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A REVIEW ON EMERGING TRENDS AND FUTURE PERSPECTIVES IN AQUATIC TOXICOLOGY: FROM CONVENTIONAL ECOTOXICOLOGY TO PREDICTIVE AND INTEGRATED RISK ASSESSMENT

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Abstract:

Aquatic toxicology is rapidly evolving from conventional single-contaminant toxicity testing toward an integrated discipline capable of addressing complex chemical mixtures, emerging contaminants, climate-related stressors, and ecosystem-level responses. Aquatic ecosystems are increasingly exposed to pharmaceuticals, pesticides, endocrine-disrupting chemicals, per- and polyfluoroalkyl substances (PFAS), microplastics, nanoplastics, nanoparticles, industrial chemicals, antibiotics and transformation products. At the same time, climate change, eutrophication, habitat alteration and changing hydrological conditions can modify contaminant fate, bioavailability and toxicity. Recent advances in high-resolution mass spectrometry, non-target chemical analysis, multi-omics, environmental DNA (eDNA), adverse outcome pathways (AOPs), exposomics, biosensors and artificial intelligence are transforming aquatic toxicology. Emerging research increasingly emphasizes environmentally realistic concentrations, chronic exposure, mixture toxicity, trophic transfer and interactions between chemical and non-chemical stressors. Multi-omics approaches can connect molecular initiating events with physiological and ecological outcomes, while machine learning can assist contaminant identification, toxicity prediction and risk assessment. Micro- and nanoplastics are particularly important because they can act as both toxicants and vectors for other contaminants. Future aquatic toxicology should integrate field observations, laboratory experimentation, computational modelling and real-time environmental monitoring. Standardization, validation, transparency and environmentally relevant experimental designs will be essential for translating technological advances into effective ecological risk assessment and management.

Keywords: Aquatic toxicology, emerging contaminants, microplastics, PFAS, multi-omics, exposomics, artificial intelligence, environmental DNA, mixture toxicity, ecological risk assessment.

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Introduction:

Aquatic ecosystems are continuously exposed to complex combinations of natural and anthropogenic stressors. Rivers, lakes, reservoirs, estuaries and oceans receive contaminants originating from domestic wastewater, agriculture, industries, mining, urban runoff, aquaculture and atmospheric deposition. Recent UNEP assessments indicate widespread degradation of freshwater systems, with increasing pollution and multiple pressures affecting rivers, lakes and aquifers. (UNEP - UN Environment Programme., 2024).

Historically, aquatic toxicology focused primarily on individual pollutants such as heavy metals, pesticides and petroleum hydrocarbons. Standard laboratory organisms, acute toxicity tests, LC_{50}/EC_{50} values and selected biochemical biomarkers formed the foundation of environmental risk assessment. However, environmental contamination is rarely characterized by exposure to a single chemical at a constant concentration. Aquatic organisms encounter mixtures of chemicals, particulate pollutants, pathogens, temperature changes, hypoxia and nutritional stress.

Consequently, modern aquatic toxicology is shifting toward mechanistic, predictive, ecosystem-based and data-intensive approaches. The objective is increasingly not simply to determine whether a chemical is toxic, but to understand how, under what environmental conditions, at what concentrations and in which organisms' toxicity occurs.

Emerging Contaminants and New Exposure Scenarios:

One of the most important developments is the recognition of contaminants of emerging concern (CECs). Pharmaceuticals, personal-care products, antibiotics, endocrine-disrupting chemicals, PFAS, flame retardants and transformation products are now important subjects of aquatic toxicology.

Pharmaceutical residues can enter aquatic systems through wastewater treatment plants, hospital discharges, agricultural runoff and improper disposal. Recent reviews indicate that pharmaceuticals may occur from nanogram-per-litre to microgram-per-litre concentrations and can influence growth, reproduction, immune function and behaviour of aquatic organisms. (Aib, H.*et al*.,2025).

PFAS represent another major research frontier because of their environmental persistence and ability to occur in aquatic environments and biological tissues. Recent research has increasingly examined PFAS bioaccumulation, biomagnification, trophic magnification and toxic effects across aquatic organisms (Cunlong Wang *et al*., 2025). Future research will therefore need to expand from conventional priority pollutants toward chemical classes, transformation products and previously unidentified contaminants.

Microplastics and Nanoplastics

Microplastics and nanoplastics have become central topics in contemporary aquatic toxicology. Plastic particles can enter freshwater and marine ecosystems through wastewater, agricultural runoff, industrial activities, fishing activities and degradation of larger plastic debris.

Microplastics may produce physical and biochemical effects, including oxidative stress, inflammation, immune disruption, behavioural changes, reproductive toxicity and altered growth. Their surfaces can also interact with metals, pharmaceuticals, hydrophobic organic pollutants and microorganisms. Recent reviews emphasize that microplastics may modify the bioavailability and fate of co-occurring contaminants. (Mahdi Banaee*et al*., 2025).

Importantly, recent research is moving beyond studying microplastics alone toward combined exposure experiments. A 2025 meta-analysis reported that combined exposure to microplastics and emerging contaminants can affect fish behaviour, development and reproduction, although responses depend on particle characteristics and contaminant combinations (Weiming Wu *et al.,* 2025).

Nanoplastics present an additional challenge because their smaller size may facilitate interactions with biological membranes and tissues. Recent literature identifies oxidative stress, membrane damage, developmental effects and immune and neurological alterations among reported responses, while also emphasizing

limitations in environmentally realistic chronic-exposure data. (Kargar M *et al.,* 2026). Future studies should therefore standardize particle characterization, including polymer type, size, shape, surface chemistry, weathering state and environmental concentration.

Multi-Omics and Molecular Aquatic Toxicology:

A major transition in aquatic toxicology is the incorporation of genomics, transcriptomics, proteomics, metabolomics, lipidomics and microbiomics.Traditional biomarkers such as catalase, superoxide dismutase, glutathione, acetylcholinesterase and malondialdehyde provide useful information but may represent only a small portion of pollutant-induced molecular responses. Multi-omics approaches can simultaneously examine thousands of molecular changes and identify biological pathways affected by environmental stressors.

Recent reviews indicate that integrated multi-omics can reconstruct molecular toxicity cascades and facilitate earlier biomarker discovery, particularly when microbiome and metabolome information are combined. (Li B, *et al*., 2025). Future aquatic toxicology will increasingly connect:

Chemical exposure → molecular initiating event → cellular response → tissue/organ alteration → organismal effect → population/ecosystem consequence.

Such mechanistic integration can strengthen the connection between laboratory observations and ecological risk assessment.

Adverse Outcome Pathways and Mechanistic Toxicology:

The Adverse Outcome Pathway (AOP) framework provides an important conceptual bridge between molecular mechanisms and adverse biological outcomes. Instead of treating toxicity as an isolated endpoint, AOP-based research identifies a sequence of biological events beginning with a molecular initiating event and progressing through key events toward an adverse outcome.

This approach is particularly valuable for emerging contaminants for which conventional toxicity data are limited. It can help organize evidence from molecular biology, physiology, pathology and ecological studies. Future research should combine AOPs with multi-omics, computational toxicology and high-throughput screening. Such integration could support more efficient identification of mechanisms of toxicity and prioritization of chemicals requiring further testing.

Exposomics and Mixture Toxicology:

Environmental organisms experience complex chemical exposomes rather than isolated pollutants. Mixture effects may be additive, synergistic or antagonistic and can vary with concentration, exposure duration, chemical ratios and biological characteristics. Consequently, future aquatic toxicology must increasingly address real-world mixtures. This requires combining chemical monitoring with biological-response measurements.

High-resolution mass spectrometry and non-target analysis are becoming particularly important because targeted monitoring can detect only chemicals for which analytical standards and predefined targets are available. Recent work indicates that machine learning can assist non-target analysis by improving chemical identification, quantification and toxicity prediction. (Alexa Cancholaet *al.,* 2025) .The future direction is therefore toward effect-directed analysis, in which chemical identification is combined with biological activity rather than relying solely on chemical concentration.

Artificial Intelligence and Machine Learning:

Artificial intelligence (AI) and machine learning (ML) represent rapidly developing areas in aquatic toxicology. Large datasets

generated through chemical monitoring, toxicity testing, omics, imaging and environmental sensors create opportunities for predictive modelling.

ML can potentially assist in:

- prediction of chemical toxicity;
- identification of emerging contaminants;
- prediction of environmental fate;
- species-specific toxicity modelling;
- mixture toxicity assessment;
- bioaccumulation prediction;
- identification of molecular biomarkers;
- environmental risk prioritization.

A recent 2025 review describes applications of ML across pollutant exposure prediction, detection, biotoxicity and environmental behaviour modelling, including multi-species and environmental-variable-informed approaches. (Xinyue Dong *et al*., 2025).

However, AI should complement rather than replace experimental toxicology. Model reliability depends on data quality, representativeness, external validation and interpretability. Recent work on AI for mixture toxicology particularly emphasizes the need for experimentally validated mixture datasets and transparent applicability domains. (Domingo JL *et al*., 2026).

Environmental DNA and Advanced Biomonitoring:

Environmental DNA (eDNA) is emerging as an important tool for aquatic ecosystem monitoring. DNA released by organisms into water can be collected and analysed to identify species or communities without requiring direct capture.Recent reviews describe applications of eDNAmetabarcoding for biodiversity assessment and marine pollution monitoring. (*SakibTahmidRishanet al.,* 2024).

Integration of eDNA with chemical monitoring could provide a more comprehensive picture of ecosystem responses. For example, chemical measurements can indicate what pollutants are present, while eDNA and molecular biomarkers can provide information about which biological communities are responding. Future monitoring systems may combine eDNA, biosensors, automated sampling, satellite observations and real-time water-quality measurements.

Climate Change and Multiple Stressors:

Climate change is increasingly recognized as an important modifier of aquatic toxicity. Increasing temperature, altered rainfall, drought, flooding, salinity changes, acidification and hypoxia can influence pollutant transport, degradation, bioavailability and organismal sensitivity.Climate-related stressors may interact with chemical contaminants rather than acting independently. Toxicological frameworks incorporating the exposome and AOP concept provide opportunities to understand interactions between climate-associated stressors and chemical pollution. (Barouki R. 2024).Future aquatic toxicology should therefore incorporate multiple-stressor experiments instead of examining chemical toxicity under constant laboratory conditions alone.

Future Perspectives:

The future of aquatic toxicology is likely to be characterized by greater integration of technologies and disciplines. Five priorities are particularly important:

1. **Environmentally realistic exposure conditions** – experiments should use realistic concentrations, exposure durations and environmental matrices.
2. **Mixture-based assessment** – risk assessment should increasingly consider chemical mixtures and multiple stressors.
3. **Mechanistic integration** – multi-omics and AOP approaches should connect molecular responses with ecological outcomes.

4. **Predictive toxicology** – AI, ML, QSAR and computational modelling can help prioritize chemicals and reduce unnecessary testing.
5. **Real-time ecosystem surveillance** – biosensors, eDNA, high-resolution mass spectrometry and automated monitoring can support rapid detection of ecological changes.

Standardization is particularly important for micro/nanoplastics, where differences in particle preparation, characterization and exposure protocols currently make comparisons between studies difficult. (LinyongZhi*et al.,* 2025).

Conclusion:

Aquatic toxicology is entering a transformative phase in which traditional toxicity testing is being integrated with molecular biology, analytical chemistry, computational science and ecological monitoring. Emerging contaminants such as pharmaceuticals, PFAS, microplastics and nanoplastics require assessment under environmentally realistic exposure scenarios, particularly because organisms are exposed to complex mixtures rather than isolated chemicals.

Multi-omics, exposomics, AOPs, eDNA, high-resolution mass spectrometry and artificial intelligence provide complementary tools for understanding toxicity from molecular mechanisms to ecosystem responses. Nevertheless, technological advancement must be accompanied by standardized methods, transparent datasets, experimental validation and strong ecological interpretation.

The future discipline will therefore be increasingly predictive, mechanistic, multidisciplinary and ecosystem-oriented, enabling earlier identification of environmental hazards and more comprehensive protection of aquatic biodiversity and ecosystem services.

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