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# MODELLING AND MITIGATING ANTIMICROBIAL RESISTANCE (AMR) THROUGH DATA-DRIVEN SURVEILLANCE, AI-POWERED DRUG DISCOVERY, AND PUBLIC HEALTH INTERVENTION DESIGN

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## Abstract

Antimicrobial resistance (AMR) has become arguably the greatest threat to global health, eroding decades of progress in the control of infectious disease and straining public health infrastructure, especially in low- and middle-income countries (LMICs). The accelerating trend of multidrug-resistant microorganisms, driven by the misuse of antibiotics, poor surveillance, and constrained drug development, calls for a combined, evidence-based approach that unites technology and public health interventions. The objective of this research is to design and validate a comprehensive model for modelling and managing

**Keywords:** Antimicrobial Resistance, Artificial Intelligence, Machine Learning, Drug Discovery, Surveillance, Simulation Modelling, Public Health, AMR Policy, Predictive Analytics.



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AMR using quantitative techniques such as epidemiological surveillance analysis, artificial intelligence-based antimicrobial compound discovery, and simulation model-based public program design. Retrospective multi-phased quantitative research was used. AMR surveillance data (2010–2024) were retrieved from GLASS, NCDC, and Nigeria hospitals to determine resistance prevalence, risk factors, and geospatial distribution. Statistical and machine learning algorithms, such as logistic regression and random forest, were used to make predictions of multidrug resistance. Molecular descriptors of 10,000 molecules from ZINC15 and ChEMBL were explored using AI models (XGBoost, GNNs) to make predictions of antimicrobial activity for drug discovery. Molecular docking and ADMET profiling were conducted on high-confidence compounds. Agent-based and system dynamics models then simulated the effects of diverse public health interventions on a 10-year time scale. Surveillance data analysis showed a 42.3% prevalence of AMR, and E. coli and K. pneumoniae were the strongest resistant microorganisms. Prior antibiotic exposure history (OR = 3.42) and hospital-acquired infection (OR = 2.91) were strong predictors. Excellent accuracy was predicted by machine learning models (XGBoost AUC = 0.93) and identified 25 new compounds with high binding propensity (up to –10.2 kcal/mol) against resistance proteins. Simulation findings indicated that coordination among antibiotic stewardship, public education, and restricting the sales of OTC products would reduce AMR rates by 55% in 10 years and save about $11.3 million in healthcare every year. This study shows that the combination of AI, large data analysis, and predictive simulation offers a powerful framework for AMR modelling and intervention planning. The results show how multisectoral policies with combined technological advances and behaviour-specific public health interventions are needed. Implementation of such a combined model can safely limit AMR trends, advise national antimicrobial policy, and hasten the development of new treatment avenues in Nigeria and other comparable LMIC settings.

## INTRODUCTION

Antimicrobial resistance (AMR) has risen as a major global health emergency, compromising the effectiveness of life-saving antibiotics and jeopardizing advances in contemporary medicine. The World Health Organization (2022) stated that AMR accounts for an estimated 1.27 million deaths each year, with most occurring in low- and middle-income countries (LMICs), mostly in sub-Saharan Africa. Nigeria, the most populous country in Africa, is under growing threats of AMR caused by the rampant misuse of antibiotics, ineffective regulatory systems, poor diagnostic capabilities, and suboptimal public health facilities.



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Epidemiologic surveillance in Nigeria has shown elevated levels of resistance among prevalent bacterial pathogens such as Escherichia coli, Klebsiella pneumoniae, and Staphylococcus aureus, particularly to important drug classes such as cephalosporins, fluoroquinolones, and carbapenems (Olayemi et al.,2020; Okeke et al., 2019). These drivers are also driven by the ready over-the-counter availability of antibiotics, poor health literacy, poor sanitation, and misuse of empirical treatment due to poor access to quick diagnostics. Although national AMR action plans exist, their implementation is slow, with surveillance systems continuing to be fragmented.

Additionally, the inability to create new antibiotics also guarantees to make the crisis even worse. Conventional drug development takes a long time, is expensive, and increasingly delivers decreasing dividends. Nevertheless, developments in artificial intelligence (AI) and machine learning (ML) present a revolutionary opportunity to identify new antimicrobial entities by leveraging enormous molecular data and predictive modelling (Stokes et al., 2020; Chen et al., 2021). Aside from drug discovery and monitoring, public health interventions mass education, drug supply regulation, and antibiotic stewardship are critical to preventing spread. These interventions are, however, typically implemented in a standalone fashion and without an illumination by predictive models that can make predictions or optimize resource allocation. This research tackles the issue of AMR from several sides with a holistically integrated solution that includes data-driven monitoring, AI-facilitated drug development, and simulation-informed public health policy making. Targeting Nigeria as a case study, it employs a quantitative, multi-stage methodology to measure patterns of resistance, forecast new compounds, and simulate the effect of compounded interventions.

Through the connection of clinical epidemiology, data science, and health policy, the study seeks to build workable insights that inform local and international AMR mitigation policies.

**RESEARCH QUESTIONS**

- How best can an integrated data-informed system of AMR surveillance analytics, AI-driven drug discovery, and simulation of public health policy model and resist the burden of antimicrobial resistance in Nigeria?
- What are the current spatial and temporal patterns of AMR among priority bacterial pathogens in Nigeria based on surveillance and clinical data?
- Which epidemiological, behavioural, and clinical factors most strongly predict the emergence of multidrug-resistant infections?
- Can machine learning and molecular docking approaches identify and prioritize novel compounds with predicted activity against resistant pathogens?

- How do different combinations of interventions such as antimicrobial stewardship programs, stricter regulation of antibiotic sales, and public education campaigns affect projected AMR trends over the next decade?
- What is the cost-effectiveness and implementation feasibility of the proposed integrated strategies in guiding national AMR action plans?

**STATEMENT OF THE PROBLEM**

The antimicrobial resistance (AMR) is on the rise at a speed previously unknown, threatening health systems globally in an unprecedented manner. It is even more critical in low- and middle-income nations such as Nigeria due to widespread misuse of antibiotics, absence of real-time capacity for surveillance, unregulated drug market, and over-the-counter sale of prescription drugs. The subsequent spread of multidrug-resistant pathogens not only adds to morbidity and mortality but also raises healthcare expenditure and defeats the efficacy of traditional medical treatment.

Despite national plans for antimicrobial resistance action, these have been marred by non-coordinated implementation, weak data integration, and poor technical capacity. Worse, there is a dwindling pipeline of new antibiotics. These traditional drug discovery approaches are generally wasteful, costly, and time-consuming, and before new treatments are even developed, resistance emerges. Moreover, existing public health interventions are seldom informed by predictive models that can simulate their actual effect under a range of demographic and behavioural conditions.

There is a wide knowledge gap and practice in designing an integrated, evidence-based policy that uses surveillance analytics, artificial intelligence (AI) for compound screening at speed, and policy simulation platforms to model the impact of various AMR control interventions. This has led to reactionary policymaking, inefficient expenditure in the Nigerian health system, and makeshift interventions.

Thus, an evidence-based, science-strengthened, and multidisciplinary framework is essential to track, forecast, and contain AMR efficiently. The framework must marry the power of AI with evidence from real-world surveillance and model the effect of behavioural, institutional, and pharmacological interventions in a resource-limited setting.

**RESEARCH OBJECTIVES**

The general aim of this study is to conceptualize and validate a general framework for the prediction and prevention of antimicrobial resistance in Nigeria through data analytics, artificial intelligence, and public health modelling. In order to attain this objective, the study is guided by the following particular aims:

**Surveillance and Epidemiological Modelling**

To estimate the size and temporal-spatial pattern of antimicrobial resistance in Nigeria based on clinical surveillance data from 2010-2024.

To detect high-burden pathogens and resistance rates against major antibiotics by statistical and geospatial analysis, respectively.

To find the strongest predictors of multidrug-resistant infection by multivariate logistic regression, based on patient age, previous antibiotic exposure, and source of infection.

**AI-Assisted Antimicrobial Compound Discovery**

- To develop and train machine learning models (e.g., XGBoost, GNNs) for predicting antimicrobial activity from molecular descriptors of chemical compound libraries (e.g., ZINC15, ChEMBL).
- To select and prioritize new compounds of high predicted activity against target resistant bacteria.
- To screen top compounds by molecular docking experiments and determine their affinities to bind target resistance enzymes (e.g., β-lactamase, DNA gyrase).
- To carry out in silico ADMET profiling to predict pharmacokinetics and toxicity of lead compounds.

**Simulation of Public Health Interventions**

- To design agent-based and system dynamics models to simulate the effect of combinations of different control measures against AMR over a decade (2025–2035).
- To compare estimated effects of different combinations of interventions e.g., antibiotic stewardship programs, public campaigns, and prohibitions on selling antibiotics over-the-counter (OTC) on AMR levels and healthcare expenditure.
- To conduct sensitivity analysis to compare the impact of variations in compliance rates, drug availability, and public actions on intervention success.

**Policy and Implementation Guidance**

- To project the cost-effectiveness of interventions simulated in this study with health economic metrics like DALYs saved and cost per infection saved.
- To design evidence-based policy recommendations to incorporate AI, surveillance analytics, and public health interventions into Nigeria's National AMR Action Plan and general global AMR strategies.

**The Growing Threat of Antimicrobial Resistance (AMR)**

Antimicrobial resistance (AMR) is no longer a looming threat it is a current and growing crisis. Projections currently suggest that in 2050, AMR can cause up to 10 million deaths annually and as much as $100 trillion in economic costs globally (Murray et al., 2022). The most severe impact is seen in low- and middle-income countries (LMICs), where uncontrolled use of antibiotics, substandard medicines, and under-resourced healthcare systems fuel the development of resistance (Hernando-Amado et al., 2023).

The status of AMR in Nigeria is worsening because of self-medication, improper hygiene, poor diagnostic services, and the availability of antibiotics free of charge without prescription (Nwafia et al., 2022). For instance, Abuja and Enugu teaching hospitals have provided recent evidence that over 60% of isolates of E. coli are resistant to three or more classes of antibiotics (Chukwu et al., 2022). The World Bank (2022) warns that without firm measures, AMR could push up to 24 million people into extreme poverty by 2030, with African nations disproportionately affected.

**AMR Monitoring Surveillance Gaps and Predictive Analytics**

Surveillance is the key to successful control of AMR. The Global Antimicrobial Resistance and Use Surveillance System (GLASS) lies at the heart, but data integration and coverage are still poor in all the LMICs (Rafiqul Islam et al., 2023). Nigeria's membership of GLASS has enhanced reporting, but issues regarding data quality, under-reporting, and heterogeneity of laboratories persist (Idoko et al., 2023).

Emerging predictive analytics advances have current tools to strengthen AMR surveillance. Machine learning (ML) models such as logistic regression, support vector machines (SVM), and ensemble models have been used in predicting AMR trends using clinical and genomic information (Kang et al., 2022). Random forest models, for example, have been shown by Shah et al. (2022) to predict accurately antibiotic resistance in K. pneumoniae with a staggering 87% accuracy based on electronic health records.

However, there is very little country-specific real-time data integration with the predictive models, particularly for West Africa. The majority of the available models are Western-trained, compromising generalizability across differences in prescribing behavior, microbial strains, and healthcare facilities.

**Artificial Intelligence in Antimicrobial Drug Discovery**

AI transformed drug discovery with the capacity of high-throughput screening of compound libraries and the prediction of molecular interactions at record speed. DeepMind's AlphaFold2 made precise protein structure predictions that greatly facilitated target-based antimicrobial discovery (Jumper et al., 2021).

Some of these approaches now utilize deep neural networks, graph convolutional networks, and reinforcement learning to identify new compounds with antibacterial activity (Yang et al., 2022). For instance, Ragoza et al. (2023) employed a deep docking pipeline to identify more than 5,000 candidate Mycobacterium tuberculosis inhibitors from a collection of 1 billion compounds. Even with these advances, AI-assisted drug discovery is not yet fully utilized in LMICs due to technical limitations, limited infrastructure, and low levels of computational literacy. In addition, few research endeavours have incorporated AI-made drug candidates into larger AMR policy and surveillance frameworks an issue that this study seeks to address.

**Molecular Docking and In Silico Validation Techniques**

Molecular docking is still crucial in lead ranking of candidate compounds selected by AI methods. Methods like Auto Dock Vina and Glide mimic ligand-receptor binding and predict free binding energy to predict compound activity (Duan et al., 2023).

In silico ADMET screening for bioavailability and safety supplements docking experiments increasingly. Bender et al. (2023) stated that early ADMET filtering decreases candidate attrition by as much as 60% in preclinical development.

For AMR, docking is typically against resistance enzymes like β-lactamase, DNA gyrase, or penicillin-binding proteins. The overwhelming majority of such studies are though abstract, theoretical exercises that see no subsequent validation or policy implementation. This study closes that gap by merging compound discovery with surveillance trend analysis and intervention modelling.

**Simulation Modelling of Public Health Interventions**

Agent-based and system dynamics modelling offer a platform to simulate the long-term effect of AMR interventions. Agent-based and system dynamics models can capture heterogeneity across the population, dynamics of behaviour, and health system capacity to study scenarios prior to actual implementation (Willis et al., 2022).

It is only now, such as in the work of Ferreira et al. (2023), that researchers have employed ABMs to model the impact of antibiotic stewardship, vaccination, and community education to cut AMR levels in Brazil by as much as 45% over 10 years. Oladipo et al. (2022) constructed a hybrid ABM-SEIR model to evaluate control options for AMR in Lagos in Africa, though without real-time compound development and AI technologies.

Marriage of such simulation models with AI-driven surveillance and drug discovery is a new frontier and the primary contribution of this research.

**Integrated Framework Research Rationale and Gaps**

Whereas earlier work has progressed each of AMR surveillance, drug discovery, or intervention design separately, few studies have put all three together as one policy-guiding platform. Nigeria-focused research has mostly neglected to examine the unification of predictive epidemiology, compound screening using AI, and simulation modelling for strategic health planning applications.

The deficits of this research are overcome by:

Combining surveillance and compound innovation through AI and molecular docking that is responsive to clinical resistance patterns; Computer simulation of long-term scenarios of intervention to guide cost-effective AMR mitigation strategies; Contextualization of the findings to the Nigerian healthcare and regulatory environment to facilitate implementation feasibility.

Through a convergence of data science, pharmacology, and public health policy, this research provides a new route to sustainable and scalable control of AMR in Nigeria and other similar LMIC settings.

**Genomic Insights and Molecular Epidemiology for AMR Control**

In the last few years, whole-genome sequencing (WGS) has been a key driver of the understanding of resistance mechanisms and identifying the source of resistant isolates. Genomic epidemiology yields high-resolution information that cannot be mimicked by traditional phenotypic monitoring (Andrade et al., 2023). For example, genomic research in West African healthcare settings has illustrated the clonal spread of extended-spectrum β-lactamase (ESBL) producing Enterobacteriaceae at an accelerated pace, stressing the need for genomic incorporation into national AMR action plans (Boateng et al., 2023).

In addition, bioinformatics pipelines can now connect genomic data to hospital surveillance data and detect outbreaks in their early phase and customize infection control interventions. This also helps to understand horizontal gene transfer among pathogens, an important cause of multidrug resistance in high-burden environments (Fernandez-Martinez et al., 2023). Their inclusion in predictive models can significantly increase the specificity of AMR interventions.

**Behavioural and Socio-Cultural Determinants of AMR**

Whereas technological innovation is of most significance, trends in behavior and socio-cultural factors have a significant contribution to antimicrobial abuse. Current literature determines that for most of the LMICs, patient pressure, cultural practices, and misinformation contribute to inappropriate use of antibiotics (Ndir et al., 2023). In Nigeria's case, self-prescribing of antibiotics by individuals without diagnosis occurs largely through community pharmacies as the first port of entry (Gidado et al., 2023).

Public health programs, therefore, must address not only deficits in knowledge but also health system trust and illness and treatment cultural practices. Quantitative evidence in Kenya indicated that integrated community outreach programs reduced the rate of self-medication by nearly 30% over a period of two years (Mutai et al., 2024). These findings suggest that technical solutions such as AI and surveillance must be accompanied by context-appropriate behavioural interventions to achieve sustainable AMR reduction.

**Economic Effects and Health System Limitation**

The economic impact of AMR in LMICs is not limited to healthcare expenditure but also impacts productivity and household income. For example, a recent health economics review in Uganda found that resistant infection patients spent an average of 40% more on their treatment and had longer lengths of stay in the hospital (Okiria et al., 2023). This imparts the importance of incorporating cost-effectiveness analysis in the formation of AMR policy.

Further, systemic weaknesses like supply chain problems, poor pharmacovigilance, and poor implementation of stewardship hinder AMR control (Abubakar et al., 2024). Evidence from Ghana was that even when stewardship protocols were in place, staff training shortages and drug stock levels undermined compliance (Mensah et al., 2023). Such systemic limitations make the introduction of real-world constraints into simulation models more important than assuming ideal conditions.

**AI and Public Health Policy Integration**

Although AI has already been shown to function effectively in the detection of drug candidates, its use in public health decision-making is still in progress. In Southeast Asia, proof has been shown regarding the potential of AI-assisted decision support systems to assist clinicians in the prescription of antibiotics, lowering inappropriate prescribing by 18% in pilot implementation (Suwantarat et al., 2023). The same technologies may be utilized in Nigerian contexts where electronic health record systems are being implemented incrementally. At the policy level, integrated data-driven dashboards of surveillance outputs, predictive models, and simulations of interventions can support evidence-based decision making through health ministries (Vong et al., 2023). The dashboards enable real-time tweaking of stewardship programs and can detect developing resistance trends before they become widespread. It demands cross-sectoral action and long-term investment.

**Towards an Integrated Framework**

Together, the above research highlights that while enormous breakthroughs have occurred in surveillance technology, AI-facilitated discovery, and intervention modeling,

they are in silos. A common, data-driven platform which integrates these domains is yet to be thoroughly mapped out, especially in LMIC settings like Nigeria. Through genomic surveillance, socio-behavioral understanding, economic appraisal, and AI-facilitated discovery integrated into a coherent simulation-informed policy development, this research here discusses an essential gap in the AMR literature directly.

## METHODOLOGY

This research utilizes a quantitative, multi-step, data-driven strategy that includes epidemiological surveillance data analysis, artificial intelligence-based computational drug screening, and simulation-based assessment of public health interventions. The research takes three consecutive sections to mirror the extent, drivers, and solutions of Antimicrobial Resistance (AMR).

### Research Design and Approach

The study employs a retrospective experimental quantitative design with three analysis components:

- Analytical analysis of AMR trends based on real datasets
- AI-supported discovery and validation of novel antimicrobial products

Modelling based on simulations of intervention approaches to act against AMR effect. Such formal strategy allows systematization of quantification of AMR determinants as well as investigation of solution possibilities.

### Data Collection

#### Epidemiological Surveillance Data

Sources: WHO Global Antimicrobial Resistance Surveillance System (GLASS), Nigeria Centre for Disease Control (NCDC), tertiary hospital databases (e.g., LUTH, UNTH), and Resistance Map (CDDEP).

Time Frame: 2010–2024

**Variables:**

Bacterial species (e.g., E. coli, K. pneumoniae, Staphylococcus aureus)

Resistance outcomes from antimicrobial susceptibility testing (AST)

Minimum Inhibitory Concentrations (MIC), Patient demographics (age, sex, treatment duration, hospital ward)

Geographic and temporal indicators

#### Drug Discovery Dataset

Chemical libraries: ZINC15, PubChem, ChEMBL

Resistance gene targets: NCBI GeneBank, CARD (Comprehensive Antibiotic Resistance Database)
Protein structures: Retrieved from the Protein Data Bank (PDB) for docking and interaction modelling

**Data Analysis and Modelling Techniques**
**Statistical and Predictive Modelling of AMR Patterns**
Descriptive statistics: Prevalence rates, incidence trends, mean MIC values by region and pathogen

**Inferential statistics:**
Chi-square tests for pathogen-resistance associations, Multivariate logistic regression to identify predictors of multidrug resistance
Geospatial mapping: GIS-based hot spot analysis to identify regional variations in AMR
Software utilized: SPSS v27, R (epitools, tidyverse), QGIS 3.34

**AI-Antimicrobial Compound Design**
**Feature Engineering:**
Physicochemical properties (molecular weight, logP, hydrogen bond donors/acceptors)
Molecular fingerprints (ECFP4, MACCS)

**Model Development:**
Supervised machine learning classifiers: Random Forest (RF), Support Vector Machines (SVM), and XGBoost for binary classification (active vs. inactive compounds)
Deep Learning (Graph Neural Networks, GNNs) for structure–activity prediction
Validation Metrics: Accuracy, ROC-AUC, Precision, Recall, F1-score (through 10-fold cross-validation)
Software utilized: Python (scikit-learn, PyTorch, RDKit)

**Molecular Docking and In Silico Validation**
Top AI-identified compounds will be docked to target proteins (e.g., β-lactamase, DNA gyrase) using Auto Dock Vina
Binding affinity (ΔG), hydrogen bonds, and active site interactions will be calculated. ADMET properties will be predicted by SwissADME and pkCSM packages

**Simulation-Based Public Health Intervention Modelling**
Modelling Approach: Agent-Based Modelling (ABM) and System Dynamics Modelling (SDM)


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**Intervention Scenarios:**

Antibiotic stewardship programs (hospital-based)

Public education campaigns (community-based)

Regulatory limits on over-the-counter antibiotics

Model Parameters, Resistance transmission rates, Antibiotic consumption rates, Policy compliance rates

Simulation horizon: 2025–2035

Outputs: Decrease in AMR prevalence, antibiotic consumption, and healthcare cost savings

Software: AnyLogic 8.8, Vensim DSS

**Model Evaluation and Sensitivity Analysis Predictive Model Evaluation: ROC curves, confusion matrices, and Kappa statistics**

Simulation Validation: Replication of historical trends and expert validation

Sensitivity Analysis: One-at-a-time (OAT) and Latin Hypercube Sampling (LHS) to examine robustness of intervention effects over parameter ranges

**Ethical Considerations**

Ethical clearance received from National Health Research Ethics Committee (NHREC), Nigeria

Deidentified patient-level data housed consistent with GDPR and Nigerian Data Protection Regulation (NDPR)

Publicly accessible data sets used consistent with the terms of open-access license agreements

No biological testing or human experimentation

**Table 1: Summary of Methodology**

| Phase | Objective | Data/Tools | Outcome |
|---|---|---|---|
| 1 | Model AMR trends and predictors | Epidemiological data, SPSS, R, GIS | Resistance maps, risk factors, trend analysis |
| 2 | Discover novel antimicrobials using AI | Compound libraries, ML models, docking tools | Novel candidate compounds with binding efficacy |
| 3 | Simulate and quantify public health impacts | Agent-Based & System Dynamics models (AnyLogic) | Forecasts of intervention effectiveness and savings |



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## RESULTS

Epidemiological Analysis of AMR Trends (2010–2024)

### Descriptive Statistics

Descriptive analysis of 18,724 de-identified patient records from tertiary health facilities and surveillance registries identified the following:

Overall prevalence among bacterial isolates was 42.3% with 19.7% as multidrug-resistant (MDR) strains.

Most common MDR pathogens were:

Escherichia coli – 26.1%

Klebsiella pneumoniae – 21.4%

Staphylococcus aureus – 19.2%

AMR trends were greater in urban tertiary hospitals (47.8%) than in rural centres (31.4%).

### Temporal and Geographic Trends

Between 2010 and 2024, AMR rates rose by 18.6%, the highest resistance of 2020–2022, coinciding with mass self-medication during the COVID-19 pandemic.

Geospatial analysis with QGIS revealed AMR "hotspots" in Lagos, Kano, and Port Harcourt.

Resistance to third-generation cephalosporins and fluoroquinolones rose by 35% and 28%, respectively, in the past 5 years.

### Inferential Analysis

Logistic regression revealed significant predictors of multidrug resistance:

History of past use of antibiotics over the last 6 months (OR = 3.42, $p < 0.001$)

Nosocomial infection (OR = 2.91, $p < 0.005$)

Age >65 years (OR = 1.84, $p = 0.018$)

Chi-square test revealed significant association between K. pneumoniae and resistance to carbapenem ($\chi^2 = 46.83$, $p < 0.001$).

AI-Assisted Antimicrobial Drug Discovery

### Machine Learning Model Performance

Among 10,000 ZINC15 and ChEMBL screened compounds:

Feature matrices of 1,024 molecular descriptors were created using RDKit.

Three models were trained to perform binary classification (active/inactive):

Random Forest (RF): AUC = 0.91, F1-score = 0.88

XGBoost: AUC = 0.93, Precision = 0.90

Support Vector Machine (SVM): AUC = 0.89, Recall = 0.87

The XGBoost model had the best performance in both training and validation sets.

**Compound Selection and Docking Results**

25 top high-confidence active compounds (confidence > 0.95) were chosen for molecular docking against three resistance proteins:

β-lactamase (PDB ID: 1ZG4)

Table 2: DNA gyrase subunit B (PDB ID: 4Z2C), Efflux pump protein AcrB (PDB ID: 2GIF).

| Compound ID | Target Protein | Binding Affinity (kcal/mol) | H-Bond Interactions |
|---|---|---|---|
| ZINC2034761 | β-lactamase | -9.6 | 4 |
| ZINC8743612 | DNA gyrase | -8.8 | 3 |
| ZINC1476935 | AcrB efflux pump | -10.2 | 5 |

All of the top 5 molecules possessed good ADMET properties with oral bioavailability scores > 0.75 and no toxicological prediction.

**QSAR and ADMET Profiling**

Quantitative Structure–Activity Relationship (QSAR) models presented high correlation ($R^2 > 0.82$) between antimicrobial activity and compound structure.

ADMET screening revealed low hepatotoxicity risk and excellent gastrointestinal absorption for 21 out of the 25 compounds.

**Simulation of Public Health Interventions**

An agent-based 10-year model was established to run three scenarios in a population of 500,000 modelled for high-burden AMR countries.

**Table 3: Intervention Scenarios and Impact**

| Scenario | Resistance Prevalence (2035) | Reduction (%) | Cost-effectiveness ($/DALY) |
|---|---|---|---|
| **No intervention (baseline)** | 48.2% | 0% | – |
| **Stewardship program only** | 33.6% | 30.2% | $812 |
| **Stewardship + Awareness + Ban OTC** | **21.5%** | **55.4%** | **$506** |

Combining stewardship interventions, public education, and restriction of over-the-counter antibiotics yielded the largest incidence reduction in AMR.



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Intensity of public education and adherence to programs were found by sensitivity analysis to have the greatest impact on intervention effectiveness.

**Simulation Results to Policy**

System dynamics modelling estimated ~20,000 fewer resistant infections annually under universal intervention by 2035.

Net healthcare cost savings estimated: $11.3 million/year (largely due to shorter hospital stays and antibiotic consumption).

**Model Validation**

Predictive models were robust in external validity (XGBoost test AUC = 0.92).

Simulations captured historical trends well with <5% deviation.

Sensitivity analysis validated robustness in ±10% change of influential parameters.

**Table 4: Key Findings Summary**

| Objective | Key Result |
|---|---|
| **Epidemiological Modelling** | 42.3% AMR prevalence; high MDR in *E. coli* and *K. pneumoniae* |
| **Predictive Risk Analysis** | Prior antibiotic use and hospital-acquired infections significantly predictive |
| **AI Drug Discovery** | 25 novel candidate compounds; top binding score -10.2 kcal/mol |
| **Simulation of Interventions** | Full policy package reduces AMR by 55% and saves $11.3M annually |

**DISCUSION**

The current study presents a data science-based solution that covers modelling and prevention of antimicrobial resistance (AMR), taking advantage of epidemiological surveillance, artificial intelligence (AI)-driven drug discovery, and simulation of public health interventions. The results provide strong evidence of the potential of integrative quantitative methods to unravel the worldwide AMR pandemic, especially in low- and middle-income nations such as Nigeria.

**Epidemiological Patterns and Predictors of AMR**

The study revealed a general AMR prevalence rate of 42.3%, with about 20% contributed by multidrug-resistant bacteria. These are symptomatic of increasing resistance burden, consistent with WHO reports that one of the fastest developing rates of resistance existed in Africa because of inadequate surveillance and abuse of antibiotics (WHO, 2022). Temporal trends found a significant rise between the years 2020–2022 during the COVID-19 period, confirming concerns and hypotheses of earlier research (Haque et al., 2021) that

antibiotic utilization in emergency conditions during health crises accelerates resistance. Geospatial mappings also determined hotspots for the AMR prevalent in high-density urban cities such as Lagos and Port Harcourt, in support of Olayemi et al. (2020), whose focus lay in urban crowding and overloading of the health system as places of stress development for emerging clusters of resistance.

Remarkably, logistic regression model previously mentioned listed earlier antibiotic exposure, hospital-acquired infection, and advanced age as predictors of strong resistance. These findings are in agreement with previous studies by Okeke et al. (2019), which had established similar correlation in Nigerian teaching hospitals. The findings reinforce the importance of improved control of prescription and infection control, especially among elderly patients.

**Artificial Intelligence in Drug Discovery: A Revolutionary Approach**

Use of AI models, specifically XGBoost and Graph Neural Networks, for prediction of active compounds resulted in satisfactory outcomes with an AUC of 0.93 and F1-scores of more than 0.88. They were better than conventional QSAR models, showing the enhanced ability of AI to represent intricate nonlinear associations in molecular data (Chen et al., 2021).

The in silico docking simulations were demonstrated to have remarkable binding affinities between selected compounds and targets of resistance like β-lactamase and DNA gyrase. ZINC1476935, with a binding affinity of –10.2 kcal/mol, was the most highly promising lead molecule. The findings are in line with the trend of recent studies into structure-based AI-enabled drug design, for example, studies by Stokes et al. (2020), who found using deep learning a new antibiotic halocin.

Moreover, ADMET profiling revealed favourable pharmacokinetic and toxicity scores for the majority of candidates, and this suggests the potential to expedite early-stage drug discovery with less opportunity for failure. This is especially important in LMICs, where cost of development is generally a limitation for new antimicrobial discovery.

**Modelling Public Health Interventions: Strategic Pathways for AMR Control**

The intervention scenarios simulated in the report illustrated that bundling antibiotic stewardship programs, public awareness campaigns, and oversight of over-the-counter sales of antibiotics could decrease cases of AMR by as much as 55% a decade from now. The outcome is consistent with previous modelling by Laxminarayan et al. (2016), which indicated that bundled interventions most heavily influence AMR.

The agent-based model specifically focused on the pivotal role of behaviour change at the community level to avert AMR. The results were sensitive to parameters like the compliance rate and health literacy. Interestingly, while stewardship had a moderate

effect in isolation, it was overall policy framework mass education and OTC regulation that provided the most cost-saving and sustainable outcome. They highlight an important observation: technical innovation (surveillance, AI) needs to be accompanied by strong public health policy and social mobilization to be most effective. They also observe that Nigeria and such contexts need to put AMR at the level of national health policy, invest in community-level outreach efforts, and rigidly implement sale regulation on drugs.

**Policy Implications**

The results have several implications for public health policy and antimicrobial regulation:

- **Antibiotic Stewardship Expansion**: Hospital-based interventions must be scaled and supported with clinical decision support systems that incorporate local resistance data.
- **Community Awareness and Behavioural Interventions**: Targeted education campaigns using culturally relevant messaging are vital to altering antibiotic use behaviour, especially in rural and underserved areas.
- **Regulation of Antibiotic Sales**: Enforcing prescription-only antibiotic laws through pharmacy inspections and digital tracking of drug sales can help limit unauthorized access.
- **AI Integration in National Health Strategy**: Government research institutions should be equipped with AI infrastructure to support predictive modelling and rapid drug discovery.

**Limitations**

While the study offers substantial insights, several limitations must be acknowledged:

- **Retrospective Nature**: Reliance on historical datasets may introduce reporting bias or inconsistencies in data recording across hospitals and regions.
- **Lack of Experimental Validation**: Although docking and ADMET simulations were used, laboratory-based validation (e.g., MIC testing, cytotoxicity assays) was not performed, which would be essential for drug candidate confirmation.
- **Behavioural Simulation Assumptions**: The agent-based models rely on assumptions that may not fully capture real-world complexities such as informal drug markets, sociocultural resistance to change, and government enforcement capacity.

Nonetheless, these limitations are counterbalanced by the study's rigorous modelling, large dataset size, and methodological triangulation.

**Contribution to Knowledge**

This research contributes significantly to the interdisciplinary field of AMR by:

- Demonstrating how AI can be practically integrated into AMR drug discovery in resource-limited settings
- Providing a predictive surveillance framework for AMR risk analysis and hot spot detection
- Offering a tested simulation model for policymakers to assess the long-term impacts of intervention strategies

It bridges the gap between computational innovation and actionable health policy, providing a model that can be adapted by other LMICs facing similar AMR challenges.

**Future Research Directions**

- **Wet lab validation** of the top candidate compounds in bacterial culture studies
- **Real-time surveillance integration** with electronic health records using automated AI tools
- **Behavioural economics modelling** to understand and influence prescribing and consumption practices
- **Longitudinal cohort studies** to monitor the impact of implemented interventions over time

**CONCLUSION**

The present research has proven the efficacy of an integrated, evidence-based approach to the growing world threat of antimicrobial resistance (AMR). Through the integration of epidemiological modelling, drug discovery empowered by artificial intelligence (AI), and simulation-supported public health policy analysis, the present work presents a menu of AMR mitigation that is revolutionary but practical, especially in resource-limited environments such as Nigeria.

Surveillance analysis revealed a striking and increasing trend of AMR, specifically multidrug-resistant Escherichia coli, Klebsiella pneumoniae, and Staphylococcus aureus, and major cities like Lagos and Port Harcourt as hubs of resistance. Predictive statistical modelling also corroborated prior exposure to antibiotics, nosocomial acquisition of infection, and advanced age as predictors of robust resistance, highlighting the necessity for targeted interventions.

The AI-based drug discovery process produced candidate molecules with high binding affinities and acceptable ADMET profiles, indicating the potential of machine learning and deep learning algorithms in accelerating antimicrobial drug discovery. The fact that the combination of predictive analytics tools and molecular docking software reinforced the strength of AI in filling the shrinking antibiotic pipeline is an extremely strong argument.

These simulated intervention scenarios also confirmed that single-action initiatives hospital stewardship programs, for example are insufficient when used alone. The

optimal approach was a multifaceted policy system that included antibiotic stewardship, public education, and control over the over-the-counter dispensing of drugs. This multi-pronged strategy was predicted to reduce the prevalence of AMR by over 50% and save millions annually in healthcare cost.

In sum, this study presents an adaptable and scalable model for AMR response that bridges clinical microbiology, data science, and public health planning. It affirms that technical innovations must be supported by behavioural and institutional reforms to ensure sustainable outcomes.

**RECOMMENDATIONS**

Based on the research findings and analysis, the following recommendations are proposed to enhance the surveillance, prevention, and mitigation of antimicrobial resistance in Nigeria and similar settings:

**1. Enhance AMR Surveillance Infrastructure**

Implement national electronic surveillance networks connecting hospital data with national reporting systems (e.g., NCDC, GLASS). Create real-time data analysis capabilities in tertiary hospitals and public health facilities to facilitate early detection and response to AMRs. Make uniform antimicrobial susceptibility testing (AST) guidelines mandatory for both public and private laboratory complexes.

**2. Institutionalize AI in Antimicrobial Drug Research**

Enable inter-institutional collaborations among research institutions, AI laboratories, and pharmaceutical industries in order to facilitate the application of machine learning models towards compound optimization and screening. Create a national drug discovery AI strategy with training programs, open data bases, and funding incentives. Enable development of local compound libraries to limit foreign chemical data base dependency.

**3. Scale Up Stewardship and Prescription Governance**

Implement clinical antibiotic stewardship practices in all tertiary and secondary care hospitals through policy requirements and enforcement for compliance. Implement decision-support tools as part of hospital electronic health records to enable rational prescribing of antibiotics. Set up antimicrobial stewardship task forces at the institutional and regional levels.

**4. Restrict Community Antibiotic Use and Access**

Prohibit over-the-counter marketing of key antibiotic classes and uphold prescription-only policies through the Pharmacists Council of Nigeria and NAFDAC. Implement culturally relevant public health interventions on self-medication risks, resistance.

Employ mobile health education platforms (e.g., text messages, radio spots, mobile apps) that address peri-urban, rural populations.

**5. Support Policy-Driven Multi-Sectoral Action**

Create a National AMR Control Council in the Federal Ministry of Health to enable cross-sectoral action across agriculture, education, health, and environment sectors (One Health approach).

Enable integration of AMR mitigation strategies into national development plans and budgets. Enhance civil society participation in awareness campaigns, monitoring, and feedback mechanisms.

**6. Investments in Future Research and Innovation**

Influence federal research grants for wet-lab validation of AI-discovered antimicrobial compounds.

Support longitudinal investigations to track the long-term effects of rolled-out AMR control interventions.

Facilitate the establishment of hybrid AI-simulation platforms for policy planning and emergency readiness for new resistance patterns.

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