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Review Article

Application of Artificial Intelligence and Molecular Docking in Early Detection of Antimicrobial Resistance: A Systematic Review

***Musa, F. M.[1], Nuhu, A. M.[2], and Abdullahi, A. M.[3]**

[1]Department of Microbiology, Faculty of Life Sciences, Kaduna State University, Kaduna, Nigeria
[2]Department of Pure and Applied Chemistry, Faculty of Physical Sciences, Kaduna State University, Kaduna, Nigeria
[3]Department of Applied Chemistry, Kaduna Polytechnic, Kaduna, Nigeria
****Corresponding Author's email*: fatima.mohammed@kasu.edu.ng; Phone: +2347066292280**

ABSTRACT
Antimicrobial resistance (AMR) poses a growing global health threat, resulting in increased morbidity, mortality, and increased cost of health care. Traditional diagnostic methods for AMR, relying on phenotypic culture and susceptibility testing, are time-consuming and often fail to provide rapid insights necessary for effective treatment decisions. Computational approaches, particularly artificial intelligence (AI) and molecular docking, offer promising alternatives for early detection of resistance by analyzing genomic, proteomic, a paradigm shift by enabling rapid target identification, ligand screening, drug optimization and structural data. This systematic review examines recent advances in AI algorithms and molecular docking techniques applied to AMR detection, evaluates their predictive performances and discusses integration challenges into clinical workflows. Findings suggest that AI-driven models can accurately predict resistance patterns, while molecular docking provides mechanistic insights into drug-target interactions and resistance mutations. Hybrid AI-docking approaches demonstrate enhanced predictive capacity, offering potential for early intervention and personalized antimicrobial therapy. Future research should focus on multi-omics integration, standardization of data pipelines, and real-world validation.

Keywords: Antimicrobial resistance; Artificial intelligence; Early detection; *In silico* modeling; Machine learning; Molecular docking

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INTRODUCTION

Antimicrobial resistance is a complex multifactorial public health challenge fueled by microbial evolution, antibiotic misuse, and insufficient infection prevention measures (Murray *et al*., 2022; Rawson *et al*., 2023). The World Health Organization reports escalating resistance across key bacterial pathogens, threatening routine surgeries and immunocompromised patient care alike (WHO, 2022).

Resistant infections cause substantial economic burden on healthcare systems globally. Over 1.27 million deaths per year are reported globally and are projected to surpass cancer as a leading cause of mortality by 2050 if left unchecked Pathogens such as *Escherichia coli*, *Klebsiella pneumoniae*, *Staphylococcus aureus*, and *Mycobacterium tuberculosis* have shown increasing multidrug-resistant (MDR) profiles, complicating standard treatment regimens (Perez *et al*., 2018). Delays in identifying resistance mechanisms contribute to ineffective therapy, prolonged hospital stays, and

elevated healthcare costs. For example, the proliferation of multidrug-resistant (MDR) and extensively drug-resistant (XDR) *E. coli, K. pneumoniae* and *S. aureus* has rendered many frontline antibiotics less effective (Rawson *et al*., 2023).

Conventional antimicrobial discovery relies on empirical screening and iterative laboratory validation, often resulting in protracted timelines of 10–15 years per new antibiotic candidate (Stokes *et al.*, 2020). In many clinical microbiology laboratories, conventional methods such as disk diffusion and broth dilution require extended incubation periods, often delaying effective therapy. The integration of artificial intelligence into these workflows has emerged as a transformative solution to improve turnaround times and diagnostic precision. Artificial Intelligence enables the analysis of extensive microbiological and genomic datasets beyond human capacity. By learning complex patterns from data for instace, AI accelerates antimicrobial susceptibility testing (AST) interpretation, enhances genomic resistance prediction, and facilitates robust AMR surveillance (Stokes *et al.*, 2020). These computational approaches, coupled with molecular docking, are increasingly used to accelerate discovery by predicting drug-target interactions, identifying resistance mechanisms, and optimizing molecular structures. The AI models learn complex genotype-to-phenotype relationships, allowing detection of both known and emergent resistance determinants. Integrating these computational approaches bridges the gap between genomic insights and experimental validation, offering predictive and mechanistic power (Arango-Argoty *et al*., 2021).

This review systematically examines the current AI applications coupled with molecular docking in clinical microbiology relevant to AMR detection.

COMPUTATIONAL APPROACHES IN AMR DETECTION

Traditional phenotypic approaches, including broth microdilution, disk diffusion, and automated susceptibility platforms, typically require 24–72 hours for bacterial culture growth and interpretation. While reliable, these methods are resource-intensive and limited in throughput. Molecular PCR-based assays and next-generation sequencing (NGS) provide faster insights but often require specialized laboratory infrastructure and may not fully capture the functional impact of resistance mutations. However, advances in computational biology have introduced AI and molecular docking as complementary tools for AMR detection (Perez *et al*., 2018).

ARTIFICIAL INTELLIGENCE ARCHITECTURES ENHANCING DOCKING

Machine learning (ML) and deep learning (DL) algorithms can process large genomic and proteomic datasets, identifying resistance-associated features that may not be data, apparently through classical analysis (Nguyen *et al.*, 2023). These models can predict resistance phenotypes before clinical manifestation. More so, ML and DL architectures have enhanced docking accuracy and predictive capacity. The ML techniques, such as Random Forests, Support Vector Machines, and Gradient Boosting, can classify ligand binding affinities and resistance phenotypes based on structural and genomic features (Nguyen *et al*., 2022).

Deep learning models, including Convolutional Neural Networks (CNNs) and Graph Neural Networks (GNNs), capture complex three-dimensional interactions between ligands and protein targets. Examples include Atomnet (one of the earliest deep CNN models for structure-based drug design. These models are particularly effective in modeling non-linear relationships between protein conformations and ligand orientation (Arango-Argoty *et al.*, 2021). Generative models, such as Variational Autoencoders (VAEs) and Generative Adversarial Networks (GANs), facilitate *de novo* design of antimicrobial compounds, optimizing chemical structures based on predicted docking outcomes (Stokes *et al*., 2020).

Recent studies have employed transfer learning and federated learning to improve model generalizability across diverse datasets while preserving data privacy, particularly in collaborative multi-center studies (Chen *et al*., 2024; Khalifa *et al*., 2024).

MOLECULAR DOCKING AND ITS PRINCIPLES

Molecular docking is a computational technique that simulates the binding of ligands to biological macromolecules, predicting both orientation and binding affinity.

In silico docking evaluates the binding interactions between antibiotics and bacterial targets, allowing assessment of how mutations in resistance genes alter drug efficacy (Chen *et al*., 2021). Docking simulations can predict resistance hotspots and rationalize drug design strategies. It relies on two core components: the search algorithm, which explores ligand conformational space, and the scoring function, which estimates the strength of interactions

(Papp-Wallace *et al*., 2021). Docking has been applied to characterize inhibitors for beta-lactamases, topoisomerases, and efflux pumps in resistant pathogens.

Despite its utility, conventional docking faces limitations. Rigid receptor assumptions, incomplete solvent modeling, and simplified scoring functions may reduce accuracy. AI integration can dynamically refine scoring functions, incorporate receptor flexibility, and leverage large training datasets to improve predictive performance. Hybrid AI-docking approaches can prioritize promising compounds for experimental validation, reduce false positives, and optimize lead selection offering positive and mechanistic power (Stokes *et al*., 2020; Arango-Argoty *et al*., 2021; Khalifa *et al.*, 2024).

APPLICATIONS IN RESISTANT PATHOGENS

Artificial Intelligence-enhanced docking has been applied to a wide range of clinically significant resistant organisms. For *K. pneumoniae*, docking simulations identified compounds targeting carbapenem-resistant β-lactamases (Papp-Wallace *et al*., 2021). Artificial Intelligence-assisted virtual screening reduced candidate libraries from thousands of molecules to top hits validated experimentally.

Similarly, MDR *E. coli* and methicillin-resistant *S. aureus* have been studied using AI-guided docking pipelines to predict inhibitor binding energies and optimize chemical scaffolds. Coupling genomic surveillance with AI predictions enables precision-targeted therapeutics against emerging resistance determinants, improving clinical applicability and reducing unnecessary laboratory testing (Rawson *et al.*, 2023).

IMPLEMENTATION IN LOW-RESOURCE SETTINGS

Deploying AI-docking pipelines in low-resource settings poses infrastructural and expertise challenges. Cloud computing platforms, open-source docking software, and publicly available structural databases offer scalable solutions (WHO, 2022). Training programs in bioinformatics and computational chemistry, coupled with collaborative networks, enhance local capacity.

Low-cost AI solutions can provide predictive analytics for hospitals lacking advanced microbiology laboratories, enabling early detection of resistance patterns and informed antimicrobial stewardship (Chen *et al*., 2024). Investment in digital infrastructure is essential to ensure equitable access to AI-enabled drug discovery.

ETHICAL, REGULATORY, AND DATA CONSIDERATIONS

AI-driven discovery requires transparent governance to address algorithmic bias, reproducibility, and equitable access (Chen *et al.*, 2024). Data privacy and ethical concerns arise when integrating genomic or patient-derived data. Regulatory agencies are increasingly developing frameworks to evaluate AI-based drug discovery tools, emphasizing validation, reproducibility, and explainability (Khalifa *et al.*, 2024).

International data-sharing agreements and standardized reporting are essential to prevent misuse while enabling collaborative research across institutions. Implementing ethical and regulatory safeguards ensures responsible AI deployment in both high- and low-resource contexts.

PROSPECTS FOR FUTURE RESEARCH

Future Researches include explainable AI frameworks, hybrid AI-quantum docking simulations, integration with real-time pathogen surveillance Federated learning.

Approaches allow secure multi-institutional data analysis, enhancing model robustness. Integrating AI pipelines with clinical decision support systems and antimicrobial stewardship programs will optimize empirical treatment strategies and reduce resistance emergence (Rawson *et al*., 2023; Khalifa *et al*., 2024). Emerging research in protein structure prediction (e.g., AlphaFold) and AI-driven compound optimization is expected to accelerate discovery of novel antimicrobial agents. Interdisciplinary collaboration between microbiologists, computational scientists, and policy stakeholders is essential for global impact.

CONCLUSION

AI and molecular docking have emerged as complementary tools for early detection of AMR. AI models offer high-throughput predictive capabilities, while docking provides mechanistic insight into drug-target interactions. Hybrid approaches show promise in improving prediction accuracy and guiding personalized antimicrobial therapy. Strategic implementation in low-resource settings can accelerate therapeutic development, strengthen surveillance, and support global efforts to combat antimicrobial resistance. Continued research should

focus on integration, multi-omics integration standardization, and prospective clinical validation.

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