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Review

# Computational Veterinary Toxicology: A Translational Framework for One Health, Food Safety, and Antimicrobial Resistance

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## Abstract

The application of computational technologies in veterinary biochemistry and toxicology is revolutionizing translational science and making it more compatible with the One Health approach. With the distinction between animal, human, and environmental health diminishing in importance, technologies like molecular modelling, systems toxicology, vetinformatics, and artificial intelligence (AI) help in making integrated and predictive decisions. This brief review aims to highlight advancements in computational veterinary biochemistry and toxicology with special emphasis on its importance for One Health, food safety, and antimicrobial resistance (AMR). Advances in predictive toxicology, multi-omics, and AI offer new and innovative solutions for the early detection of biochemical disorders, simulation of toxicant exposure, and prediction of AMR in different species. These advancements highlight the importance of making connections between laboratory science and policy-making for animal health with the help of a multidisciplinary computational approach for global food security and AMR in a data-driven world.

**Keywords:** computational toxicology; vetinformatics; one health; food safety; antimicrobial resistance; translational veterinary biochemistry; systems modelling; predictive analytics

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## 1. Introduction

Significant transformation in the field of translational veterinary biochemistry and toxicology has been witnessed over the past two decades, primarily owing to the digital revolution in biomedical, environmental, and life sciences. Traditionally, veterinary biochemistry and toxicology were primarily descriptive in nature, with a focus on the identification of biochemical abnormalities and toxicity in animals, primarily based on empirical observations and *in vivo* studies. Although the traditional approach has provided a foundation for veterinary toxicology, it was always limited in its scope. However, veterinary biochemistry and toxicology are currently influenced by a variety of computational strategies, primarily based on the integration of molecular mechanisms and population outcomes, thus promoting the concept of One Health, which emphasizes the intrinsic interrelatedness of human, animal, and environmental health. [1,2].

This paradigm shift has become more imperative in the wake of emerging issues like antimicrobial resistance (AMR), food contamination, agricultural intensification, and environmental degradation. The aforementioned issues are not independent of one another; rather, they are the culmination of intricate biochemical and microbial interactions that share common ecosystems [3]. Therefore, veterinary science needs to be advanced beyond species-specific evaluations and embrace integrative tools that bridge the link between biochemical events and public health outcomes.

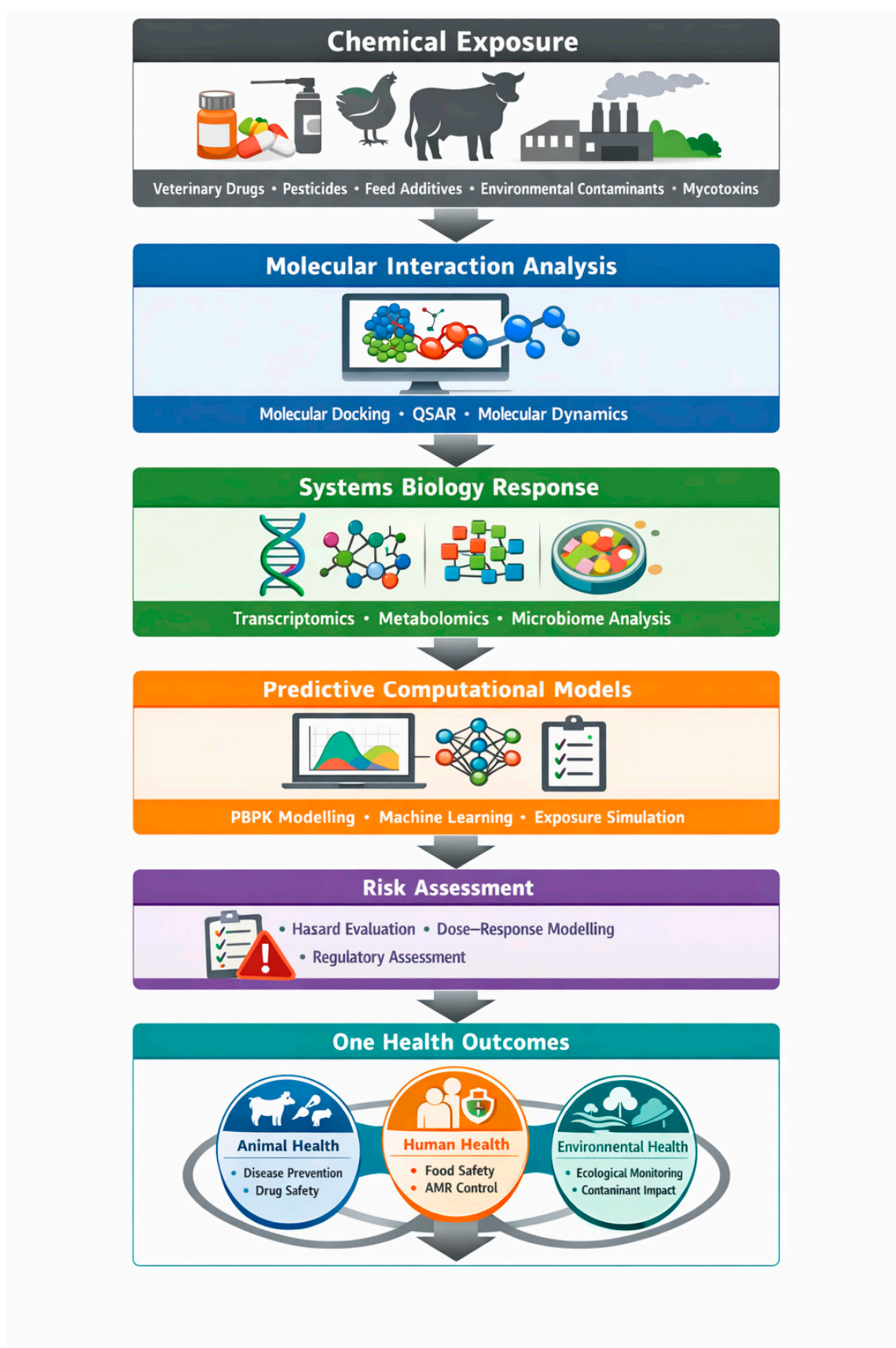
The One Health concept has been established as an important guiding philosophy to address these crises. The globalisation of food production systems, the intensification of animal production systems, and environmental changes due to climate change have resulted in an increased risk of chemical exposure, pathogen transmission, and the emergence of resistance. These events occur

through the action of common biochemical mechanisms that involve the use of similar targets and routes of exposure among species [4]. Veterinary biochemistry and toxicology play an important role as they offer mechanistic explanations that have direct implications for food safety, occupational health and safety, environmental toxicology, and human health risk assessment.

At the heart of the change in the disciplinary approach is the concept of computational toxicology. With the aid of *in silico* tools that can forecast the hazards of chemicals, their toxicokinetics, and their biological effects in various species, it is now possible to move away from the identification of hazards and towards the prediction of risk. Techniques that allow for the use of physiologically based pharmacokinetic modeling, quantitative structure-activity relationships, network toxicology, and adverse outcome pathways offer mechanistic continuity between the molecular initiating events and adverse outcomes [5]. Most importantly, they minimize the use of animal testing and thus meet the ethical and economic needs of veterinary toxicology.

Parallel to these advancements, vetinformatics, bioinformatics, systems biology, and computational veterinary science have revolutionized the field of biochemical regulation in livestock and companion animals. These techniques include transcriptomics, proteomics, metabolomics, and microbiomics data integration to identify relevant information on biomarkers and risk factors for various applications in toxicology, nutrition, and infectious diseases [6]. These computational techniques enable scientists to simulate how xenobiotics, antibiotics, and environmental pressures affect metabolic networks, immune systems, and gene expression profiles, providing predictive information from individual to population levels [7].

Significantly, computational methods in veterinary biochemistry and toxicology are no longer confined to conducting research in laboratories. These methods are increasingly being used to shape regulatory science, surveillance systems, and global health governance under the One Health approach. For instance, AI-based analytics enable the timely recognition of AMR determinants, forecasts of drug-toxin interactions, and tracking of chemical contaminants along food chains [8,9]. In this regard, computational toxicology is not only a scientific approach but a “translating bridge” between molecular science and health and well-being on a planetary scale (Figure 1).



**Figure 1.** Computational framework for translational veterinary toxicology within the One Health Paradigm.

## 2. Computational Strategies in Veterinary Biochemistry and Toxicology

Computational methodologies have become indispensable to modern veterinary biochemistry and toxicology, enabling high-throughput analysis, multidimensional data integration, and predictive modelling. These tools address long-standing challenges in the field, including experimental variability, species extrapolation, and the ethical limitations of extensive *in vivo* testing (Table 1).

**Table 1.** Key Computational Approaches in Veterinary Toxicology.

Method	Application	Example
QSAR	Predict chemical toxicity	Feed additives
PBPK	Tissue residue modelling	Veterinary drugs
Molecular docking	Drug–target interactions	Transporter inhibition
Toxicogenomics	Biomarker discovery	Hepatotoxicity
AI / ML	AMR prediction	Antibiotic resistance

### 2.1. Vetinformatics and Systems Integration

Vetinformatics represents the convergence of veterinary science, systems biology, and computational modelling to decode complex molecular interactions underlying animal health, disease progression, and toxicant exposure. According to Pathak and Kim (2023), vetinformatics integrates comparative genomics, transcriptomic profiling, proteomic mapping, and metabolic network reconstruction, tailored to the physiological and biochemical diversity of animal species. The integration of multi-omics datasets has been particularly transformative. Combining genomic, proteomic, metabolomic, and microbiome data, researchers can reconstruct toxicity pathways and identify regulatory nodes affected by chemical exposure. Systems-based analyses can, for example, elucidate how environmental contaminants disrupt hepatic xenobiotic metabolism or interfere with endocrine signalling in food-producing animals, with downstream consequences for productivity, reproduction, and food safety [10,11]. These insights support the development of molecular biomarkers for exposure assessment, early disease detection, and risk stratification.

Computational annotation tools further facilitate cross-species translation of biochemical pathways. This capability is especially important in veterinary toxicology, where data availability varies widely across species. Model organisms such as rodents or zebrafish are frequently used to infer toxicological effects in livestock species. Comparative systems biology approaches enable informed extrapolation by accounting for species-specific differences in metabolism, enzyme expression, and physiological parameters [12].

### 2.2. Predictive and Computational Toxicology

Predictive toxicology employs computational techniques to anticipate biological effects of chemicals prior to *in vivo* testing. Central to this approach are QSAR models, machine learning classifiers, and PBPK simulations that collectively describe absorption, distribution, metabolism, and excretion. As highlighted by Thomas et al. (2019), predictive toxicology is increasingly integral to translational risk assessment, enabling efficient hazard prioritisation for veterinary medicines, feed additives, and environmental contaminants.

PBPK modelling is particularly valuable in veterinary contexts, as it incorporates species-specific physiological parameters such as organ size, blood flow, and enzyme activity. These models simulate time-dependent xenobiotic concentrations in target tissues, facilitating cross-species extrapolation where experimental data are limited [13,14]. Integration of PBPK models with AOP frameworks establishes mechanistic continuity between molecular interactions, such as receptor binding or enzyme inhibition, and adverse outcomes, including hepatotoxicity, endocrine disruption, or neurotoxicity.

Recent advances in artificial intelligence have further accelerated predictive toxicology. Deep learning architectures trained on large chemical and biological datasets can predict toxicity endpoints, metabolic liabilities, and genotoxic potential with increasing accuracy. In antimicrobial development, these models are particularly valuable for forecasting off-target effects, environmental persistence, and selective pressures that contribute to AMR emergence [15–17].

### 2.3. Computational Pharmacology and Drug–Toxin Interaction Modelling

Computational pharmacology has reshaped toxicological risk assessment in veterinary medicine by enabling atomic-level analysis of drug–target and toxin–target interactions. Techniques such as molecular docking, pharmacophore modelling, and molecular dynamics simulations provide detailed insights into how small molecules interact with detoxification enzymes, transporters, and nuclear receptors, including cytochrome P450 isoforms and ABC transport proteins [18–20].

With these interactions between veterinary drugs and metabolic enzymes, researchers can predict potential drug–toxin synergies, metabolic inhibition, or altered clearance pathways that may lead to adverse effects. For example, *in silico* docking studies can assess whether antibiotic residues interact with hepatic receptors or transporters, potentially affecting detoxification capacity in food-producing animals. Those insights are critical for maintaining residue levels within regulatory limits and safeguarding consumer health [21].

### 2.4. Data-Driven Toxicogenomics

Toxicogenomics has become a cornerstone of mechanistic toxicology, enabling systematic characterisation of gene expression responses to chemical exposure. Computational analysis of toxicogenomic datasets allows comparison of transcriptomic signatures across compounds, doses, and exposure scenarios, revealing conserved pathways associated with stress responses, inflammation, or organ-specific injury [22].

Machine learning algorithms increasingly support biomarker discovery within these datasets. Methods such as random forests and neural networks can identify gene expression patterns predictive of hepatotoxicity, nephrotoxicity, or endocrine disruption. These computational biomarkers can subsequently be validated experimentally, enhancing translational confidence while reducing animal use [23].

Comparative toxicogenomics further strengthens the One Health framework by identifying conserved molecular responses across species. Shared transcriptional signatures enable extrapolation of veterinary or environmental exposure data to human health risk assessment, embodying the translational ethos of modern toxicology [24].

### 2.5. Environmental and Food Chain Modelling

Veterinary toxicology increasingly encompasses environmental and food system dimensions. Computational models describing environmental fate, exposure dynamics, and bioaccumulation are essential for assessing the broader impact of veterinary medicines, pesticides, and feed additives. These models evaluate not only animal safety but also ecological and human health risks associated with chemical residues in soil, water, and food products [25].

Integration of geographic information systems (GIS) and spatial modelling enhances detection of exposure hotspots and prediction of contaminant migration. When combined with toxicokinetic and toxicodynamic models, these tools provide a comprehensive view of risk across the One Health continuum, linking biochemical mechanisms to population-level outcomes [26,27].

## 3. Translational Applications within the One Health Framework

The One Health framework emphasises the interconnectedness of biological systems across species and environments. Translational computational approaches are central to operationalising

this concept, transforming molecular toxicological data into actionable insights for surveillance, regulation, and public health intervention [28,29].

Veterinary toxicology serves as a critical interface between animal exposure and human health outcomes. Traditionally, toxicological data derived from animals were often isolated from human risk assessment processes [30]. Computational approaches now enable bidirectional translation, allowing animal-derived molecular data to inform human toxicology and vice versa. Integrated surveillance systems combining veterinary diagnostics, food safety monitoring, and public health databases represent a major achievement in this regard. Machine learning-based pattern recognition enables early detection of AMR emergence, chemical contamination, and zoonotic spillover, facilitating timely intervention [31].

Computational toxicology also underpins predictive epidemiology by enabling simulation of disease emergence driven by chemical, microbial, or ecological factors. Models integrating exposure data, toxic effects, and microbial evolution can identify AMR hotspots in animal production systems. Probabilistic risk models, supported by Bayesian inference and Monte Carlo simulations, quantify uncertainty and enable transparent decision-making within One Health policy frameworks [32].

AMR represents a paradigmatic One Health challenge. Computational biochemistry and toxicology elucidate resistance mechanisms at both the molecular and systems levels. AI-driven models integrate genomic, biochemical, and environmental data to predict resistance emergence and assess the co-selective effects of non-antibiotic stressors such as heavy metals and biocides [33,34]. PBPK and environmental exposure models further support risk-based prioritisation of compounds likely to promote resistance [35].

#### 4. Computational Toxicology and Food Contaminant Assessment

Computational toxicology provides a predictive framework for evaluating feed additives, veterinary medicines, and food contaminants. QSAR, PBPK, and molecular docking approaches enable early hazard identification, residue prediction, and regulatory compliance assessment, particularly in food-producing animals [40–44]. PBPK models are especially valuable for predicting tissue-residue depletion and for establishing withdrawal periods in accordance with regulatory frameworks, such as maximum residue limits. Computational models also intersect with food microbiology by simulating microbial growth, toxin production, and contamination dynamics across the farm-to-fork continuum [45–47].

Network-based models trace AMR gene flow across livestock, processing environments, and ecosystems. When integrated with ecotoxicological data, these models quantify the role of chemical stressors in co-selection for resistance [48–50]. Machine learning models further support AMR risk prioritisation by integrating molecular, environmental, and epidemiological data to rank threats by public health impact [51].

#### 5. Conclusion

Translational computational strategies have fundamentally redefined veterinary biochemistry and toxicology. Once primarily descriptive, these disciplines are now predictive, integrative, and central to the One Health agenda. Computational tools bridge molecular mechanisms with food safety, environmental protection, and global AMR surveillance. Future progress will depend on ethical governance, open science, and equitable access to computational infrastructure. In this evolving landscape, computational toxicology functions not merely as a methodological advance but as a translational conduit linking scientific knowledge to planetary health stewardship.

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