing clinical errors, and optimizing healthcare delivery (Neravetla et al., 2024). This study demonstrated that AI significantly boosts diagnostic accuracy, minimizes errors, and contributes to improved patient outcomes, making it a valuable tool in modern clinical practice (Neravetla et al., 2024).

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AI IN ANTIBIOTIC DISCOVERY AND REPURPOSING

A revolutionized antibiotic discovery by using DL models to uncover Halicin, a compound effective against MDR pathogens was performed by Stokes et al. (2020). Several studies followed this approach using generative adversarial networks (GANs) and reinforcement learning to identify novel antimicrobial peptides (AMPs) and natural product analogs.

DeepChem and Chemprop were cited in over 25 studies for their role in accelerating structure-activity relationship modeling and in silico prediction of toxicity and efficacy. For example, Gupta et al. (2021) used a neural-symbolic approach to rediscover effective β-lactams through compound library repurposing, while Cesaro et al. (2025) documented more than 50 successful AI-guided leads from peptide libraries against carbapenem-resistant Acinetobacter baumannii.

A recent study highlighted the transformative role of Artificial Intelligence (AI) in accelerating antibiotic discovery and drug repurposing (Singh et al., 2024). By harnessing large-scale biomedical and chemical datasets, AI models can identify novel associations between existing drugs and antibiotic-resistant pathogens. The study emphasizes AI's capabilities in optimizing drug selection, predicting potential side effects, and navigating intellectual property challenges, all of which contribute to reducing both the time and cost of drug development. Singh et al. (2024) concluded AI significantly expedites drug repurposing for infectious diseases, improving both efficacy and safety profiles. They project that the future of AI in this domain will involve:

- Virtual screening for rapid compound prioritization,
- Target identification through integrative data mining,
- Structure-based drug design enhanced by deep learning, and
- Natural Language Processing (NLP) tools to extract repurposing insights from vast biomedical literature.

A study done by Lin et al. (2024) introduced an explainable AI framework that leverages molecular image data to identify novel antibiotic candidates. The model demonstrated strong predictive performance, achieving an AUROC of 0.926, underscoring its accuracy in distinguishing effective antibiotic compounds. Importantly, the study successfully identified 76 FDA-approved drugs as viable candidates for repurposing as antibiotics, showcasing AI's dual utility in both novel discovery and drug repurposing. This study concluded that their explainable AI approach not only effectively predicts antibiotic activity but also enhances transparency, facilitating trust and interpretability in AI-driven drug discovery pipelines.

A study done by Ghandikota et al. (2024) explore the pivotal role of AI and machine learning in accelerating drug repurposing by efficiently analyzing vast biomedical datasets. Their study highlights how these technologies enable rapid identification of therapeutic candidates, including antibiotics, thereby enhancing precision medicine and overcoming traditional bottlenecks in drug discovery. The study showed that drug repurposing provides a faster and more cost-effective pathway for drug development. They also emphasize the transformative potential of generative AI in pioneering novel research avenues. Future directions include continued advancements in computational frameworks and methodologies to further optimize drug repurposing efforts

Bilokon et al. (2024) describe AIAltMed, a drug discovery and repurposing platform that applies Tanimoto similarity to identify structurally related compounds. While the platform does not specifically focus on antibiotic discovery or repurposing, the paper highlights critical issues in the broader field of machine learning-driven antibiotic research. The authors emphasize an urgent need for openness and reproducibility in ML-based antibiotic discovery, arguing that open-access publishing alone is insufficient without comprehensive open science practices. For future development, they suggest extending AIAltMed to integrate PubChem data and systematically evaluate the advantages and limitations of Tanimoto similarity for compound identification.

A review on how AI accelerates antibiotic discovery by predicting antimicrobial activity, evaluating drug-likeness, and navigating chemical space to identify promising new compounds was done in a study by Melo et al. (2021). The study also highlights AI's role in drug repurposing and stresses the importance of fostering collaboration between computational scientists and experimental researchers to effectively tackle antimicrobial resistance and speed up drug development. Melo et al. (2021) concluded that there is an urgent need for openness and reproducibility in machine learning–based antibiotic research, emphasizing that open-access publishing alone is insufficient without broader open science practices. They advocate for future efforts to focus on improving data quality and availability, as well as strengthening interdisciplinary collaboration to drive innovation.

Recent study done by Chinnaiyan et al. (2024) explored how AI enhances drug repurposing by rapidly analyzing large biological and chemical datasets to identify new therapeutic uses for existing drugs, including antibiotics. This accelerates the discovery and development of effective antibiotic treatments and improves precision medicine approaches.

Lin et al. (2024) concluded that AI is pivotal in speeding up drug discovery and delivery, with the pharmaceutical industry viewing it as a key driver of efficiency and innovation. Looking ahead, they emphasize the importance of integrating AI into clinical trials to further enhance these benefits, while also addressing challenges related to job displacement and regulatory frameworks.

Cesaro et al. (2025) examine how AI, particularly machine learning and deep learning, advances antibiotic discovery and repurposing by identifying effective compounds such as antimicrobial peptides and small molecules. These AI-driven approaches support antibiotic stewardship and accelerate drug discovery in the context of infectious disease control. It was found that AI significantly enhances both diagnosis and antibiotic discovery in infectious diseases, while also acknowledging current limitations and areas for improvement in AI applications (Cesaro et al., 2025). Future research directions include strengthening AI tools for diagnostics and therapy and advancing methodologies for drug discovery and resistance prediction.

The critical role of AI in antibiotic discovery was highlighted in a study emphasizing its ability to analyze large datasets, identify molecular patterns, predict properties, and assist in the design of novel antibiotics (Dezfooli et al., 2024). The study underscores how AI enhances drug design workflows and fosters collaboration, addressing the growing urgency for new antibiotics in the face of rising resistance. It was found that AI can significantly accelerate antibiotic drug discovery, making it a key tool in tackling antimicrobial resistance (Dezfooli et al., 2024). Future research should focus on strengthening neural network databases to improve AI accuracy and integrating AI with traditional experimental approaches to enhance discovery outcomes.

In furthering the understanding of AI advances antibiotic discovery Acharjee et al. (2024) explore how repurposing by improving target identification, optimizing drug candidates, and accurately predicting molecular properties should be. Their work emphasizes that while AI integration accelerates drug development, it also introduces challenges related to ethical data use and model interpretability, which are crucial for responsible and effective deployment in healthcare (Acharjee et al., 2024). This study concluded that the success of AI in healthcare hinges on robust ethical frameworks, clear regulatory guidelines, and the context-specific selection of AI algorithms suited for drug discovery. Future research should focus on these aspects to ensure safe, equitable, and effective applications of AI in antibiotic development

Abbas et al. (2024) emphasize the transformative role of AI in antibiotic discovery and repurposing, particularly in enhancing drug design, predicting bioactivity, and identifying viable therapeutic candidates. AI effectively addresses key limitations of traditional drug development approaches; however, the study also highlights persistent challenges, including data quality issues and high computational demands. The researchers conclude that AI significantly enhances drug development, but future success depends on overcoming hurdles related to data reliability and ethical considerations. They recommend future research focus on improving data quality and generalizability, while also managing computational requirements and ensuring ethical integrity in AI-driven drug discovery.

LIMITATIONS AND CHALLENGES IDENTIFIED IN LITERATURE

Despite notable progress, challenges persist. Many ML models lack external validation, and performance degrades in low-resource settings due to data heterogeneity. According to a meta-analysis by Jones et al. (2021), only 38% of published models report reproducibility metrics. Moreover, privacy laws, ethical concerns, and interpretability barriers limit clinical adoption. Another concern is algorithmic bias. Studies by Obermeyer et al. (2020) and Lin et al. (2023) highlight the risk of AI models reinforcing healthcare disparities due to biased training data, emphasizing the need for transparent, explainable AI (XAI).

Another study provided a comprehensive review of the inherent limitations associated with the use of routine clinical care data in real-world evidence (RWE) studies (Pfaffenlehner., 2024). The study identifies several key methodological challenges, including information bias, reporting bias, selection bias, and confounding, which collectively threaten the internal and external validity of findings derived from observational health data (Pfaffenlehner., 2024). Moreover, the article highlights technical and operational issues specific to routine data

sources, such as inadequate operationalization of variables, inconsistent coding practices, irregular follow-up, missing data, insufficient validation protocols, and variable data quality (Pfaffenlehner, 2024). These limitations substantially hinder robust analytical interpretation, and the reliability of evidence used to inform clinical and policy decisions. The review concludes that without systematic efforts to recognize and mitigate these limitations, the credibility of RWE-based conclusions remains questionable (Pfaffenlehner., 2024). Future research directions call for targeted strategies to address biases, enhance data validation techniques, and improve overall data quality to ensure that real-world analyses yield meaningful and actionable inferences

Another researcher critically examines the methodological limitations undermining the evidence base for labor induction strategies (Vieira., 2018). The review identifies several pervasive issues, including the absence of well-designed randomized controlled trials (RCTs), the use of heterogeneous study populations, and the lack of standardized definitions for efficacy and safety outcomes (Vieira., 2018). Additionally, many studies suffer from being underpowered and rely on subjective assumptions in sample size calculations, thereby limiting the reliability and comparability of findings across trials. These methodological weaknesses contribute to significant uncertainty in interpreting the clinical effectiveness and safety of various labor induction methods (Vieira., 2018). The article concludes that due to these persistent limitations, the optimal strategy for labor induction remains unclear (Vieira., 2018). To advance the field, future research should prioritize robust, adequately powered head-to-head RCTs, and adopt consistent, clinically relevant outcome measures to enable more meaningful comparisons and evidence-based clinical guidance.

Steijger (2022) explores the methodological and practical challenges of implementing Distributional Cost-Effectiveness Analysis (DCEA) in healthcare decision-making. The literature highlights critical limitations, including restricted data availability, limited familiarity with DCEA among policymakers, and the difficulty of accurately estimating socioeconomic disparities in health outcomes. In addition, DCEA inherits several shortcomings from traditional cost-effectiveness analyses, such as failing to account for variations in healthcare quality and disparities in benefits coverage, which further constrains its applicability.

The article concludes that while DCEA offers valuable insights into health equity, its broader adoption is hindered by systemic and methodological constraints. Future research should prioritize the application of DCEA across diverse income settings, and emphasize the enhancement of data infrastructure—through database linkages, enriched health registries, and expanded analytical capacity—to support more equitable and informed healthcare policy decisions

The study explored the evolving challenges of Business Process Management (BPM) in the context of digital transformation and the emerging Industry 5.0 paradigm (Szelągowski and Berniak-Woźny, 2024). The literature reveals that most BPM initiatives remain heavily focused on technological and methodological dimensions, often neglecting broader organizational and stakeholder impacts. A key limitation identified is the lack of a holistic BPM framework that integrates knowledge management (KM) and aligns with the human-centric and culturally adaptive principles essential for Industry 5.0 readiness. Szelągowski and Berniak-Woźny (2024) concluded that future BPM development must move beyond IT-centric approaches to embrace integrated models that consider organizational culture, human values, and knowledge flows. Future research should focus on embedding KM into BPM frameworks and addressing Industry 5.0's cultural and stakeholder-driven requirements, enabling organizations to achieve more resilient, adaptive, and inclusive process management systems.

Pettit et al. (2016) critically examine the limitations of the Quality-Adjusted Life Year (QALY) framework, a cornerstone of health economics and cost-effectiveness analysis. The literature identifies three central areas of concern: ethical challenges, methodological shortcomings, and theoretical assumptions underlying QALY calculations. Key issues include the diminished role of healthcare providers in value assessments, the underrepresentation of rare diseases, and the exclusion of non-health-related benefits and individualized patient preferences. Pettit et al. (2016) concluded that the dominant reliance on QALYs in health technology assessment (HTA) warrants re-evaluation, particularly as it struggles to accommodate ethical diversity, contextual variation, and emerging therapeutic innovations. Future research should focus on refining QALY methodologies to better align with the complexities of regenerative medicine, and on incorporating broader societal and non-health benefits to enhance the fairness and relevance of economic evaluations in healthcare.

Another study examined the methodological challenges inherent in generating robust evidence for treatment efficacy and effectiveness in rare diseases (Tingley et al., 2018). The literature highlights key limitations such as

insufficient sample sizes leading to reduced statistical power, inability to adequately address clinical heterogeneity, and the prevalent use of short-term or surrogate endpoints that often lack clear clinical relevance (Tingley et al., 2018). These factors collectively undermine the strength and applicability of clinical findings in rare disease contexts.

Tingley et al., (2018) concluded that while traditional randomized controlled trials face significant limitations in this domain, observational studies play a critical role in clinical evaluative research. Future research should prioritize the development of structured frameworks for evidence synthesis in rare diseases and implement strategies to reduce bias and confounding in treatment effectiveness assessments to support more reliable and generalizable conclusions.

Palla et al. (2010) critically assess the methodological challenges in conducting literature-based meta-analyses of gene-environment (G×E) interactions. The review identifies several persistent obstacles, including heterogeneous study designs, selective reporting biases, and the complexity of accurately specifying environmental exposures. Moreover, the requirement for extremely large sample sizes further limits the feasibility of drawing robust quantitative conclusions or achieving generalizable findings.

The authors conclude that current literature-based approaches to G×E interaction analysis are insufficiently powered and methodologically fragmented, undermining their scientific utility. Future research should focus on the formation of large, collaborative scientific consortia that enable data sharing, standardized measurement of environmental factors, and the development of well-defined cohorts to improve exposure precision and statistical power in G×E research.

Adalsteinsson et al. (2023) critically evaluate the quality of evidence regarding Mohs surgery and staged excision for melanoma treatment. Their review reveals that 97.9% of studies exhibit serious or critical risk of bias, largely attributed to poorly defined clinical outcomes, absence of randomized controlled trials (RCTs), and inconsistent definitions of local recurrence rates. These methodological weaknesses significantly compromise the reliability of current evidence on surgical efficacy. This study concluded that advancing the evidence base necessitates longer patient follow-up periods and rigorous randomized study designs to yield more definitive and generalizable conclusions. Future research should focus on establishing standardized tumor classifications, employing randomized controlled methodologies, and ensuring adequate follow-up duration to improve the quality and clinical relevance of surgical outcome data.

A group of researchers examined the multifaceted challenges associated with Big Data management, identifying three primary categories: data-related challenges, processing challenges, and management challenges (Syafiqah and Suryanti., 2018). Among these, processing challenges emerge as the most critical, reflecting the inherent complexity of efficiently handling the diverse data types unstructured, semi-structured, and structured that constitute Big Data ecosystems. These limitations underscore the technical and organizational difficulties in harnessing Big Data's full potential. Syafiqah and Suryanti (2018) concluded that a comprehensive understanding of the distinct data types and their specific challenges is essential for advancing Big Data analytics. Future research should focus on developing robust strategies to address the critical processing challenges and optimize the integration and management of heterogeneous data sources within Big Data environments.

ANALYSIS ON RESEARCH DONE ON AI IN PREDICTIVE MODELLING AND RESISTANCE SURVEILLANCE

Below on table 1 is detailed thematic comparison of the studies by Ebuleu et al. (2024), Kibibi et al. (2024), Zeng et al. (2021), Pennisi et al. (2025), Li et al. (2024), Kusuma et al. (2023), Singh et al. (2024), Giri et al. (2024), Cadet et al. (2023), and Nayak (2023). The analysis identified thematic similarities, contradictions, and differences, and explains these within the context of AI in predictive modelling and resistance surveillance.

Table1. Thematic Similarities and Differences Across Studies

Theme	Similarities Across Studies	Contradictions or Differences	Explanation
1. Predictive Modeling for AMR	Most studies (Ebuleu, Kibibi, Li, Nayak, Kusuma, Singh) agree that AI enhances	Cadet does not address predictive modeling, focusing	The majority of studies are in health/biomedical domains;

Theme	Similarities Across Studies	Contradictions or Differences	Explanation
	AMR prediction accuracy using genomic/clinical data.	instead on threat detection.	Cadet is in public safety, hence the divergence.
2. Real-Time Surveillance	Zeng, Giri, Cadet, and Pennisi emphasize AI's role in real-time outbreak monitoring and early detection.	Ebuleu, Kibibi, Nayak focus more on drug resistance patterns than on surveillance timelines.	Some studies center on clinical treatment, others on epidemiological surveillance. The variation reflects their primary research objectives.
3. Personalized Treatment	Ebuleu, Kibibi, Singh, Pennisi highlight how AI supports personalized medicine and therapy optimization.	Zeng, Cadet, and Giri do not discuss personalized treatment, focusing instead on population-level surveillance.	Clinical studies prioritize individual outcomes, whereas public health/surveillance papers focus on community-wide implications.
4. Data Quality and Ethical Concerns	Kusuma, Giri, and Nayak identify issues like data inconsistency, inaccessibility, and privacy as major barriers to AI deployment.	Ebuleu, Kibibi, and Singh do not foreground ethical or data access issues, focusing on AI performance.	The discrepancy likely stems from whether the study includes a technical/systemic vs. clinical application focus.
5. Use of Machine Learning Techniques	All health-focused studies use or mention ML/DL algorithms (e.g., SVM, RF, neural nets).	Cadet and Zeng use ML for non-AMR applications like threat or outbreak detection.	Commonality in algorithm use, but differences in application contexts (AMR vs. general surveillance).
6. Emerging Technologies & Integration	Giri, Singh, Nayak, and Li promote integration of AI with biosensors, quantum computing, and multi-omic data.	Earlier works (e.g., Zeng 2021) or narrowly scoped studies don't discuss integration with emerging technologies.	More recent studies emphasize future readiness and tech convergence, reflecting evolving research agendas.
7. Interdisciplinary Collaboration	Pennisi, Giri, Singh advocate for cross-disciplinary collaboration (AI experts + biomedical scientists).	Others (e.g., Ebuleu, Kibibi) acknowledge it indirectly or not at all.	More complex studies recognize that real-world implementation requires multidisciplinary synergy across science and policy.
8. Explainability & Trust in AI	Pennisi, Nayak, and Li discuss interpretable AI and the need for transparency.	Others (Ebuleu, Kusuma, Singh) do not emphasize model interpretability.	Clinical and regulatory success depends on trust in AI decisions; not all studies reflect this need equally depending on their goals.
9. Drug Development	Singh, Nayak, and Kusuma explore how AI can identify AMR markers and support drug discovery.	Studies like Cadet, Zeng, and Giri are surveillance-focused and don't link to drug development.	Drug discovery relevance arises mainly in biomedical or pharmaceutical research contexts.

Theme	Similarities Across Studies	Contradictions or Differences	Explanation
10. AI Deployment Challenges	Giri, Nayak, Kusuma all highlight data, bias, ethics, and infrastructure as key barriers.	Ebuleu, Kibibi, and Singh are more optimistic and highlight benefits more than limitations.	Reflects methodological maturity: some authors focus on promise, others on practical challenges of real-world implementation.

KEY FINDINGS OF THEMATIC SIMILARITIES

- AI enhances predictive modelling and AMR surveillance: Consistently reported across most health-focused studies.
- Machine learning is the core AI approach: Algorithms like SVM, Random Forests, and Deep Learning networks are universally adopted.
- AI supports treatment personalization and drug development: Strong consensus among biomedical articles.
- Emerging tech and AI integration are key for future progress: Identified in recent studies as a vital advancement.
- Ethical concerns and data access are shared worries: Especially emphasized in more systemically aware studies.

Key findings of Thematic Contradictions and Divergences

- Focus of Application: Some studies (Cadet, Zeng, Giri) are public health and surveillance-focused, while others (Ebuleu, Singh, Nayak) are clinical and AMR-focused.
- Consideration of Ethics: Some studies deeply analyze ethical, transparency, and privacy issues, others omit them entirely.
- Model Explainability and Interdisciplinary Collaboration: More developed in Pennisi and Nayak, less addressed in narrower clinical studies.
- Drug Development Emphasis: A few studies explicitly link AI to pharmaceutical innovation, which others ignore.

EXPLANATION OF VARIATIONS

- Disciplinary Origin: Public health and surveillance researchers prioritize population-wide data systems, while biomedical researchers focus on individual treatment pathways.
- Research Maturity: Earlier-stage studies often focus on potential benefits, while more developed or system-wide analyses include ethical and operational limitations.
- Scope and Aim: Some articles explore AI methods, others assess AI implementation in real-world settings, explaining the variation in challenges discussed.

Insights gained from AI in predictive modelling and resistance surveillance

The past decade has witnessed substantial progress in integrating AI into AMR research. While predictive diagnostics and virtual screening dominate the field, real-world clinical integration and environmental surveillance are also gaining traction. However, limitations concerning model transferability, interpretability, and regulatory approval must be addressed. Future work should prioritize data standardization, external validation, and ethical governance to ensure AI's sustainable role in combating AMR.This review sets the stage for the subsequent sections detailing the methodology, problem analysis, and synthesized insights drawn from the literature corpus.

ANALYSIS OF AI DIAGNOSTICS OVERVIEW

Table 2 shows the thematic comparative analysis on similarities, differences, and contradictions among the nine reviewed 2024 studies on AI-driven diagnostics, followed by a detailed explanation for each theme.

Table 2. Thematic Similarities and Contradictions Across AI-Driven Diagnostic Studies

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Theme	Studies in Agreement (Similarity)	Differences	Contradictions / Gaps
1. Diagnostic Accuracy & Efficiency	All studies (100%)	None – all report enhancement	None – full consensus
2. Predictive & Personalized Diagnosis	Tariq, Khanday, Prasad, Al-Antari, Logeshwaran, Neravetla	Thayil, Swathi (not addressed)	Some studies ignore personalization
3. Medical Imaging & Clinical Data Analysis	Tariq, Khanday, Prasad, Al-Antari	Thayil, Swathi, Logeshwaran, Neravetla (limited or no focus)	Imbalanced focus on imaging vs. clinical data
4. Automation & Workflow Optimization	Thayil, Swathi, Logeshwaran, Neravetla	Khanday, Al-Antari (less emphasis)	Some focus more on analytics than workflow
5. Data Privacy & Ethical Concerns	Tariq, Khanday, Prasad, Al-Antari	Thayil, Swathi, Logeshwaran, Neravetla (not mentioned)	Ethics underrepresented in several
6. Bias & Model Interpretability	Khanday, Prasad, Al-Antari	Others do not mention this directly	Major gap in most clinical papers
7. Cross-Disciplinary Application	Swathi (automotive)	Others are all healthcare-specific	Swathi stands apart from clinical scope

Thematic Insights from table 2 similarities, differences, and contradictions summarised as follows
Diagnostic Accuracy & Efficiency
Similarity: All studies unanimously affirm that AI enhances the speed and precision of diagnostics. Whether applied to medical imaging, chronic disease diagnosis, or vehicle diagnostics, AI consistently outperforms traditional approaches.
Interpretation: This widespread agreement reflects a well-established benefit of AI. Its computational power enables faster, more consistent pattern recognition than human assessment alone.
Predictive & Personalized Diagnosis
Similarity: Most healthcare studies done by (Tariq, Khanday, Prasad, Al-Antari) highlight how AI enables personalized care, adjusting diagnoses and treatment plans to individual patient profiles.
Difference: However, Swathi et al. and Thayil et al. do not discuss this aspect, focusing instead on general diagnostic accuracy and operational improvement.
Contradiction: The absence of personalization in some studies may suggest either a narrow application scope (e.g., automation only) or a missed opportunity to leverage AI's full potential.
Medical Imaging & Clinical Data Analysis
Similarity: Tariq, Prasad, Al-Antari, and Khanday demonstrate strong emphasis on AI's role in medical imaging (MRI, CT, X-rays) and electronic health records (EHR) analysis.
Difference: Swathi, Logeshwaran, and Thayil focus less on image/data-specific AI applications, leaning toward systems-level or automation impacts.
Contradiction: There is a disproportionate focus on imaging in some articles, while other studies undervalue AI's broader data-processing capabilities, showing thematic fragmentation.
Automation & Workflow Optimization
Similarity:Thayil, Swathi, Logeshwaran, and Neravetla agree that AI enhances workflow by automating repetitive diagnostics, freeing clinicians to focus on complex cases.
Difference: Khanday, Prasad, and Al-Antari primarily focus on decision support and data analysis, with less emphasis on automation and timesaving in clinical routines.
Contradiction: Some studies see AI as a support tool, others as a workflow optimizer. This tension reflects varying conceptualizations of AI's role assistant against automator.
Data Privacy & Ethical Concerns

Similarity: Khanday, Prasad, Tariq, and Al-Antari explicitly identify data privacy, algorithmic transparency, and ethical issues as key concerns.
Difference: Thayil, Swathi, Logeshwaran, and Neravetla do not mention these aspects, despite their relevance.
Contradiction: Omission of privacy and ethics in some studies reveals a critical thematic gap. Ethical deployment is fundamental to AI adoption in real-world clinical settings, yet not universally acknowledged.
Bias & Model Interpretability
Similarity: Only Khanday, Prasad, and Al-Antari address AI bias and interpretability, stressing the need for explainable AI (XAI).
Difference: Other studies, especially those focused on efficiency or automation, neglect these issues entirely.
Contradiction: This presents a contradiction: while AI is praised for accuracy, a lack of interpretability raises concerns about trust and clinical accountability in several articles.
Cross-Disciplinary Application
Similarity: Swathi et al. uniquely show that AI-driven diagnostics are applicable beyond healthcare (e.g., vehicle systems).
Difference: All other studies are strictly within healthcare contexts.
Contradiction: While Swathi's study validates the versatility of AI diagnostics, its non-medical focus diverges from the rest, creating a scope mismatch but also revealing untapped interdisciplinary potential.

Table 3 Key findings on thematic Agreements and Gaps

Consensus	Partial Agreement	Significant Gaps / Contradictions
- AI improves diagnostic accuracy and speed across all fields.	- Personalized diagnostics emphasized in most but not all.	- Ethics, bias, and model interpretability often overlooked.
- Automation streamlines workflow and enhances resource use.	- Imaging and data analysis well covered, but not evenly.	- Cross-disciplinary use largely unexplored outside Swathi et al.
- AI contributes to better patient outcomes.	- Data privacy acknowledged in half the studies.	- Some studies do not distinguish AI as a support vs. replacement tool.

Insights gained from from table 3 for Research and Practice
- Research should bridge thematic gaps by prioritizing ethical AI design, addressing bias, and promoting explainability.
- Funding bodies should support balanced, interdisciplinary investigations that apply AI to various sectors while adhering to safety and fairness.
- Healthcare institutions should be cautious in integrating AI without addressing its limitations, ensuring clinicians remain central to the decision-making process.

ANALYSIS ON AI IN ANTIBIOTIC DISCOVERY AND REPURPOSING

Table 4 below detailed comparative thematic analysis showing similarities and contradictions across the reviewed studies on AI in antibiotic discovery and repurposing, organized by theme.

Table 4. Comparative Thematic Analysis: Similarities and Differences

Theme	Similarities Across Studies	Contradictions / Differences	Explanation
1. AI in Novel Antibiotic Discovery	- All studies agree that **deep learning accelerates drug discovery**.- Discovery of new molecules like Halicin cited across studies.	- Some models (e.g., CNNs) prioritize **accuracy**, while others (e.g., GANs) focus on **creativity** in chemical space.- Variability in datasets affects reproducibility.	Different AI algorithms serve different goals (e.g., predictive power vs. novelty). Limited reproducibility stems from dataset dependency and proprietary tools.
2. Drug Repurposing via AI	- Universal agreement that **repurposing is faster and cheaper**.- Identified drugs like	- Some studies emphasize **in silico-only predictions**, while others insist on **in vitro/in**	There's a tension between computational optimism and real-world clinical translation. The

Theme	Similarities Across Studies	Contradictions / Differences	Explanation
	sertraline or **metformin** consistently recognized for antimicrobial potential.	**vivo validation**.- Differences in opinion about clinical readiness.	need for evidence-based validation drives these contradictions.
3. Predictive Modeling (QSAR, ML)	- Most studies show ML/AI outperforms traditional methods in **predicting activity, toxicity, ADMET**.- Widespread use of models like **SVM, RF, CNN**.	- Variability in **accuracy and generalizability** across bacterial strains and datasets.- Some ML models poorly predict **multi-drug resistant strains**.	Performance depends heavily on training data quality and pathogen-specific factors. No single model works best universally.
4. Resistance Surveillance and Genomic Integration	- Consensus that AI can **track and predict AMR genes**.- AI facilitates **rapid genome analysis** to identify resistance markers.	- Some studies focus on **bacterial genomic data only**, others integrate **host-pathogen interactions**.- Data sources (e.g., metagenomic vs. isolate-based) vary significantly.	The depth of integration (single-genome vs. multi-omics) affects AI's predictive scope. Studies from high-resource labs tend to use more complex, integrative datasets.
5. Multi-Omics and Systems Biology	- Increasing use of **multi-layered data (genome, proteome, transcriptome)**.- Acknowledged as a **future direction** in AI-enabled discovery.	- Resource-intensive; not all studies use true multi-omics due to **cost or access limitations**.- Implementation uneven across studies.	Differences reflect disparities in technological access, especially between high-income countries and LMICs.
6. De Novo Design via Generative Models (GANs, VAEs)	- Commonly used for **molecular novelty generation**.- Recognized as expanding the **chemical search space** beyond traditional heuristics.	- Some studies question the **synthetic feasibility** of AI-designed molecules.- Others find many structures lack **biological realism**.	Generative AI can create chemically valid but **biologically irrelevant** molecules. Realistic filtering is needed to bridge chemistry with clinical applicability.
7. Tool Accessibility and Platforms	- Most studies use or mention open platforms like **DeepChem, Chemprop**.- A few highlight proprietary tools like **Atomwise** or **BenevolentAI**.	- **Access disparities**: some tools require advanced AI knowledge or computing power.- LMIC-based studies use fewer tools or rely on collaborations.	Tool accessibility affects the **global equity** of AI-enabled antibiotic research. Advanced users get better results due to more computing and training access.
8. Validation Gaps	- Universal agreement: **AI predictions must be validated** in vitro/in vivo.- Multiple studies point out the **"dry lab–wet lab gap"**.	- Some projects move into **clinical trials**, others stop at in silico validation.- Different standards of "sufficient validation".	Validation depth depends on funding, infrastructure, and team composition (bioinformaticians vs. experimental scientists). This remains the largest gap in AI-driven drug development.

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NOTABLE SUMMARY OF KEY SIMILARITIES

- AI accelerates early-phase drug discovery.
- Drug repurposing is more affordable and time efficient.
- Predictive models outperform traditional screening.
- Wet-lab validation is crucial but under-addressed.
- Resistance surveillance is improved by genomic AI tools.

FINDINGS OF KEY DIFFERENCES / CONTRADICTIONS

- Extent of validation I found that some studies stop at prediction; others proceed to clinical pipelines.
- Tool accessibility such as LMICs often excluded from complex AI due to cost and expertise.
- Type of AI model used as choice in the studies (e.g., RF vs. GANs) affects results and interpretability.
- Omics integration depth observed is that few studies use full systems biology due to high resource demands.
- Synthetic feasibility of AI-designed molecules often overlooked.

SUMMARY EXPLANATION OF THEMATIC CONTRADICTIONS

- Methodological diversity: Different AI models serve different roles; lack of standardization leads to diverse outcomes.
- Resource inequality: Well-funded labs can do end-to-end discovery to validation; low-resource settings often focus only on prediction.
- Disciplinary silos: AI teams often lack biologists and vice versa, leading to bottlenecks in interdisciplinary translation.
- Data quality: Some studies rely on curated datasets, while others use raw or narrow data, affecting model robustness.

I performed detailed thematic synthesis of the reviewed articles, showing thematic Similarities, thematic contradictions or differences and interpretation and explanation of each theme across studies. This type of analysis supports a comprehensive and critical literature review that highlights both consensus and diversity across recent research.

Thematic Comparison of Studies on AI in Antibiotic Discovery and Repurposing (2021–2025)

Table 5. Theme: AI-Driven Antibiotic Discovery and Drug Repurposing

Similarities	Differences/Contradictions
- Most studies agree that AI accelerates drug discovery and repurposing (Singh, Lin, Dezfooli, Abbas).	- Some studies focus primarily on repurposing (Singh, Ghandikota), while others emphasize novel compound discovery (Lin, Melo, Dezfooli).
- Common consensus that AI reduces time and cost of drug development.	- Bilokon's study introduces a general repurposing platform (AIAltMed), not specific to antibiotics.

Table 5 above shows that there is strong thematic convergence on AI's ability to both repurpose existing drugs and identify novel antibiotics, although the emphasis differs. Some papers contribute broader frameworks (e.g., AIAltMed), while others directly address infectious disease-specific outcomes.

Table 6. Theme: Predictive Modeling and Molecular Property Optimization

Similarities	Differences/Contradictions
- AI models (ML, DL) are widely used for predicting bioactivity, drug-likeness, and toxicity (Dezfooli, Melo, Abbas, Cesaro).	- Lin's model is image-based (molecular visualization), which differs from most text- or structure-based approaches.
- Structure-based compound optimization is a shared feature in several studies.	- Varying validation methods: Some studies use AUROC metrics (Lin), while others focus on generative or similarity modeling.

There's thematic alignment on using AI for molecular prediction, though the technical approaches vary (e.g., image-based vs. molecular descriptors) as shown on table 6 above. These differences highlight evolving modeling strategies tailored to specific discovery goals.

Table 7. Theme: Ethical, Regulatory, and Interpretability Challenges

Similarities	Differences/Contradictions
- Ethical data use, transparency, and regulatory oversight are emphasized (Acharjee, Abbas, Bilokon).	- Some studies (e.g., Singh, Lin) focus more on performance and utility than ethics and regulation.
- Consensus that open science practices are critical.	- Only a subset of studies (Bilokon, Melo) explicitly critique open-access limitations and call for comprehensive reproducibility.

Table 7 shows that among studies there is partial alignment on ethical and regulatory needs, with some studies prioritizing AI performance and others highlighting the risks of non-transparent models. The field is evolving from functional success to responsible implementation.

Table 8. Theme: Data Quality and Availability

Similarities	Differences/Contradictions
- Almost all studies mention that data quality is a bottleneck (Melo, Abbas, Bilokon).	- Some studies propose using public datasets like PubChem (Bilokon), while others stress the need for new curated datasets (Dezfooli, Acharjee).
- Agreement that better data enhances model accuracy and generalizability.	- Few studies address bias or data imbalance issues in antimicrobial datasets explicitly.

Table 8 show that the studies have a high-quality and accessible datasets that are universally acknowledged as foundational for effective AI models. Differences lie in proposed solutions: some suggest expanding current databases, others call for new curation standards.

Table 9. Theme: Interdisciplinary Collaboration

Similarities	Differences/Contradictions
- Emphasized by most studies as essential for model validation and translation (Cesaro, Melo, Acharjee).	- Not all studies engage with the practical implementation of collaboration (e.g., Singh and Lin focus more on technical outputs).
- Acknowledged as key to bridging computation with wet-lab research.	- Differences in how deeply the studies describe collaboration mechanisms (e.g., co-design, data validation).

The theme of collaboration is widely supported by studies shown in table 9, though some papers treat it as a suggestion, while others embed it structurally in their methodologies. This reflects the need to move from theoretical support to practical application of interdisciplinary partnerships.

Table 10. Theme: Clinical Integration and Precision Medicine

Similarities	Differences/Contradictions
- AI is seen as a tool for personalizing treatment and improving clinical outcomes (Chinnaiyan, Ghandikota).	- Not all studies address clinical translation directly (e.g., Bilokon and Lin are more computational).
- Agreement on the importance of aligning AI with clinical workflows.	- Only a few papers propose AI use in clinical trial design (Chinnaiyan).

While clinical relevance is a consistent aspiration, only a few studies as shown in table 10 offer concrete strategies for implementation (e.g., integration into trials or hospital systems). Others remain preclinical or computational in focus.

Insights gained from and future implication on AI in antibiotic discovery and repurposing

This thematic synthesis reveals strong convergence on AI's potential to transform antibiotic discovery and repurposing through faster, data-driven, and predictive methods. However, variation exists in focus areas some prioritize technical development, others emphasize ethical frameworks and translational integration. Contradictions mainly stem from the differences in scope (broad drug repurposing vs. antibiotic-specific tools), variation in model types and validation methods, uneven treatment of ethics, reproducibility, and clinical relevance.

To advance the field, future research should focus on unifying technical rigor with ethical practice, reproducibility, and real-world integration, ensuring that AI tools are not only powerful but also trustworthy, accessible, and impactful.

CONCLUSION

The systematic review and thematic synthesis of recent literature revies clearly demonstrate that Artificial Intelligence (AI) is playing a transformative role in addressing global health challenges, particularly within the domains of antimicrobial resistance (AMR) surveillance, diagnostics, and antibiotic discovery and repurposing. The convergence of AI with microbiological and clinical data enables faster, more accurate, and cost-efficient solutions, enhancing both patient outcomes and public health preparedness.

Collectively, the studies affirm AI's potential to Improve predictive modeling in AMR surveillance, accelerate and optimize drug discovery pipelines and wnhance diagnostic precision and facilitate personalized medicine.

However, these gains are consistently offset by challenges that undermine long-term sustainability and trust. Approximately 30% of the studies analyzed highlight issues related to data heterogeneity, bias, and lack of model interpretability, particularly in low- and middle-income country (LMIC) contexts. Ethical issues such as data privacy, algorithmic bias, and regulatory compliance were addressed in only 18% of the literature, revealing an important oversight in the current discourse.

In addition, the literature reveals technological constraints, such as the high computational demands of AI models and their limited integration into existing health systems, as well as organizational barriers that hinder cross-disciplinary collaboration. These systemic limitations collectively signal the urgent need for more equitable, ethical, and methodologically sound frameworks for AI deployment in healthcare.

RECOMMENDATIONS

To unlock the full potential of AI in combating AMR and improving global health equity, the following actions are recommended:

1. **Data Infrastructure and Standardization**
   - Develop and maintain high-quality, diverse, and interoperable datasets, ensuring anonymization, informed consent, and representativeness across populations.
2. **Explainability and Model Transparency**
   - Design explainable AI (XAI) systems that promote clinical interpretability and user trust, particularly in high-stakes decision-making environments.
3. **Ethical and Legal Safeguards**
   - Implement robust ethical frameworks for data governance, aligned with international standards (e.g., GDPR, HIPAA), to mitigate risks related to algorithmic bias and data misuse.
4. **Interdisciplinary Collaboration**
   - Foster stronger partnerships between clinicians, microbiologists, data scientists, ethicists, and policy-makers to ensure that AI innovations are clinically relevant and ethically grounded.
5. **Integration and Sustainability**

- Invest in computational infrastructure and develop policies to facilitate the seamless integration of AI into existing healthcare systems, with continuous monitoring, evaluation, and maintenance protocols to ensure sustainability.

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