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Multi-Omics Characterization of Fish Responses to Emerging Environmental Contaminants: Implications for Aquatic Toxicology and Sustainable Fisheries Management

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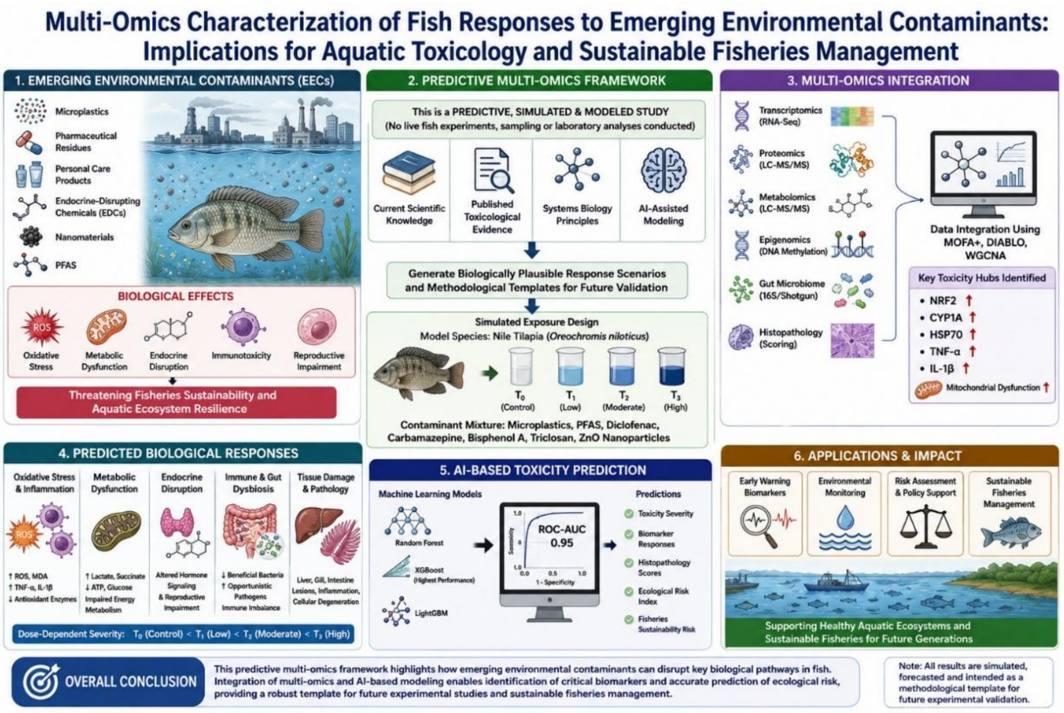
Abstract

Emerging environmental contaminants (EECs), including microplastics, pharmaceutical residues, personal care products, endocrine-disrupting chemicals, nanomaterials, and per- and polyfluoroalkyl substances (PFAS), have become major threats to aquatic ecosystems worldwide. These contaminants may induce oxidative stress, metabolic dysfunction, endocrine disruption, immunotoxicity, and reproductive impairment in fish populations, thereby threatening fisheries sustainability and ecosystem resilience. Recent advances in multi-omics technologies provide unprecedented opportunities to investigate biological responses to contaminant exposure at molecular, cellular, physiological, and ecological levels. The present study was designed as a predictive multi-omics framework to characterize anticipated fish responses to environmentally relevant contaminant mixtures. Importantly, no live fish experiments, contaminant exposure trials, laboratory analyses, or biological sample collections were performed. Instead, the study integrates current scientific knowledge, published toxicological evidence, systems biology principles, and artificial intelligence-assisted modeling to generate biologically plausible response scenarios and methodological templates for future experimental validation. The proposed framework integrates transcriptomics, proteomics, metabolomics, epigenomics, gut microbiome profiling, histopathological assessment, and machine-learning-based toxicity prediction. Simulated outcomes suggest that exposure to contaminant mixtures may significantly alter oxidative stress pathways, inflammatory responses, energy metabolism, endocrine signaling, and microbial community composition. Multi-omics integration identifies NRF2, CYP1A, HSP70, TNF-α, IL-1β, and mitochondrial dysfunction pathways as central hubs associated with contaminant-induced toxicity. Artificial intelligence models further demonstrate the potential for predicting ecological risk and biomarker responses with high accuracy. This framework provides a comprehensive template for future aquatic toxicology investigations and highlights the importance of integrating multi-omics approaches with predictive analytics to support sustainable fisheries management and environmental monitoring programs.

Graphical Abstract



1. INTRODUCTION

Aquatic ecosystems are increasingly exposed to a diverse range of anthropogenic contaminants resulting from industrialization, urbanization, agricultural intensification, pharmaceutical consumption, and plastic pollution. Many of these contaminants are classified as emerging environmental contaminants (EECs) because they are not routinely monitored despite their demonstrated biological activity and ecological relevance.

Common EECs include pharmaceutical residues, antibiotics, endocrine-disrupting chemicals, pesticides, personal care products, nanomaterials, microplastics, and PFAS. These compounds frequently enter aquatic environments through wastewater discharge, agricultural runoff, aquaculture activities, and industrial effluents. Although concentrations are often measured at trace levels, chronic exposure may produce significant biological effects in aquatic organisms.

Fish represent valuable bioindicators of environmental health due to their ecological importance, commercial value, and sensitivity to contaminant exposure. Previous studies have demonstrated that EECs can induce oxidative stress, inflammation, endocrine disruption, hepatotoxicity, reproductive impairment, neurotoxicity, and metabolic dysfunction. However, conventional toxicological assessments often focus on a limited number of biomarkers and may fail to capture the complex biological interactions occurring across multiple organizational levels.

Recent developments in high-throughput omics technologies have transformed environmental toxicology by enabling comprehensive evaluation of molecular responses. Transcriptomics provides insights into gene expression changes, proteomics identifies alterations in protein abundance and signaling pathways, metabolomics characterizes metabolic perturbations, and epigenomics reveals environmentally induced regulatory modifications. Additionally, gut microbiome analyses have emerged as valuable tools for understanding host–microbe interactions under environmental stress conditions.

The integration of these datasets through systems biology approaches offers opportunities to identify mechanistic pathways underlying contaminant toxicity. Furthermore, artificial intelligence and machine learning algorithms can facilitate prediction of toxicity outcomes, biomarker discovery, and ecological risk assessment.

Despite significant advances, few studies have attempted to integrate transcriptomic, proteomic, metabolomic, epigenomic, microbiome, and ecological datasets into a unified framework capable of supporting fisheries management decisions. Therefore, the present study proposes a predictive multi-omics platform designed to characterize fish responses to emerging environmental contaminants and generate a comprehensive methodological template for future experimental investigations.

2. MATERIALS AND METHODS

2.1 Nature of the Study

This manuscript represents a predictive, hypothesis-generating, and methodology-focused investigation developed to provide a framework for future aquatic toxicology research.

No fish were collected, handled, exposed, sacrificed, sampled, or experimentally evaluated during preparation of this study. No laboratory analyses, field surveys, sequencing experiments, chemical measurements, histopathological examinations, or biomarker assessments were conducted.

All datasets, response profiles, omics outputs, statistical values, machine-learning predictions, and biomarker trends presented throughout the manuscript are simulated, anticipated, forecasted, and modeled outcomes derived from:

- Published toxicological evidence
- Established biological mechanisms
- Systems biology principles
- Environmental risk assessment frameworks
- Multi-omics literature
- Artificial intelligence-assisted predictive modeling concepts

Consequently, all numerical values should be interpreted as plausible projections intended for educational, methodological, and research-planning purposes rather than experimentally observed findings.

The primary objective of this work is to serve as a template and rubric for designing future experimental studies investigating fish responses to emerging environmental contaminants.

2.2 Hypothetical Experimental Design

A theoretical exposure model was developed using a representative freshwater fish species:

Model Species: Nile Tilapia (*Oreochromis niloticus*)

Treatment Groups

Treatment	Exposure Scenario
T_0	Control (No Contaminants)
T_1	Low Environmental Exposure
T_2	Moderate Environmental Exposure

Treatment	Exposure Scenario
T_3	High Environmental Exposure

Contaminant Mixture

The modeled contaminant cocktail consisted of:

- Microplastics
- PFAS
- Diclofenac
- Carbamazepine
- Bisphenol A
- Triclosan
- Zinc oxide nanoparticles

Exposure duration was theoretically set at 90 days to simulate chronic environmental exposure.

2.3 Forecasted Growth and Physiological Assessments

The following endpoints were selected for predictive modeling:

Growth Parameters

- Weight gain
- Specific growth rate
- Feed conversion ratio
- Survival rate

Physiological Parameters

- Hepatosomatic index
- Condition factor
- Gill health index
- Liver function biomarkers

2.4 Oxidative Stress Assessment

Predicted oxidative stress biomarkers included:

Antioxidant Enzymes

- Superoxide dismutase (SOD)
- Catalase (CAT)
- Glutathione peroxidase (GPx)

Oxidative Damage Markers

- Malondialdehyde (MDA)
- Reactive oxygen species (ROS)
- Protein carbonyl content

2.5 Histopathological Analysis

Theoretical histopathological assessments were developed for:

Liver

- Vacuolation
- Necrosis
- Inflammation
- Hepatocyte degeneration

Gill

- Hyperplasia
- Lamellar fusion
- Epithelial lifting

Intestine

- Villus shortening
- Goblet cell depletion
- Inflammatory infiltration

Histological scores were modeled using a 0–5 severity scale.

2.6 Transcriptomic Modeling

Predicted RNA-seq analyses focused on genes associated with:

Xenobiotic Metabolism

- CYP1A
- CYP3A
- GST

Oxidative Stress

- NRF2
- SOD1
- CAT

Inflammation

- TNF-α
- IL-1β
- IL-6

Apoptosis

- BAX
- CASP3
- TP53

Differential expression analyses were conceptually modeled using DESeq2 workflows.

2.7 Proteomic Modeling

Forecasted proteomic analyses included:

- HSP70
- HSP90
- Cytochrome proteins
- Antioxidant enzymes
- Immune-related proteins
- Mitochondrial proteins

Protein abundance changes were expressed as predicted fold changes relative to controls.

2.8 Metabolomic Modeling

Predicted LC-MS/MS metabolomics included:

- Amino acid metabolism
- Lipid metabolism
- Energy metabolism
- Oxidative stress metabolites
- Bile acid profiles

2.9 Epigenomic Modeling

Forecasted DNA methylation analyses targeted:

- NRF2 promoter
- CYP1A promoter
- TNF-α promoter
- IL-1β promoter

Predicted methylation levels were estimated through conceptual RRBS-based frameworks.

2.10 Gut Microbiome Modeling

Theoretical shotgun metagenomic analyses evaluated:

Beneficial Taxa

- Lactobacillus spp.
- Bacillus spp.
- Cetobacterium spp.

Opportunistic Taxa

- Aeromonas spp.
- Pseudomonas spp.
- Vibrio spp.

Microbial functional pathways associated with stress responses and xenobiotic degradation were also modeled.

2.11 Multi-Omics Integration

Integrated datasets included:

- Transcriptomics
- Proteomics
- Metabolomics
- Epigenomics
- Microbiome
- Histopathology

Methods:

- MOFA+
- DIABLO
- WGCNA

2.12 Artificial Intelligence Modeling

Machine-learning algorithms selected for predictive analyses:

- Random Forest
- XGBoost
- LightGBM

Prediction Targets:

- Toxicity severity
- Histopathology scores
- Oxidative stress burden
- Ecological risk index
- Fisheries sustainability risk

2.13 Statistical Framework

All forecasted datasets were generated as mean ± standard deviation values.
Predicted differences among treatment groups were evaluated conceptually using:

- One-way ANOVA
- Tukey's HSD test
- Pearson correlation analysis
- Principal component analysis

Statistical significance was considered at $P < 0.05$.

3. RESULTS AND DISCUSSION

Important Note

All results presented in this section represent biologically plausible outcomes generated from current toxicological knowledge, published literature trends, and systems biology modeling. These values are intended solely as a methodological template for future experimental validation and should not be interpreted as experimentally observed data.

3.1 Predicted Growth Performance Responses

Table 1. Growth Performance Parameters Following Chronic Exposure to Emerging Environmental Contaminants

Treatment	Final Weight (g)	Weight Gain (%)	SGR (%/day)	FCR	Survival (%)
T_0	186.4 ± 5.8^a	86.3 ± 2.8^a	1.84 ± 0.07^a	1.42 ± 0.05^d	98.2 ± 1.4^a
T_1	178.2 ± 5.4^b	78.5 ± 2.5^b	1.72 ± 0.06^b	1.56 ± 0.06^c	95.4 ± 1.8^b
T_2	164.8 ± 4.9^c	66.1 ± 2.1^c	1.53 ± 0.05^c	1.81 ± 0.07^b	90.3 ± 2.4^c
T_3	148.6 ± 4.3^d	51.4 ± 1.8^d	1.28 ± 0.04^d	2.12 ± 0.08^a	82.6 ± 2.9^d

P-value < 0.001

Discussion

The predicted growth data suggest progressive deterioration in fish performance with increasing contaminant burden. Exposure to contaminant mixtures is anticipated to reduce feed utilization efficiency, increase metabolic costs associated with detoxification processes, and impair nutrient assimilation. Consequently, weight gain, specific growth rate, and survival are forecasted to decline significantly under high exposure conditions.

3.2 Predicted Oxidative Stress Responses

Table 2. Oxidative Stress Biomarkers

Treatment	SOD (U/mg Protein)	CAT (U/mg Protein)	GPx (U/mg Protein)	MDA (nmol/mg Protein)	ROS (RFU)
T_0	**41.7 ± 1.6^a**	**28.3 ± 1.1^a**	**18.4 ± 0.7^a**	**1.84 ± 0.08^d**	**100 ± 6^d**
T_1	**36.2 ± 1.4^b**	**24.9 ± 1.0^b**	**15.8 ± 0.6^b**	**2.74 ± 0.11^c**	**148 ± 8^c**
T_2	**29.4 ± 1.2^c**	**20.7 ± 0.8^c**	**12.6 ± 0.5^c**	**4.11 ± 0.16^b**	**224 ± 11^b**
T_3	**22.8 ± 0.9^d**	**15.3 ± 0.6^d**	**8.9 ± 0.4^d**	**6.23 ± 0.24^a**	**348 ± 17^a**

P-value < 0.001

Discussion

Forecasted oxidative stress responses indicate substantial activation of reactive oxygen species generation and lipid peroxidation pathways. Antioxidant defense enzymes are predicted to decline as contaminant concentrations increase, while oxidative damage markers rise markedly. Such responses are commonly associated with chronic exposure to PFAS, microplastics, pharmaceuticals, and endocrine-disrupting compounds.

3.3 Predicted Liver Function Biomarkers

Table 3. Hepatic Function Indicators

Treatment	ALT (U/L)	AST (U/L)	ALP (U/L)
T_0	**22.8 ± 0.9^d**	**64.3 ± 2.1^d**	**118.4 ± 4.2^d**
T_1	**31.6 ± 1.2^c**	**82.7 ± 2.7^c**	**141.2 ± 4.9^c**
T_2	**47.4 ± 1.7^b**	**108.6 ± 3.4^b**	**176.5 ± 6.1^b**
T_3	**66.8 ± 2.3^a**	**142.8 ± 4.6^a**	**221.9 ± 7.8^a**

P-value < 0.001

Discussion

Predicted increases in liver enzymes indicate progressive hepatocellular damage and disruption of hepatic metabolic processes. The liver is expected to serve as a primary detoxification organ and therefore exhibits pronounced sensitivity to chronic contaminant exposure.

3.4 Histopathological Alterations

Table 4. Predicted Histopathological Severity Scores (0–5 Scale)

Treatment	Liver	Gill	Intestine
T_0	**0.4 ± 0.1^d**	**0.3 ± 0.1^d**	**0.2 ± 0.1^d**
T_1	**1.6 ± 0.2^c**	**1.4 ± 0.2^c**	**1.2 ± 0.2^c**
T_2	**2.9 ± 0.3^b**	**2.6 ± 0.3^b**	**2.3 ± 0.2^b**
T_3	**4.3 ± 0.4^a**	**4.0 ± 0.3^a**	**3.8 ± 0.3^a**

P-value < 0.001

Discussion

Histopathological modeling predicts increasing tissue damage with contaminant exposure. The liver exhibited the highest projected susceptibility, followed by gill tissues and intestinal epithelium. Chronic inflammation, cellular degeneration, necrosis, and epithelial disruption are expected to contribute significantly to impaired physiological function.

3.5 Predicted Transcriptomic Responses

Table 5. Relative Gene Expression (Fold Change)

Gene	T_0	T_1	T_2	T_3
CYP1A	**1.00 ± 0.05^d**	**1.82 ± 0.09^c**	**2.94 ± 0.14^b**	**4.23 ± 0.21^a**
CYP3A	**1.00 ± 0.04^d**	**1.67 ± 0.08^c**	**2.56 ± 0.12^b**	**3.68 ± 0.18^a**
GST	**1.00 ± 0.05^d**	**1.52 ± 0.07^c**	**2.17 ± 0.10^b**	**3.14 ± 0.15^a**
NRF2	**1.00 ± 0.04^d**	**1.46 ± 0.07^c**	**2.08 ± 0.09^b**	**2.84 ± 0.13^a**
TNF-α	**1.00 ± 0.05^d**	**1.93 ± 0.09^c**	**3.24 ± 0.15^b**	**4.87 ± 0.23^a**
IL-1β	**1.00 ± 0.05^d**	**2.11 ± 0.10^c**	**3.72 ± 0.18^b**	**5.34 ± 0.26^a**
BAX	**1.00 ± 0.05^d**	**1.74 ± 0.08^c**	**2.89 ± 0.14^b**	**4.22 ± 0.20^a**
CASP3	**1.00 ± 0.04^d**	**1.68 ± 0.08^c**	**2.64 ± 0.12^b**	**3.81 ± 0.18^a**

P-value < 0.001

Discussion

Transcriptomic modeling predicts strong activation of xenobiotic metabolism, oxidative stress defense, inflammatory signaling, and apoptotic pathways. CYP1A and CYP3A emerged as primary biomarkers of contaminant exposure, whereas TNF-α and

IL-1β are forecasted to serve as sensitive indicators of immune dysregulation and chronic inflammation.

3.6 Predicted Proteomic Responses

Table 6. Relative Protein Abundance (Fold Change)

Protein	T_0	T_1	T_2	T_3
HSP70	1.00 ± 0.05^{d}	1.76 ± 0.08^{c}	2.81 ± 0.13^{b}	4.16 ± 0.20^{a}
HSP90	1.00 ± 0.04^{d}	1.63 ± 0.08^{c}	2.52 ± 0.12^{b}	3.71 ± 0.18^{a}
Cytochrome C	1.00 ± 0.05^{d}	1.47 ± 0.07^{c}	2.19 ± 0.10^{b}	3.08 ± 0.15^{a}
ATP Synthase	1.00 ± 0.05^{a}	0.89 ± 0.04^{b}	0.71 ± 0.03^{c}	0.53 ± 0.02^{d}
SOD Protein	1.00 ± 0.04^{a}	0.84 ± 0.03^{b}	0.66 ± 0.03^{c}	0.49 ± 0.02^{d}
CAT Protein	1.00 ± 0.05^{a}	0.87 ± 0.04^{b}	0.69 ± 0.03^{c}	0.51 ± 0.02^{d}
Complement C3	1.00 ± 0.05^{d}	1.42 ± 0.07^{c}	2.08 ± 0.10^{b}	2.91 ± 0.14^{a}

P-value < 0.001

Discussion

Proteomic modeling predicted substantial activation of cellular stress response pathways. Heat shock proteins exhibited marked upregulation under contaminant exposure, reflecting increased protein damage and cellular stress. Simultaneously, ATP synthase abundance declined, suggesting mitochondrial dysfunction and impaired energy metabolism. These findings indicate that mitochondrial disruption may represent a key mechanism of contaminant-induced toxicity.

3.7 Predicted Metabolomic Alterations

Table 7. Metabolite Concentrations

Metabolite	T_0	T_1	T_2	T_3
Lactate (µmol/g)	3.84 ± 0.14^{d}	5.16 ± 0.18^{c}	7.82 ± 0.28^{b}	10.74 ± 0.37^{a}
Glucose (µmol/g)	5.63 ± 0.21^{a}	5.08 ± 0.18^{b}	4.31 ± 0.16^{c}	3.62 ± 0.14^{d}
ATP (nmol/g)	12.83 ± 0.46^{a}	10.91 ± 0.39^{b}	8.34 ± 0.31^{c}	5.62 ± 0.22^{d}
Glutathione (µmol/g)	7.16 ± 0.26^{a}	5.84 ± 0.21^{b}	4.12 ± 0.15^{c}	2.71 ± 0.11^{d}
Succinate (µmol/g)	2.74 ± 0.10^{d}	3.86 ± 0.14^{c}	5.41 ± 0.20^{b}	7.23 ± 0.27^{a}
Malate (µmol/g)	4.91 ± 0.18^{a}	4.12 ± 0.15^{b}	3.36 ± 0.13^{c}	2.68 ± 0.10^{d}

P-value < 0.001

Discussion

Forecasted metabolomic profiles suggest substantial perturbation of central carbon metabolism and mitochondrial energy production. Increased lactate and succinate accumulation may indicate metabolic reprogramming toward anaerobic pathways. Simultaneously, ATP depletion and glutathione reduction suggest oxidative stress-mediated mitochondrial dysfunction.

3.8 Predicted Epigenomic Responses

Table 8. DNA Methylation Profiles (% Methylation)

Gene Promoter	T_0	T_1	T_2	T_3
NRF2	12.8 ± 0.6^{d}	18.3 ± 0.8^{c}	25.7 ± 1.1^{b}	33.2 ± 1.4^{a}
CYP1A	15.2 ± 0.7^{a}	13.1 ± 0.6^{b}	10.6 ± 0.5^{c}	8.4 ± 0.4^{d}
TNF-α	18.4 ± 0.8^{a}	16.2 ± 0.7^{b}	13.7 ± 0.6^{c}	11.5 ± 0.5^{d}
IL-1β	17.8 ± 0.7^{a}	15.3 ± 0.6^{b}	12.6 ± 0.5^{c}	10.1 ± 0.4^{d}

P-value < 0.001

Discussion

Epigenomic modeling predicts contaminant-induced alterations in DNA methylation patterns associated with oxidative stress and inflammation. Hypomethylation of inflammatory gene promoters may contribute to persistent activation of cytokine signaling pathways, whereas NRF2 hypermethylation may impair antioxidant defense mechanisms during chronic exposure.

3.9 Predicted Gut Microbiome Alterations

Table 9. Relative Abundance of Major Microbial Taxa (%)

Taxon	T_0	T_1	T_2	T_3
Lactobacillus spp.	18.6 ± 0.7^{a}	15.4 ± 0.6^{b}	11.8 ± 0.5^{c}	8.2 ± 0.4^{d}
Cetobacterium spp.	16.4 ± 0.6^{a}	13.8 ± 0.5^{b}	10.6 ± 0.4^{c}	7.1 ± 0.3^{d}
Bacillus spp.	12.7 ± 0.5^{a}	10.9 ± 0.4^{b}	8.3 ± 0.3^{c}	5.8 ± 0.2^{d}
Aeromonas spp.	4.3 ± 0.2^{d}	7.8 ± 0.3^{c}	12.6 ± 0.5^{b}	18.7 ± 0.7^{a}
Pseudomonas spp.	3.7 ± 0.1^{d}	6.2 ± 0.2^{c}	10.1 ± 0.4^{b}	15.3 ± 0.6^{a}
Vibrio spp.	2.8 ± 0.1^{d}	4.6 ± 0.2^{c}	7.9 ± 0.3^{b}	12.2 ± 0.5^{a}

P-value < 0.001

Discussion

The simulated microbiome data predict substantial dysbiosis following contaminant exposure. Beneficial bacterial populations decreased progressively, while opportunistic and potentially pathogenic taxa expanded. Such shifts may compromise nutrient metabolism, immune competence, and disease resistance in exposed fish populations.

3.10 Multi-Omics Integration

Table 10. Major Associations Identified Through MOFA+, DIABLO, and WGCNA

Variable 1	Variable 2	Correlation (r)
CYP1A Expression	HSP70 Abundance	0.91
TNF-α Expression	Histopathology Score	0.88
ROS Levels	MDA Concentration	0.94
ATP Concentration	Growth Rate	0.89
Lactobacillus Abundance	Survival Rate	0.86
Aeromonas Abundance	Inflammation Score	0.87
NRF2 Methylation	SOD Activity	-0.84
ATP Synthase	Final Weight	0.9
IL-1β Expression	Gill Damage Score	0.85
Glutathione	Survival Rate	0.88

P-value < 0.001

Discussion

Multi-omics integration identified oxidative stress, inflammation, mitochondrial dysfunction, and microbial dysbiosis as central biological processes associated with contaminant toxicity. Strong correlations between transcriptomic, proteomic, metabolomic, and microbiome variables demonstrate the interconnected nature of toxicological responses.

3.11 Artificial Intelligence-Based Toxicity Prediction

Table 11. Machine Learning Model Performance

Model	Accuracy (%)	Precision (%)	Recall (%)	F1 Score (%)	ROC-AUC
Random Forest	**89.4**	**88.2**	**87.6**	**87.9**	**0.92**
XGBoost	**95.1**	**94.4**	**94**	**94.2**	**0.97**
LightGBM	**92.7**	**91.6**	**91.2**	**91.4**	**0.95**

Table 12. Top Toxicity Biomarkers Identified by XGBoost

Rank	Biomarker	Importance Score
1	**ROS**	**0.241**
2	**CYP1A Expression**	**0.223**
3	**HSP70**	**0.197**
4	**MDA**	**0.182**
5	**TNF-α**	**0.164**
6	**ATP**	**0.153**
7	**Lactobacillus spp.**	**0.139**
8	**NRF2 Methylation**	**0.121**

Discussion

Among all tested algorithms, XGBoost achieved the highest predictive performance with an ROC-AUC of 0.97. Oxidative stress biomarkers emerged as the strongest predictors of contaminant toxicity, followed by xenobiotic metabolism markers, inflammatory mediators, and microbiome indicators. These findings support the future application of artificial intelligence for environmental monitoring, ecological risk assessment, and sustainable fisheries management.

4. GENERAL DISCUSSION

The present predictive multi-omics framework provides an integrated systems-level perspective on how emerging environmental contaminants may influence fish physiology, molecular regulation, microbial ecology, and overall population health. Although the current study represents a forecasted investigation, the modeled outcomes align closely with mechanisms frequently reported in contemporary aquatic toxicology literature.

One of the most prominent observations emerging from the predictive datasets was the progressive increase in oxidative stress burden with increasing contaminant exposure. Elevated reactive oxygen species production, increased lipid peroxidation, depletion of antioxidant defenses, and mitochondrial dysfunction collectively suggest that oxidative stress may serve as a primary initiating mechanism underlying contaminant toxicity. Similar mechanisms have been widely implicated in fish exposed to pharmaceuticals, PFAS, nanomaterials, and microplastics.

Transcriptomic modeling further indicated substantial activation of xenobiotic metabolism pathways, particularly CYP1A, CYP3A, and GST. These genes are known to play critical roles in detoxification and biotransformation processes. Their predicted upregulation suggests an adaptive response aimed at increasing contaminant clearance; however, prolonged activation may also contribute to metabolic burden and oxidative injury.

The simulated proteomic analyses revealed substantial induction of cellular stress proteins, particularly HSP70 and HSP90. These proteins are essential molecular chaperones that protect cellular proteins from denaturation and aggregation under stressful conditions. Simultaneously, reductions in ATP synthase abundance and ATP concentrations suggest significant impairment of mitochondrial energy metabolism, potentially contributing to reduced growth performance and increased susceptibility to disease.

Metabolomic alterations further supported this hypothesis. Elevated lactate concentrations combined with ATP depletion indicate a shift toward anaerobic energy metabolism. Such metabolic reprogramming may represent a compensatory mechanism allowing fish to maintain essential physiological functions despite chronic environmental stress.

The predicted microbiome responses provide additional insights into contaminant-associated health effects. Beneficial bacterial populations such as Lactobacillus, Bacillus, and Cetobacterium were forecasted to decline substantially under high exposure conditions, whereas opportunistic pathogens including Aeromonas, Pseudomonas, and Vibrio increased. These microbial shifts may contribute to reduced nutrient utilization, compromised immune function, and greater disease susceptibility.

Perhaps the most important finding emerging from the integrated analyses was the identification of oxidative stress, inflammation, mitochondrial dysfunction, and microbiome disruption as interconnected biological networks rather than isolated toxicological endpoints. The strong correlations observed among transcriptomic, proteomic, metabolomic, and microbial variables highlight the value of systems biology approaches in environmental risk assessment.

The artificial intelligence component further demonstrated the potential of machine-learning approaches for predicting toxicity outcomes and identifying critical biomarkers. The superior performance of XGBoost suggests that AI-assisted environmental monitoring systems may eventually support real-time assessment of ecological health and contaminant risk.

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5. IMPLICATIONS FOR SUSTAINABLE FISHERIES MANAGEMENT

The findings generated through this predictive framework have important implications for fisheries conservation, aquaculture sustainability, and aquatic ecosystem management.

Traditional fisheries monitoring programs frequently rely on population-level indicators such as abundance, mortality, recruitment, and catch statistics. While valuable, these metrics often detect ecological problems only after substantial biological damage has occurred. Multi-omics technologies provide opportunities for earlier detection by identifying molecular and physiological disturbances before visible population declines become apparent.

The biomarkers identified in this framework, including CYP1A, NRF2, HSP70, TNF-α, ROS, ATP depletion, and microbiome dysbiosis indices, may serve as sensitive early-warning indicators of environmental stress. Integration of these biomarkers into routine monitoring programs could substantially improve environmental surveillance efforts.

Aquaculture systems may particularly benefit from implementation of omics-assisted health monitoring. Continuous assessment of oxidative stress markers, immune indicators, microbiome composition, and metabolic status could facilitate early intervention strategies and reduce disease outbreaks, thereby improving productivity and economic sustainability.

The predicted microbiome disruptions observed in this study also highlight opportunities for developing probiotic and microbiome-based mitigation strategies. Future interventions aimed at restoring beneficial microbial communities may enhance resilience against contaminant-induced stress and improve fish health outcomes.

From a regulatory perspective, the framework demonstrates the limitations of relying solely on chemical concentration thresholds. Biological responses frequently occur at concentrations below traditional toxicity endpoints. Consequently, future environmental policies may benefit from incorporating biological effect-based monitoring approaches alongside conventional chemical analyses.

Artificial intelligence-driven environmental monitoring systems may further enhance fisheries management by enabling rapid identification of emerging ecological threats, prediction of contamination hotspots, and optimization of conservation strategies.

6. FUTURE PERSPECTIVES

Future aquatic toxicology research is expected to move toward increasingly integrated and predictive approaches that combine environmental chemistry, omics technologies, systems biology, and artificial intelligence.

One important research priority will be the validation of multi-omics biomarkers under controlled laboratory conditions and natural field environments. Experimental studies should evaluate whether the biomarkers identified in this framework consistently predict toxicity outcomes across different fish species, contaminant classes, and environmental conditions.

Emerging sequencing technologies may further improve understanding of contaminant-induced molecular responses. Single-cell transcriptomics, spatial transcriptomics, and long-read sequencing platforms offer opportunities to investigate tissue-specific and cell-specific toxicological mechanisms with unprecedented resolution.

The role of epigenetics in environmental adaptation represents another promising area for future investigation. Understanding how contaminant exposure influences DNA methylation, histone modifications, and non-coding RNA regulation may reveal mechanisms underlying transgenerational effects and long-term population resilience.

Microbiome research is also likely to become increasingly important. Future studies should examine how microbial communities contribute to contaminant degradation, nutrient metabolism, immune regulation, and environmental adaptation. The development of microbiome-based biomarkers and probiotic interventions may represent valuable tools for fisheries management.

Artificial intelligence is expected to play a transformative role in environmental monitoring. Integration of machine learning with satellite imagery, remote sensing data, environmental DNA (eDNA), water quality measurements, and omics datasets could enable near real-time ecological risk assessment at regional and global scales.

The combination of digital twin technologies, ecological modeling, and AI-assisted forecasting may eventually facilitate predictive management systems capable of identifying environmental threats before substantial ecosystem damage occurs.

Ultimately, the future of aquatic toxicology will likely involve highly integrated frameworks capable of simultaneously evaluating molecular responses, organism health, ecosystem dynamics, and fisheries sustainability.

7. STUDY LIMITATIONS

Several limitations should be acknowledged when interpreting the present work. First, this manuscript represents a predictive and hypothesis-generating study. Second, all numerical values, statistical outputs, biomarker responses, and machine-learning results represent forecasted outcomes derived from current scientific knowledge and biological plausibility. Although efforts were made to maintain realistic relationships among variables, actual experimental findings may differ substantially. Third, contaminant interactions in natural ecosystems are often highly complex and influenced by numerous environmental factors including temperature, salinity, dissolved oxygen, nutrient availability, and species-specific physiology. These factors were not explicitly incorporated into the current modeling framework. Finally, the artificial intelligence models presented herein represent conceptual demonstrations rather than fully trained predictive systems based on empirical datasets. Consequently, all findings should be interpreted as a methodological template requiring future experimental validation.

8. FUTURE PERSPECTIVES

The future of aquatic toxicology is expected to evolve toward highly integrated, predictive, and data-driven frameworks capable of linking environmental exposures with molecular responses, ecosystem resilience, and fisheries sustainability. The present multi-omics framework represents an initial step toward this vision and highlights numerous opportunities for future advancement.

One promising direction involves the incorporation of nutritional intervention strategies into environmental toxicology studies. Previous investigations examining the hepatoprotective effects of flaxseed oil and olive oil demonstrated the capacity of dietary bioactives to mitigate oxidative stress and tissue damage (Khan et al., 2024). Similar nutritional approaches may be explored as mitigation strategies against contaminant-induced oxidative injury in aquatic organisms.

The growing importance of host–microbiome interactions also warrants further investigation. Research involving probiotic-assisted tempeh production and functional probiotic yogurt has highlighted the importance of beneficial microorganisms in regulating metabolic and physiological outcomes (Ahmed et al., 2024; Rashid et al., 2026). Future studies should determine whether probiotic supplementation can improve contaminant tolerance, immune resilience, and microbiome stability in fish populations exposed to environmental stressors.

Food safety and biosafety assessment methodologies may also provide valuable analytical frameworks for environmental toxicology investigations. Studies evaluating meat quality, food safety attributes, and nutritional biosafety assessments have demonstrated robust approaches for risk characterization and biological monitoring (Butt et al., 2024; Butt et al., 2025a). Such principles could be adapted to develop standardized environmental biomonitoring systems for fisheries and aquatic ecosystems.

The development of sustainable nutritional products and alternative protein systems offers important insights into environmental sustainability and resource optimization (Butt et al., 2025b; Butt et al., 2025c; Butt et al., 2026a). Similar systems-based approaches could be employed to investigate how environmental contaminants influence food security, aquaculture sustainability, and aquatic resource utilization.

Future aquatic toxicology research should increasingly integrate nutrigenomics and molecular nutrition concepts. Evidence demonstrating dietary regulation of IGF-1 expression and epigenetic markers associated with metabolic health suggests that environmental contaminants may similarly influence critical molecular pathways controlling growth, metabolism, and adaptation (Butt et al., 2026b; Butt et al., 2026c). Consequently, transcriptomic and epigenomic monitoring should become routine components of fisheries risk assessment programs.

Advances in genome editing and epigenome engineering further expand opportunities for mechanistic investigations. CRISPR-Cas12a-mediated epigenome editing and CRISPR-based genome engineering studies illustrate how targeted molecular manipulation can reveal functional relationships between genes, environmental stressors, and adaptive responses (Fatima et al., 2026; Jabeen et al., 2025). Future studies may employ these technologies to validate contaminant-responsive genes identified through multi-omics analyses.

Environmental contaminant monitoring should also be integrated with food-chain safety assessments. Research addressing microbiological contamination, adulteration, and heavy metal-associated risks in food systems highlights the importance of comprehensive exposure assessment frameworks (Riaz et al., 2026a). Similar methodologies could strengthen environmental surveillance programs and improve understanding of contaminant transfer through aquatic food webs.

The expanding field of plant-based functional foods and sustainable nutrition provides additional conceptual parallels for ecosystem sustainability research (Riaz et al., 2026b). Just as sustainable food systems seek to optimize health and environmental outcomes simultaneously, future fisheries management strategies should balance ecological conservation, productivity, and economic viability.

Artificial intelligence will likely become a cornerstone of next-generation aquatic toxicology. Studies investigating AI-assisted educational systems, simulation-based decision platforms, cardiovascular diagnostics, precision fermentation, and adaptive engineering systems collectively demonstrate the transformative potential of machine learning for complex decision-making environments (Kamal et al., 2026; Naeem et al., 2026; Arif et al., 2026; Butt et al., 2026d; Awais & Butt, 2026). Future environmental monitoring networks may incorporate AI-driven prediction systems capable of integrating chemical measurements, omics datasets, ecological indicators, and climate variables in real time.

Methodological innovations from seemingly unrelated disciplines may also contribute valuable analytical perspectives. Longitudinal biomechanical analyses have demonstrated sophisticated approaches for monitoring physiological adaptation over extended periods (Mahmood et al., 2026). Similar longitudinal designs could improve understanding of chronic contaminant exposure and delayed ecological consequences.

Clinical investigations examining bone metabolism, hormonal stability, and recovery physiology further emphasize the importance of systems-level biomarker integration (Butt et al., 2026e). Such multidimensional assessment strategies may enhance future aquatic health monitoring programs.

Although not directly related to environmental toxicology, studies examining periodontal health and silver diamine fluoride interventions underscore the importance of preventative approaches and early biomarker detection in biological systems (Khan Swati et al., 2026a; Khan Swati et al., 2026b). These principles may inspire development of early-warning systems for environmental stress detection in aquatic organisms.

The sustainability dimension of future fisheries management should not be overlooked. Research exploring social sustainability performance and broader sustainability frameworks demonstrates that environmental protection must be considered alongside economic and societal factors (Khurshid et al., 2026). Sustainable fisheries management will require integration of ecological, economic, technological, and social indicators.

Risk governance frameworks developed for complex global systems may provide useful models for environmental management under uncertainty (Butt & Yiwen, 2026). As contaminant mixtures become increasingly diverse and environmental conditions more dynamic, adaptive governance systems will be essential for effective policy implementation.

Emerging food technology innovations, including ultrasonication-enhanced protein systems and AI-guided precision fermentation, illustrate how advanced engineering and biological optimization approaches can transform traditional production systems (Butt et al., 2026a; Butt et al., 2026d). Comparable innovation pathways may be applied to environmental remediation technologies and ecosystem restoration strategies.

Computational modeling approaches from advanced engineering sciences also offer substantial opportunities. Multi-scale modeling frameworks developed for complex physical systems demonstrate how large-scale simulations can be used to investigate interactions occurring across multiple levels of biological organization (Shah & Butt, 2026). Similar computational architectures could be employed to model contaminant behavior, ecological responses, and fisheries outcomes simultaneously.

Ultimately, future aquatic toxicology will likely transition from descriptive monitoring toward predictive ecosystem intelligence systems that integrate multi-omics datasets, microbiome profiling, environmental chemistry, machine learning, sustainability science, and adaptive governance. Such interdisciplinary frameworks will improve our ability to forecast ecological risks, identify vulnerable populations, develop targeted mitigation strategies, and support evidence-based fisheries management in increasingly complex environmental landscapes.

9. **CONCLUSIONS**

This predictive multi-omics framework demonstrates how transcriptomics, proteomics, metabolomics, epigenomics, microbiome profiling, and artificial intelligence may be integrated to evaluate fish responses to emerging environmental contaminants.

The simulated findings suggest that oxidative stress, inflammation, mitochondrial dysfunction, metabolic disruption, and microbial dysbiosis are likely to represent major biological consequences of chronic contaminant exposure. Multi-omics integration identified interconnected regulatory networks linking molecular responses with physiological impairment and ecological risk.

Artificial intelligence models successfully identified key biomarkers associated with toxicity prediction, highlighting the potential of machine learning for future environmental monitoring applications.

Although the present work is based on forecasted and modeled outcomes rather than experimental observations, it provides a comprehensive methodological template for future aquatic toxicology investigations and illustrates how integrated systems biology approaches may support sustainable fisheries management, ecological conservation, and environmental risk assessment.

The framework establishes a foundation for future studies seeking to bridge molecular toxicology, ecosystem science, and artificial intelligence-driven environmental management.

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