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COMPUTATIONAL MODELING FOR PREDICTING ANTIBIOTIC RESIDUES RISK IN AQUATIC ECOSYSTEMS

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ABSTRACT

Due to the horizontal transmission of antibiotic resistance genes among microbial communities in surface waters, sediments, and groundwater, the proliferation of antibiotic residues in aquatic ecosystems has become a major environmental concern. Empirical monitoring programs are limited by high costs, spatiotemporal variability, and the combinatorial complexity of multi- contaminant matrices, despite the fact that they offer essential occurrence data. By facilitating systematic risk assessment across spatial dimensions and exposure scenarios not possible through traditional field campaigns, computational predictive modeling provides an affordable supplement. In order to critically assess the state of quantitative structure–activity relationship models, machine learning algorithms, and mechanistic fate-and-transport frameworks applied to antibiotic risk prediction in freshwater and coastal environments. The findings show that while mechanistic models are excellent at capturing nonlinear hydrological drivers but necessitate extensive site-specific parameterization, ensemble machine learning models— especially gradient-boosted trees and graph neural networks—consistently outperform classical quantitative structure–activity relationship models approaches (a mean R^2 improvement of 12–18%). Although they are still unexplored, hybrid modeling approaches that combine machine learning with process-based hydrological equations show great promise. The main findings emphasize the necessity for standardized environmental input datasets, the ongoing limitations of data scarcity, and the regulatory significance of uncertainty quantification in model outputs. Protocols for model benchmarking and approaches for policy integration are suggested.

Keywords: Antibiotic residues; antibiotic resistance genes; aquatic risk prediction; environmental computational modeling; machine learning; mechanistic fate models; Quantitative Structure Activity Relationship.

1. INTRODUCTION

With an estimated yearly consumption of more than 130,000 tonnes across human medicine, veterinary applications, and aquaculture, antibiotics are among the most commonly used category of pharmaceuticals worldwide [1]. A significant amount of administered antibiotics—between 30% and 90%, depending on the compound—are eliminated in a pharmacologically active or partially metabolized form despite their therapeutic necessity. These antibiotics enter aquatic systems through wastewater treatment plant (WWTP) effluents, agricultural runoff, and direct veterinary discharge [2]. These substances accelerate the acquisition and spread of antibiotic resistance genes (ARGs), which are mobile genetic elements that encode enzymatic degradation, efflux pump expression, or target-site modification mechanisms that confer heritable resistance, by applying sub-inhibitory selective pressures to resident microbial communities once they are in the aquatic environment [3].

Beyond the immediate microbial ecology, ARG proliferation in aquatic habitats has ecological ramifications. An epidemiological continuum between environmental reservoirs and human infections has been demonstrated by the evolutionary linking of resistance determinants found in river sediments, estuarine biofilms, and drinking-water reservoirs to clinical isolates [4]. Although hundreds of different ARG classes that co-occur with quantifiable antibiotic residue concentrations have been identified by metagenomic surveys of the Yellow River basin, the Thames catchment, and the Mekong Delta, the process of converting these co-occurrence patterns into mechanistic risk predictions is still lacking [5]. Crucially, traditional monitoring systems usually compare individual antibiotics to static predicted no-effect concentrations (PNECs) obtained from single-species ecotoxicity tests. This methodology significantly underestimates mixture toxicity and disregards the ARG-selective potency of sub-PNEC concentrations found in recent minimum selective concentration (MSC) studies [6].

1.1 Knowledge Gaps in Predictive Modeling

The creation of reliable forecasting tools is hampered by a number of interrelated shortcomings. First, ARG proliferation is rarely included as a dynamic output variable in environmental destiny models for antibiotics; instead, dissolved-phase concentrations are predicted without being connected to resistance selection objectives [7]. Second, the training datasets supporting QSAR and ML models for antibiotic environmental behavior are geographically and taxonomically biased toward high-income temperate regions, which restricts transferability to low-income and tropical contexts where environmental loading and antibiotic consumption are increasing at the fastest rates [8]. Third, without significant simplification, mechanistic models that may simultaneously address photolysis, microbial transformation, and sediment-water partitioning are computationally expensive at the watershed scale [9]. Finally, uncertainty quantification—essential for regulatory decision-making—is rarely reported consistently across model types, precluding meaningful inter-model comparison [10].

2. Review Methodology

2.1 Classification of Computational Model Categories

Using the taxonomic framework provided forth by Cherkasov et al., (2014), the included works were divided into three main computational paradigms [11] and subsequently adapted for environmental applications by Sangion and Gramatica et al., (2016) [12]. Regression and classification techniques that link molecular descriptors to environmental fate parameters like log Kow, biodegradation half-lives, and ecotoxicity endpoints are included in the first category, QSAR and quantitative property–property relationship (QPPR) models. The second group includes deep learning and machine learning techniques such as random forest, gradient boosting, support vector machines, and graph neural networks that have been trained on physico-chemical property repositories or environmental monitoring datasets. The third group consists of mechanistic fate-and-transport models that mimic the physical, chemical, and biological processes controlling antibiotic fate from source to receptor. These models include fugacity-based multimedia compartment models, river basin hydrological models combined with chemical fate modules, and agent-based sediment transport frameworks.

2.2 Data Extraction and Quality Assessment.

The study location, target antibiotics and matrices, model type and algorithm, input variables, training/validation dataset size, performance metrics (R^2, RMSE, AUC-ROC, and Nash- Sutcliffe efficiency when reported), uncertainty reporting method, and availability of code or model outputs were all recorded in a standardized form. Risk of bias was assessed using a modified GRADE-EO framework adapted for environmental modeling studies by Pullin and Knight et al., (2001), evaluating methodological transparency, spatial and temporal representativeness of training data, and rigor of external validation procedures [13].

3. Results

3.1 QSAR and Molecular Descriptor-Based Models

Aqueous solubility, soil and sediment sorption coefficients (Kd/Koc), and algal or invertebrate ecotoxicity (EC50) were the most often simulated endpoints. A multitask deep neural network trained on 4,200 antibiotic structures from ChEMBL produced a mean absolute error (MAE) of 0.31 log units for aquatic toxicity prediction against Daphnia magna, outperforming classical partial least squares QSAR benchmarks by about 22%. Crucially, the multitask design enhanced generalization to structurally new fluoroquinolones that were not included in the training set, which was a recurring drawback of single-task QSAR models that depended on mechanistic analogies.

Li et al. (2023) used a random forest QSAR with 47 molecular descriptors and seven sediment physicochemical covariates (total organic carbon, clay content, pH, cation exchange capacity, and iron/aluminum oxide fractions) to model sorption behavior, which determines whether an antibiotic partitions into bioavailable aqueous phase or sequestrated sediment fractions. Compared to previous single-antibiotic-class QSAR models, their model obtained $R^2 = 0.89$ and RMSE = 0.34 log units on an external validation set covering sulfonamides, tetracyclines, macrolides, and fluoroquinolones over 14 soil types—a far wider chemical and pedological domain. The training data, however, were primarily obtained from batch equilibrium studies carried out at a single ionic strength, which the authors admitted could introduce systematic bias when applied to high-salinity estuarine or artificial wetland environments [15].

Liu et al. (2023) addressed photolytic transformation, a major attenuation pathway for fluoroquinolones, sulfonamides, and some tetracyclines in shallow, light-penetrable surface waters, by creating a QPPR that connected directly measured quantum yield values with 11 electronic descriptors derived from density functional theory (DFT). The model ($R^2 = 0.84$, LOO-CV $R^2 = 0.81$) demonstrated the usefulness of in silico screening to prioritize compounds for laboratory photolysis testing by predicting photodegradation half-lives for 63 developing antibiotic analogs without experimental quantum yield data. Reliance on solar irradiance parameterized for mid-latitude summer circumstances was identified as a drawback, requiring seasonal adjustment factors for Arctic or tropical applications [15].

3.2 Machine Learning Approaches

The most methodological variation was seen in machine-learning studies (n = 29; 43% of the corpus), which ranged from graph-convolutional neural networks to conventional ensemble approaches. Gradient-boosted decision tree (GBDT) algorithms, especially XGBoost and LightGBM, consistently showed better predictive accuracy for environmental concentration modeling among ensemble techniques. In order to predict downstream fluoroquinolone concentrations from upstream flow velocity, dissolved organic carbon, temperature, turbidity, and wastewater treatment plant discharge records, Lee et al. (2026) trained a LightGBM model on 8,760 hourly river antibiotic monitoring observations from seven monitoring stations in the Pearl River Delta. With far less parameterization work, the model beat a calibrated SWAT-based hydrological model at the same sites (NSE = 0.74), achieving a Nash–Sutcliffe efficiency (NSE) of 0.91 [16].

A more recent development is graph neural networks (GNNs), which eliminate the requirement for manually created descriptors by directly encoding antibiotic molecule topology as node and edge properties. For binary classification of aquatic acute toxicity (fish LC50 < 1 mg/L), Wang et al. (2024) showed that a directed message-passing neural network (D-MPNN) trained on the EPA's DSSTox database supplemented with 1,140 antibiotic-specific ecotoxicity measurements achieved an AUC-ROC of 0.93, outperforming random forest and support vector machine baselines by 8 and 11 percentage points, respectively [17]. Electron-withdrawing substituents on the aromatic core were found to be the primary structural determinants of high acute toxicity by Shapley additive explanation (SHAP) analysis, which is consistent with previous mechanistic knowledge of fluoroquinolone photosensitization mechanisms.

Müller et al. (2023) used the ChemBERTa language model architecture to assess transfer learning, which involves pre-training on large pharmacological property datasets before fine-tuning on smaller environmental datasets [18]. Compared to models trained from scratch on the same short dataset, fine-tuning on 620 antibiotic–environment paired observations increased biodegradation half-life prediction by 31%, indicating usefulness for domains with little environmental training data. Osei-Bonsu et al. (2024) used recurrent neural networks (LSTM architectures) to capture temporal autocorrelation in antibiotic monitoring time series from Ghana's Densu River, resulting in RMSE reductions of 18–27% compared to seasonal ARIMA benchmarks. This has practical implications for the design of real-time early warning systems in low-income country contexts [19].

3.3 Mechanistic Fate-and-Transport Models

The majority of the mechanistic models (n = 18; 26% of the corpus) were catchment-scale extensions of pre-existing hydrological modeling platforms that included pharmaceutical fate modules. Liu et al. (2023)

used the SWAT-CUP framework in conjunction with a first-order antibiotic transformation module at the Yangtze River tributary scale to simulate the fate of erythromycin, sulfamethoxazole, and ciprofloxacin over a ten-year period (2014–2023) under observed WWTP loading and river flow conditions [20]. The model underestimated peak concentrations during monsoon flushing events by up to 60% due to insufficient representation of resuspension-driven sediment-bound antibiotic release, but it replicated observed spatial concentration gradients for low-flow summer conditions with relative error below 25% after manual calibration against 48 monitoring observations.

In comparison to non-speciated formulations, the SimpleBox4Nano multimedia fugacity model, which was modified for ionic antibiotics by Domínguez-Moñino et al. (2023), used species-specific speciation chemistry (taking into account zwitterionic, cationic, and anionic antibiotic forms as a function of pH) to improve compartmental mass balance accuracy by 19% across freshwater scenarios in Europe [21]. Kapley et al. (2023) used coupled ocean-atmosphere modeling to project antibiotic loading to the Bay of Bengal under three socioeconomic scenarios (SSP1-2.6, SSP2-4.5, and SSP5-8.5), incorporating projected changes in antibiotic consumption and population-driven wastewater volumes through 2050. This is a methodological advancement that links pharmaceutical fate to climate scenario analysis that is uncommon in the literature [22].

3.4 Hybrid and Integrated Modeling Approaches

The most quickly expanding methodological category was hybrid models, which combined data-driven flexibility with mechanistic process insight. First-order photolysis and biodegradation kinetics were incorporated as soft constraints into a deep learning framework trained on sulfamethoxazole monitoring data from Korean rivers using a physics-informed neural network (PINN) architecture created by Park et al. (2024) [23]. In comparison to a solely data-driven LSTM (NSE = 0.87), the PINN obtained NSE = 0.94 while demonstrating superior extrapolation behavior under novel flow regime conditions. This is a significant practical advantage for regulatory scenario testing outside the observed data range. Similar to this, Hernandez-Fernandez et al. (2024) Bayesian network models allowed for joint uncertainty propagation from source to risk endpoint by conditionally linking sub-models for antibiotic loading, environmental fate, and ARG proliferation probability in a single probabilistic graphical structure. This methodological advancement is directly applicable to regulatory probabilistic risk assessment frameworks [23].

4. DISCUSSION

4.1 Comparative Model Performance in Global Context

According to the evidence compiled in this review, ensemble machine learning algorithms especially gradient-boosted tree ensembles and graph neural networks consistently outperform single-paradigm approaches across predictive endpoints, including sorption coefficients, dissolved antibiotic concentrations, and ecotoxicity endpoints. This trend is mostly in line with performance standards documented in the fields of environmental chemistry and pharmacokinetics. However, care must be taken when interpreting raw performance indicators. This corpus contains a large number of high-performance machine learning models that were validated either internally (cross-validation) or on test sets taken from the same temporal and spatial domain as training data. This practice inflates apparent accuracy when models are later applied to geographically or climatically different regions [24].

Despite lower average accuracy metrics in routine validation, mechanistic models perform better in extrapolation scenarios and extreme hydrological events because they encode domain- specific physical chemistry that data-driven models must infer implicitly from observations. Therefore, despite their lower statistical performance in retrospective fitting exercises, mechanistic models remain practically indispensable for regulatory applications requiring counterfactual scenario testing (e.g., assessing the concentration impact of new WWTP treatment technologies or projected land use change) [25].

4.2 Inconsistent Results and Model Failures

Significant variations in prediction performance were found between investigations. Wegst-Uhrich et al. (2014) attributed the high variance in Koc predictions (spanning two orders of magnitude across studies using similar descriptors) in QSAR models for tetracycline sorption to sediments to unresolved heterogeneity in sediment organic matter composition and the inadequate representation of cation-bridging sorption mechanisms in conventional descriptor sets [28]. In contrast to antibiotic concentration prediction, machine learning models applied to ARG proliferation prediction performed noticeably worse (median AUC-ROC = 0.72 versus 0.88 for concentration models). This is probably due to the additional complexity of microbiome community dynamics, horizontal gene transfer rates, and selection-coefficient non-linearity that are poorly captured by currently available training features [26].

5. Research Gaps and Limitations

Absence of ARG proliferation as a dynamic model output. Without connecting these to quantitative ARG selection results, the vast majority of models anticipate physicochemical destiny endpoints or dissolved antibiotic concentrations. Models that target human health risk through resistance selection rather than direct aquatic toxicity are desperately needed, as minimum selected concentrations for several antibiotic classes are now clearly below PNECs [31].

Geographic and taxonomic data imbalance. High-income, temperate catchments are consistently oversampled in training datasets. This gap could be partially filled without the need for politically complicated data-sharing agreements through federated learning architectures and data synthesis protocols that allow model training across jurisdictionally distinct datasets without centralizing sensitive environmental data [8].

Absence of real-time adaptive modeling systems. Although they are still in the prototype or proof-of-concept stages, operational early warning systems that combine near-real-time satellite-derived river flow, remote sensing-based land use data, and continuous biosensor antibiotic monitoring with predictive machine learning models are conceptually possible [32].

Inadequate representation of biological transformation pathways. Under aerobic sediment conditions, microbial biotransformation, a quantitatively significant attenuation pathway for sulfonamides and macrolides, is typically parameterized as a single first-order decay constant without mechanistic coupling to redox-stratified sediment biogeochemistry or microbial community structure [33].

Neglect of nanoplastic and microplastic co-contaminant interactions. Recent research indicates that nanoplastics and microplastic particles function as vectors that speed up the horizontal transport of ARG and alter the behavior of antibiotic sorption. Despite an increasing body of research on this interaction at the process level, no reviewed model included plastic-antibiotic co-contaminant dynamics [31].

Limited multi-contaminant mixture modeling. Despite persistent evidence that concentration addition models underestimate mixture toxicity at environmentally relevant ratios, risk evaluations seldom take into consideration the combined selective pressure of antibiotic mixtures. As Scholz et al. (2022) showed for pesticide mixtures, ML-based mixture toxicity prediction frameworks have not been methodically expanded to antibiotic resistance selection contexts [35].

Insufficient model validation against independent field datasets. External validation against geographically or temporally independent monitoring data was reported by less than 35% of the assessed machine learning models. Regulatory approval of computational predictions in chemical risk assessment workflows depends on community consensus on minimum validation criteria, which are comparable to the OECD QSAR validation principles [36].

6. CONCLUSION

This analysis shows that while computer modeling has significantly advanced as a prediction tool for assessing the danger of antibiotic residues in aquatic habitats, significant obstacles to regulatory implementation still exist. While mechanistic models continue to be indispensable for extrapolating to scenarios outside of reported data ranges, ensemble machine-learning models provide the highest retrospective predictive accuracy for concentration and ecotoxicity endpoints. Although more benchmarking against geographically varied validation datasets is necessary, hybrid physics-informed and Bayesian techniques show great potential in balancing these complementary strengths.

From a policy standpoint, the models' persistent underperformance in low- and middle-income country contexts highlights the necessity of international investment in standardized environmental monitoring infrastructure that can produce training data in the areas most impacted by rising antibiotic use. An existing policy architecture for incorporating predictive modeling tools into national pharmaceutical risk surveillance systems is provided by the World Health Organization's One Health AMR National Action Plan framework. It should specifically require computational risk prediction components in addition to conventional monitoring requirements.

Future research should focus on creating and adopting open benchmark datasets for model comparison, standardizing uncertainty reporting procedures to comply with regulatory probabilistic risk characterization requirements, incorporating ARG proliferation dynamics as a required predictive endpoint in aquatic environmental risk assessments, and expanding hybrid modeling techniques to catchment contexts in the tropical and Global South.

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