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Transformation products of emerging contaminants and their formation pathways, environmental fate, predictive modeling, and regulatory risk implications

Matthew Chidozie Ogwu[1*], Sylvester Chibueze Izah[2], Olugbemiga Ojo Aliu[3], Ayebapreye Kari[4] and Esther Ugo Alum[5]

*Correspondence:
ogwumc@appstate.edu

[1] Goodnight Family Department of Sustainable Development, Living Learning Center, Appalachian State University, Boone, NC, USA
[2] Department of Community Medicine, Faculty of Clinical Sciences, Bayelsa Medical University, Yenagoa, Bayelsa State, Nigeria
[3] Department of Environmental Biology, Auchi Polytechnic, Auchi, Edo State, Nigeria
[4] Department of Microbiology, Faculty of Science, Bayelsa Medical University, Yenagoa, Bayelsa State, Nigeria
[5] Department of Research and Publications, Kampala International University, P. O. Box 20000, Kampala, Uganda

Abstract

Transformation products (TPs) of emerging contaminants are emerging as a major frontier in environmental chemistry, toxicology, and regulatory science because many exhibit greater persistence, mobility, bioavailability, or biological activity than their parent compounds. These transformation-driven changes can alter exposure pathways, trophic interactions, environmental transport, and long-term ecological and human health risks, challenging conventional parent-compound-centered approaches to chemical risk assessment. This review critically examines the formation pathways, environmental fate, analytical detection, predictive modeling, and regulatory implications of TPs derived from major contaminant groups, including pharmaceuticals, pesticides, industrial chemicals, plastic additives, and per- and polyfluoroalkyl substances (PFAS). Unlike many existing reviews that focus primarily on TP occurrence, analytical detection, or individual contaminant classes, this review advances a transformation-aware predictive systems framework that integrates formation mechanisms, environmental fate, analytical monitoring, predictive modeling, toxicity assessment, and regulatory decision-making into a unified risk-governance approach. Evidence from the reviewed literature shows that selected pharmaceutical, pesticide, PFAS-related, and plastic-associated contaminants and their transformation products are commonly detected in wastewater, surface water, groundwater, drinking-water systems, sediments, and biological matrices, with reported concentrations often ranging from ng/L to µg/L levels depending on contaminant class, matrix, source intensity, and treatment conditions. Particular attention is given to coupled biotic and abiotic mechanisms governing TP formation, including microbial metabolism, photochemical reactions, hydrolysis, oxidation–reduction processes, and treatment-induced transformations across aquatic, terrestrial, atmospheric, indoor, and engineered systems. The review further evaluates how physicochemical properties influence TP persistence, partitioning, trophic transfer, bioaccumulation, and long-range transport. Advances in high-resolution mass spectrometry, suspect and non-target screening, isotope-assisted pathway tracing, and machine-learning-assisted prediction are discussed as transformative tools for identifying overlooked contaminants and anticipating

transformation-driven risks. Persistent regulatory blind spots are critically examined, particularly the limited incorporation of TPs into monitoring frameworks, exposure modeling, watch-list systems, and chemical governance. In response, the review proposes an integrated monitoring–modeling–toxicity–policy pathway to support adaptive environmental risk governance. Recognizing TPs as independent environmental risk entities rather than secondary degradation byproducts represents a necessary paradigm shift for advancing chemical safety assessment, sustainable pollution management, and proactive environmental protection in the era of emerging contaminants.

Keywords: Non-target screening, High-resolution mass spectrometry, Chemical persistence, Environmental exposure, Mixture toxicity, Watch-list monitoring, Adaptive risk governance

1 Introduction

Assessment of chemical contaminants has historically focused on parent compounds rather than (TPs). This focus creates significant gaps in environmental risk evaluation. TPs may display toxicity, persistence, and mobility exceeding those of precursor substances. Transformation products are generated across diverse anthropogenic systems, including pharmaceutical use, household and hospital wastewater, personal-care products, agriculture, livestock and aquaculture, industrial manufacturing, plastic and polymer production, landfill leachate, biosolids application, drinking-water disinfection, wastewater treatment, combustion, and remediation technologies [105, 130, 169]. Within these systems, parent contaminants may be transformed by microbial metabolism, photolysis, hydrolysis, oxidation–reduction reactions, chlorination, ozonation, and advanced oxidation, indicating that transformation products arise wherever contaminants undergo biological, chemical, or engineered transformations [169, 197].

Evidence shows that TPs from organic micropollutants can be more hazardous in aquatic systems [43]. Degradation pathway modeling demonstrates that some products exhibit strong bioaccumulation potential [9, 37, 167]. These findings indicate the importance of systematically integrating TPs into environmental assessments. Chemical transformations vary across environmental conditions, increasing analytical complexity. Introduction of new pesticides into agricultural systems requires ongoing evaluation of degradation and toxicity [64]. Studies of heterocyclic insecticides such as pyraquinil show rapid hydrolysis under defined pH and temperature conditions [64]. The resulting products may exhibit distinct physicochemical and toxicological properties. Research demonstrates that metabolites formed from parent compounds can exhibit heightened ecological risk [127]. Regulatory attention toward these products remains limited despite such findings. Recent work emphasizes that research on TPs must integrate reaction-mechanism identification, novel product discovery, and environmental implication assessment to better characterize contaminant risk beyond parent compounds [97].

Existing regulatory frameworks often emphasize the properties of the parent chemical. Agencies, including the European Chemicals Agency (ECHA) and the United States Environmental Protection Agency (EPA), prioritize established pollutants in monitoring programs [9, 142, 198]. International chemical governance also extends beyond national regulatory agencies through multilateral environmental agreements. The Basel Convention regulates the transboundary movement and disposal of hazardous wastes, while the Rotterdam Convention promotes prior informed consent in the international

trade of certain hazardous chemicals and pesticides. The Stockholm Convention specifically targets persistent organic pollutants for restriction or elimination, making it particularly relevant to persistent parent contaminants and TPs with long-range transport potential [101, 195]. In the European Union, the Industrial Emissions Directive (Directive 2010/75/EU) further strengthens chemical governance by regulating emissions from industrial installations across multiple receiving media, including air, water, and soil. These frameworks provide important policy instruments for managing problematic chemicals and reducing transformation-product risks across borders and environmental compartments. However, limited incorporation of TPs into routine assessments creates blind spots. Some TPs show greater persistence or toxicity than original compounds [36, 182, 183]. Such characteristics amplify environmental exposure risks over time. Analytical limitations further restrict the detection of many TPs [20]. Insufficient monitoring hinders accurate assessment of their distribution and effects. Wastewater treatment plants illustrate this challenge clearly. Pharmaceuticals and their metabolites may persist through treatment processes [61, 113, 178, 179]. Effluent discharge introduces TPs into aquatic environments. Accumulation in sediments and biota has been documented in several contexts. These findings highlight the need for enhanced detection and regulatory consideration.

Empirical research confirms the enhanced toxicity of certain TPs. Phototransformation of pesticides can yield byproducts that are more toxic than the parent compounds [142, 167]. Such outcomes complicate assumptions regarding degradation as a risk-reducing process. Plant-mediated back conversion of transformation products can also alter exposure pathways. For example, methyl triclosan may be converted back to triclosan in plant systems, thereby reintroducing the parent compound and affecting contaminant bioavailability and ecological exposure [41, 111]. These processes challenge linear models of contaminant degradation. Persistence also characterizes several documented TPs. Fluconazole derivatives, including 1,2,4-triazole, show stability and mobility in aquatic systems [36, 43]. Mobility enhances potential for distribution across environmental compartments. Bioaccumulation in aquatic organisms increases ecological and human health concerns. Traditional safety evaluations focused on parent compounds may underestimate long-term risks [139, 167, 182, 183]. A comprehensive evaluation requires the inclusion of TPs across exposure pathways.

The significance of TPs for human health is growing, as these compounds can enter exposure pathways that directly affect people. Transformation products can occur in drinking-water sources, wastewater-impacted surface waters, irrigated crops, aquatic foods, biosolids-amended soils, indoor air, and contaminated sediments [99, 118, 119, 131, 145]. Human exposure may occur through ingestion, inhalation, dermal contact, and food-chain transfer, particularly where treated wastewater, contaminated drinking-water supplies, or polluted aquatic food webs serve as exposure routes [99, 134, 145]. Some transformation products may retain or exceed the biological activity of parent compounds, contributing to endocrine disruption, developmental toxicity, reproductive effects, oxidative stress, antimicrobial resistance selection, and chronic low-dose mixture risks [33, 34, 134, 182, 183, 199]. These concerns help explain why transformation products should not be treated only as environmental chemistry byproducts, but as potential public-health-relevant contaminants requiring targeted monitoring and

regulatory assessment. Previous reviews have made important contributions by examining the occurrence, analytical detection, environmental fate, and class-specific behavior of transformation products of emerging contaminants [151, 200, 201]. However, much of the existing literature remains organized around either specific contaminant groups, analytical methods, or environmental compartments rather than the full risk pathway from parent-compound release to transformation, exposure, toxicity, prediction, and regulation [33, 34, 169].

This review examines the formation pathways, environmental fate, predictive modeling approaches, and regulatory implications of transformation products of emerging contaminants. It positions transformation products as distinct environmental risk entities rather than as secondary or incidental degradation outcomes of parent compounds. The review synthesizes the current literature on degradation mechanisms, environmental distribution, analytical detection, and model-based prediction to show how transformation products may differ from their precursors in terms of persistence, mobility, toxicity, bioavailability, and detectability. It also evaluates regulatory and monitoring gaps that arise when chemical assessment frameworks focus primarily on parent compounds. By integrating mechanistic, analytical, predictive, and governance perspectives, the review advances a transformation-aware framework for environmental health assessment and chemical risk management. The conceptual contribution of this review is the development of a transformation-aware risk perspective. This perspective recognizes that contaminants do not remain chemically static after release but may undergo sequential biotic and abiotic reactions across wastewater systems, surface waters, sediments, soils, the atmosphere, indoor environments, and biological tissues. As a result, exposure and hazard assessment must account for both parent compounds and their secondary or tertiary products. The novelty of this review lies in its transformation-aware risk-governance framing, which integrates mechanistic formation pathways, compartment-specific fate processes, analytical detection challenges, predictive modeling tools, and regulatory decision points into a single framework for assessing transformation products as independent risk entities. This framing advances the manuscript from a descriptive overview to an integrated risk-assessment and governance argument.

1.1 Review methodology

This review adopted a structured narrative and integrative literature review approach to synthesize current knowledge on the formation pathways, environmental fate, predictive modeling, analytical detection, and regulatory implications of TPs of emerging contaminants [33, 34, 178, 179]. Literature searches were conducted using major scientific databases, including Scopus, Web of Science, PubMed, ScienceDirect, and Google Scholar. Search terms included combinations of "TPs," "emerging contaminants," "environmental fate," "predictive modeling," "biotransformation," "photodegradation," "PFAS transformation," "non-target screening," "QSAR," "risk assessment," and "wastewater treatment byproducts." Peer-reviewed articles, review papers, regulatory reports, and selected authoritative technical documents published primarily between 2000 and 2025 were considered. Earlier seminal studies were also included where foundational concepts or analytical frameworks were relevant to transformation-product research. Inclusion criteria focused on studies addressing transformation mechanisms, occurrence, analytical

detection, environmental behavior, ecotoxicological effects, predictive approaches, and governance implications of TPs across aquatic, terrestrial, atmospheric, and engineered systems. Studies lacking direct relevance to TPs or presenting insufficient methodological detail were excluded.

The retrieved literature was screened thematically and organized into major analytical domains, including contaminant source classes, transformation mechanisms, environmental transport and persistence, ecotoxicological implications, analytical monitoring technologies, predictive modeling frameworks, and regulatory governance. Particular emphasis was placed on studies employing high-resolution mass spectrometry, suspect and non-target screening workflows, machine-learning-assisted prediction, and integrated environmental risk-assessment approaches. The review further prioritized interdisciplinary studies linking environmental chemistry, toxicology, computational modeling, and policy-oriented environmental management frameworks. This integrative methodology enabled the development of a systems-oriented synthesis that connects transformation pathways with environmental exposure dynamics, predictive toxicology, and emerging governance strategies for sustainable chemical risk management.

Although quantitative data on TPs are increasingly reported, direct cross-study integration remains limited by differences in environmental matrices, analytical methods, detection limits, reporting units, exposure durations, toxicity endpoints, and availability of reference standards. For this reason, this review does not attempt a formal meta-analysis of concentration ranges or dose–response values. Instead, this review provides a comparative synthesis using available evidence on persistence, mobility, detectability, exposure relevance, and relative risk concern, while noting where standardized quantitative datasets remain insufficient. This review treats transformation products as independent risk entities and organizes the discussion around five linked themes: formation pathways, environmental fate, analytical detection, predictive modeling, and regulatory risk governance.

2 Sources and classes of transformation products

The classification of TP adopted in this review is primarily source- and use-based rather than strictly structure-based. Emerging contaminants are grouped into broad categories according to their dominant environmental sources and applications, including pharmaceuticals and personal-care products, pesticides and herbicides, industrial chemicals, plastic additives, and PFAS. Chemical-structure groups are discussed only as sub-examples within these broader categories, where they help explain transformation behavior, persistence, mobility, or toxicity. This approach provides a consistent basis for comparing transformation products across major contaminant classes while acknowledging that some compounds may overlap across source, use, and structural classifications.

Transformation products originate from diverse contaminant sources across anthropogenic systems. Major classes include pharmaceuticals, pesticides, industrial chemicals, PFAS, and plastic additives, all of which are increasingly recognized as important contributors to environmental exposure and chemical risk [33, 34, 169]. Domestic consumption, agricultural application, and manufacturing activities contribute to environmental release. Table 1 summarizes the principal contaminant classes generating transformation products, their dominant transformation drivers, representative

examples, and key environmental concerns associated with each class. Waste disposal and industrial discharge further expand contaminant pathways [118, 119, 151]. After release, parent compounds enter wastewater treatment plants, agricultural runoff channels, and landfill leachates, where they may undergo biotic and abiotic transformations [73, 178, 179].

Microbial metabolism alters molecular structures through enzymatic reactions, while photochemical reactions driven by sunlight produce additional derivatives. Hydrolysis and oxidation–reduction processes further diversify transformation pathways [37, 43]. These mechanisms generate products with properties distinct from those of the precursor substances. Reported concentrations of transformation products vary widely across contaminant classes and environmental matrices (Table 2). Pharmaceutical TPs have been detected in wastewater-impacted rivers at ng/L to µg/L levels, with one river study reporting concentrations of 0.68–544 ng/L and broader evidence showing pharmaceuticals and TPs in surface water, groundwater, and drinking water at ng/L–µg/L levels [190]. In surface-water monitoring, pharmaceutical residues and TPs were also reported at median concentrations ranging from sub-ng/L to tens of ng/L, including metformin at median concentrations of 3.0–39 ng/L in Luxembourgish surface waters [146]. Drinking-water studies further show that pesticide TPs can reach high ng/L levels, including metolachlor SA at 772 ng/L and acetochlor OA at 882 ng/L in source and finished drinking waters [31]. These values show that TPs are not only structurally relevant but also exposure-relevant, although concentration patterns remain strongly influenced by source intensity, matrix type, season, treatment efficiency, and analytical method.

Transformation products often differ markedly in persistence and mobility. Increased polarity may enhance solubility and transport through aquatic systems, while some derivatives bind more strongly to sediments or organic matter [9, 43]. Transformation pathways are also controlled by molecular-level properties, including crystallinity, chemical bond types, ionization state, pKa, polarity, functional groups, and molecular stability. These factors influence dissolution, sorption, reactivity, degradation rate, product formation, persistence, mobility, toxicity, and analytical detectability. For example, ester, amide, ether, halogenated, and aromatic bonds differ in their susceptibility to hydrolysis, oxidation, reduction, photolysis, and thermal degradation, while ionization affects solubility, membrane permeability, and environmental transport [33, 34], (Boxall and Adams 2009), [24]. Variability in degradation rates affects long-term environmental residence. Biological activity may increase or decrease with structural modifications, complicating the prediction of ecological outcomes [33, 34, 182, 183]. Environmental compartments receiving these products include soil, surface water, groundwater, sediments, and air. Interconnected transport processes enable movement between compartments [62, 63]. Volatilization can introduce certain products into atmospheric pathways, while groundwater transport facilitates regional distribution. Sediment accumulation creates reservoirs of persistent contaminants, and sequential transformations may occur during transport, generating secondary or tertiary products [37, 43].

Figure 1 conceptualizes these relationships by mapping contaminant origins and transformation pathways. Integration of source categories with environmental entry routes establishes analytical coherence. This framework supports the identification of high-risk transformation processes. Recognition of interconnected pathways

Table 1 Comparative classes, formation pathways, environmental behavior, and risks of transformation products of emerging contaminants

Parent contaminant class	Parent compound examples	Typical transformation mechanisms / dominant formation drivers	Representative transformation products	Dominant environmental compartments	Typical environmental behavior	Main analytical challenge	Key ecological / human health concerns	Evidence / practical interpretation
Pharmaceuticals and personal-care products	Diclofenac, carbamazepine, sulfamethoxazole, triclosan	Human metabolism, wastewater treatment, microbial transformation, photolysis, and hydrolysis	Hydroxylated diclofenac metabolites, carbamazepine epoxide, acridine/acridone products, methyl triclosan/triclosan back-conversion products	Wastewater, rivers, sediments, effluent-dominated streams	Often polar, mobile, and continuously introduced into aquatic systems through wastewater discharge	Low concentrations, complex effluent mixtures, and limited analytical standards	Chronic aquatic exposure, endocrine disruption, behavioral effects, and long-term mixture toxicity	Persistent pharmaceuticals and their products may remain detectable downstream of wastewater discharge, contributing to chronic aquatic exposure and mixture effects
Pesticides and herbicides	Atrazine, fipronil, metolachlor, tebuconazole	Photodegradation, hydrolysis, soil microbial metabolism, and seasonal field application	Desethyl-atrazine, deisopropyl-atrazine, fipronil sulfone, fipronil sulfide, metolachlor ESA	Agricultural soils, surface waters, irrigation water, sediments	Highly variable persistence depending on soil type, pH, sunlight, rainfall, and microbial activity	Episodic occurrence, diverse degradation products, and variable detection windows	Toxicity to aquatic organisms, pollinators, birds, and food-web components	Pesticide transformation products may persist beyond application periods and may be more mobile or toxic than parent compounds, especially in agricultural runoff and sediment systems
PFAS precursors	Fluorotelomer alcohols, N-EtFOSE, fluorotelomer sulfonates	Oxidation, biotransformation, environmental weathering, treatment processes, and precursor degradation	Perfluoroalkyl acids, PFOS-related products, terminal PFAS products	Groundwater, drinking water, landfill leachate, sediments, wastewater	Terminal products may be extremely persistent, mobile, and difficult to remediate	Incomplete detection of precursors, unknown organofluorines, and limited total fluorine characterization	Long-term drinking-water contamination, bioaccumulation, developmental toxicity, and chronic human exposure	PFAS precursors can transform into terminal products that persist for long periods, complicating remediation and long-term exposure control

Table 1 (continued)

Parent contaminant class	Parent compound examples	Typical transformation mechanisms / dominant formation drivers	Representative transformation products	Dominant environmental compartments	Typical environmental behavior	Main analytical challenge	Key ecological / human health concerns	Evidence / practical interpretation
Plastic additives	Bisphenol A, phthalates, UV filters, flame-retardant additives	UV weathering, oxidative degradation, leaching, polymer degradation, and microbial transformation	Bisphenol derivatives, phthalate metabolites, hydroxylated or oxidized UV-filter products	Marine waters, soils, landfill leachate, sediments, food-contact materials	Variable mobility; some products remain dissolved while others sorb to particles, sediments, or organic matter	Complex additive mixtures, poorly characterized products, and limited reference standards	Endocrine disruption, developmental effects, food-chain exposure, and aquatic toxicity	Plastic additive products may retain endocrine activity and can enter food chains through packaging migration, leachate, dust, or aquatic exposure
Industrial chemicals	Chlorinated solvents, benzotriazoles, PAHs, industrial surfactants	Hydrolysis, oxidation–reduction reactions, combustion, treatment-induced transformation, and environmental weathering	Chlorinated solvent intermediates, oxidized PAH products, benzotriazole derivatives	Industrial discharge zones, sediments, air, wastewater, soils	Matrix-dependent persistence with potential for sediment accumulation or atmospheric transport	Diverse chemical structures, limited monitoring lists, and uncertain transformation pathways	Carcinogenicity, long-term ecosystem exposure, occupational/environmental health risks, and persistent contamination	Industrial transformation products may accumulate in sediments, air, or wastewater-impacted systems and require site-specific monitoring because of diverse structures and toxicity profiles

Table 2 Reported environmental concentrations of selected transformation products and related emerging contaminants

Contaminant group	Environmental matrix	Reported concentration evidence	Exposure relevance	References
Pharmaceuticals and pharmaceutical TPs	Wastewater-impacted rivers	Detected compounds ranged from 0.68 to 544 ng/L	Indicates chronic exposure in effluent-impacted rivers and supports the need for downstream monitoring	Zha et al. [190]
Pharmaceuticals and pharmaceutical TPs	Surface waters	Metformin median concentrations ranged from 3.0 to 39 ng/L across sampling periods	Shows continuous low-level pharmaceutical input into surface waters	Singh et al. [146]
Pesticide TPs	Source and finished drinking waters	Metolachlor SA and acetochlor OA reached 772 ng/L and 882 ng/L, respectively	Demonstrates that mobile pesticide TPs can occur in drinking-water sources at policy-relevant levels	Elliott et al. [31]
Pesticide TPs	Finished drinking water	Metolachlor SA reached 2470 ng/L	Highlights the potential persistence of pesticide TPs through treatment and the need for targeted monitoring	Elliott et al. [31]
PFAS and PFAS-related products	Drinking water	Individual PFAS maximum concentrations ranged from 0.943 to 33.2 ng/L	Supports long-term monitoring because PFAS-related compounds are persistent and mobile	Elliott et al. [31]
PFAS and PFAS-related products	Wastewater influent and effluent	PFAS concentrations were reported up to 107 ng/L in wastewater-related samples	Indicates wastewater as a relevant pathway for PFAS release and redistribution	Mashtare et al. (2021)
Plastic-associated contaminants	Finished drinking water	Bis(2-ethylhexyl) phthalate reached 4000 ng/L	Indicates potential exposure relevance for plastic-associated contaminants in treated water	Elliott et al. [31]
Mixed emerging contaminants	Wastewater and surface waters	Emerging contaminants are commonly reported from ng/L to µg/L ranges	Shows that low-level detection may still be relevant for chronic exposure and mixture-risk assessment	[118, 119, 197]

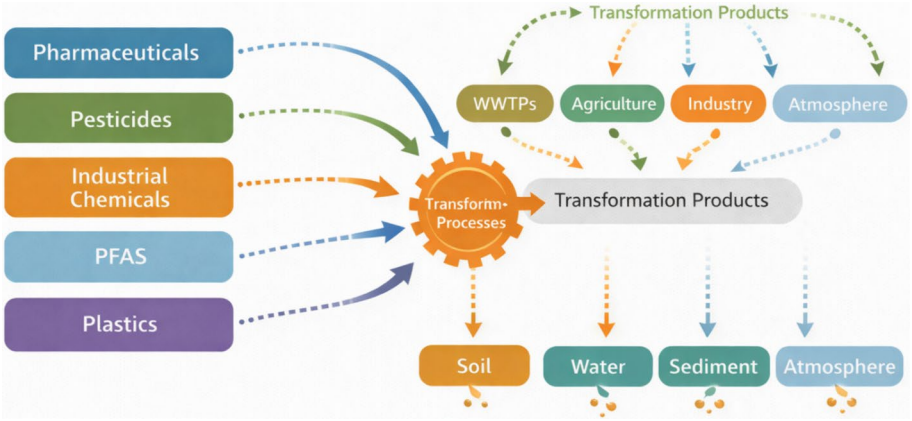

Fig. 1 Sources and Environmental Entry Pathways of Transformation Products

reinforces the need for comprehensive monitoring strategies. Examination of source classes, therefore, provides a foundational context for subsequent discussion of environmental behavior and regulatory considerations.

Across contaminant classes, transformation products differ substantially in formation mechanisms, environmental behavior, detectability, and risk relevance. Pharmaceutical transformation products are often generated through human metabolism, wastewater treatment, and microbial transformation, with many entering aquatic systems through continuous effluent discharge [178, 179, 204]. Pesticide and herbicide transformation products are more strongly influenced by application timing, soil chemistry, sunlight exposure, hydrolysis, and microbial activity, resulting in variable persistence across agricultural landscapes [154]. PFAS transformation products differ from many other classes because precursor transformation may generate terminal perfluoroalkyl acids that are extremely persistent, mobile, and difficult to remediate [47, 136]. Plastic additives and industrial chemical transformation products are more heterogeneous, with behavior shaped by polymer weathering, combustion, leaching, oxidation, and sorption to organic matter or particles [19, 180].

Apparent contradictions among studies often reflect differences in experimental design and environmental context rather than direct disagreement. A transformation product reported as persistent in one study may degrade rapidly in another because of differences in pH, temperature, redox conditions, microbial community composition, dissolved organic matter, sediment organic carbon, irradiation intensity, or treatment conditions [37, 43]. Similarly, differences in analytical platforms, detection limits, suspect lists, and availability of reference standards can influence whether specific transformation products are detected or overlooked [24, 107, 162]. Transformation-product behavior should therefore be interpreted as the outcome of interactions among chemical structure, the environmental matrix, the transformation pathway, and the analytical method.

2.1 Pharmaceuticals and personal-care products

Pharmaceuticals and personal-care products (PPCP) remain widely detected in aquatic environments, with wastewater treatment plants serving as major entry points for these compounds [178, 179]. Parent substances, metabolites, and secondary transformation products can persist through treatment processes and enter receiving waters through effluent discharge. These contaminants constitute a diverse group of emerging contaminants rather than a single homogeneous category. Pharmaceuticals include antibiotics, hormones, non-steroidal anti-inflammatory drugs, psychotropic drugs, beta-blockers, and other therapeutic agents, while personal-care products include preservatives, UV filters, fragrances, antibacterial agents, surfactants, plasticizers, siloxanes, and cosmetic microplastics. These groups differ in use patterns, transformation pathways, environmental persistence, mobility, bioaccumulation potential, and endocrine-disrupting activity. Their transformation products may form through human metabolism, wastewater treatment, photolysis, microbial degradation, hydrolysis, oxidation, and environmental weathering, making subclass-level classification important for risk assessment.

Effluents introduce complex contaminant mixtures into receiving waters, where metabolites and transformation products may exhibit toxicity equal to or greater than their precursor compounds [147, 178, 179]. Increased polarity may enhance environmental mobility and bioavailability, while continuous discharge can expose aquatic organisms to low but biologically active concentrations over long periods. Knowledge gaps persist regarding the long-term fate, mixture toxicity, and cumulative ecological effects of PPCP residues. Microbial degradation plays a central role in PPCP transformation, but biotransformation processes vary according to microbial community composition, treatment conditions, and environmental context [178, 179]. Complex mixtures may challenge conventional treatment systems, particularly when metabolites or intermediate products contribute to effluent toxicity [95]. Advanced oxidation processes and ozonation can improve removal efficiencies, although these technologies may also generate intermediate products requiring further evaluation [114, 147]. Understanding PPCP transformation pathways is therefore important for predictive modeling, monitoring design, and environmental management.

To strengthen the classification of pharmaceuticals and personal-care products, Table 3 organizes these contaminants into major functional groups and links each group to representative parent compounds, typical transformation products, dominant formation pathways, and environmental significance. This structure highlights that PPCPs are not a uniform contaminant category; rather, antibiotics, hormones, NSAIDs, psychotropic drugs, preservatives, UV filters, fragrances, antibacterial agents, surfactants, plasticizers, siloxanes, and cosmetic microplastics differ in persistence, mobility, bioaccumulation potential, endocrine-disrupting activity, and ecological relevance.

2.2 Pesticide and herbicide degradation products

Pesticides and herbicides generate numerous TPs in aquatic systems. Degradation pathways depend on molecular structure and environmental conditions [152, 153]. Microbial metabolism, photolysis, and hydrolysis contribute to structural modification. Some metabolites e xhibit greater toxicity than their parent compounds [152].

Table 3 Major pharmaceutical and personal-care product groups, transformation products, and environmental significance

Major group	Representative parent compounds	Typical metabolites/transformation products	Dominant formation pathway	Environmental significance
Antibiotics	Sulfamethoxazole, trimethoprim, and ciprofloxacin	Hydroxylated, acetylated, or oxidized metabolites	Human metabolism, wastewater treatment, microbial transformation, and photolysis	Persistence in wastewater effluents, microbial community effects, and potential contribution to antimicrobial resistance
Hormones	Estradiol, ethinylestradiol, and estrone	Hydroxylated and conjugated hormone metabolites	Human/animal excretion, deconjugation, and microbial transformation	Endocrine disruption, reproductive effects in aquatic organisms, and activity at low concentrations
NSAIDs	Diclofenac, ibuprofen, and naproxen	Hydroxylated diclofenac metabolites and carboxylated ibuprofen products	Human metabolism, photolysis, and wastewater transformation	Chronic aquatic exposure, fish toxicity, and persistence in effluent-impacted waters
Psychotropic drugs	Carbamazepine, fluoxetine, and citalopram	Carbamazepine epoxide, acridine/acridone products, desmethyl metabolites	Human metabolism, wastewater treatment, and photolysis	Persistence, behavioral effects in aquatic organisms, and long-term low-dose exposure concerns
Preservatives	Methylparaben, propylparaben, and butylparaben	Hydroxylated or chlorinated paraben products	Wastewater transformation, chlorination, photolysis	Endocrine-disruption concerns and continuous release from cosmetics and hygiene products
UV filters	EHMC, benzophenone-3, ODPABA, octocrylene	Hydroxylated, oxidized, or photodegraded UV-filter products	Photolysis, oxidation, chlorination, and wastewater treatment	Persistence, bioaccumulation potential, coral/aquatic toxicity, and endocrine activity
Fragrances	Galaxolide, tonalide, and nitro musks	Hydroxylated or oxidized musk products	Photolysis, oxidation, and wastewater treatment	Bioaccumulation, persistence in sludge and sediments, and long-range exposure potential
Antibacterial agents	Triclosan, and triclocarban	Methyl triclosan, chlorinated triclosan derivatives, dioxin-like photoproducts	Chlorination, photolysis, methylation, and wastewater treatment	Endocrine disruption, antimicrobial resistance concerns, sediment persistence, and aquatic toxicity
Surfactants	Nonylphenol ethoxylates, and octylphenol ethoxylates	Nonylphenol, octylphenol, shorter-chain ethoxylates	Wastewater biodegradation and environmental transformation	Estrogenic activity, persistence in sediments, and toxicity to aquatic organisms
Plasticizers in personal-care products	DEP, DBP, and DEHP	Monoethyl phthalate, monobutyl phthalate, MEHP, and oxidized metabolites	Hydrolysis, metabolism, leaching, wastewater transformation	Endocrine and developmental concerns, widespread human exposure, and migration from packaging or formulations
Siloxanes	D4, D5, and D6	Oxidized or hydrolyzed siloxane products	Volatilization, atmospheric oxidation, and hydrolysis	Persistence, bioaccumulation potential, sediment partitioning, and indoor/outdoor exposure relevance
Cosmetic microplastics	Polyethylene microbeads, acrylic polymers, and glitter particles	Weathered microplastic fragments and additive leachates	UV weathering, mechanical fragmentation, oxidation, and biofilm-mediated transformation	Particle transport, additive release, sorption of pollutants, and food-web exposure

Such findings raise concerns for aquatic organisms and downstream consumers. Environmental factors influence degradation kinetics and product formation. Temperature, pH, and co-contaminants alter reaction rates and pathways [153]. Variable conditions complicate predictions of persistence and ecological impact. Conventional wastewater treatment plants often remove pesticides incompletely. Residual compounds and metabolites enter surface waters through effluent discharge. Bioaccumulation of toxic derivatives has been observed in aquatic biota. Sediments and irrigation waters also contain detectable pesticide TPs [153, 178, 179]. Monitoring these compartments remains critical for comprehensive assessment. High-resolution mass spectrometry facilitates the identification and quantification of compounds in complex matrices. Analytical advances support regulatory evaluation and exposure assessment. Systematic surveillance improves understanding of long-term environmental consequences.

2.3 Industrial chemical and plastic additive transformation products

Industrial chemicals and plastic additives represent persistent sources of TPs. Compounds such as bisphenol A (BPA) and phthalates undergo environmental degradation. Resulting byproducts may retain endocrine-disrupting or toxic properties [152, 178, 179]. BPA and several phthalates are themselves recognized endocrine-disrupting chemicals, independent of the toxicity of their transformation products. However, environmental degradation, hydrolysis, oxidation, photolysis, and microbial metabolism can generate additional by-products and metabolites with altered persistence, mobility, and biological activity. Bisphenol A diglycidyl ether (BADGE) and related hydrolysis products are receiving growing attention due to their presence in epoxy resins, food-contact materials, wastewater systems, and aquatic environments. BADGE hydrolysis products can form readily under aqueous and acidic conditions and may contribute additional toxicological and endocrine-related concerns [166]. Several phthalates have also been extensively studied for environmental transformation and biodegradation. Common examples include diethyl phthalate (DEP), dibutyl phthalate (DBP), diisobutyl phthalate (DiBP), benzyl butyl phthalate (BBP), di-(2-ethylhexyl) phthalate (DEHP), and diisononyl phthalate (DiNP). These compounds can undergo hydrolysis to monoester metabolites, which are then oxidized to alcohol, ketone, and carboxylic acid derivatives, particularly in wastewater, soil, sediment, and microbial environments [66, 171].

Structural modification does not necessarily reduce biological activity. Transformation rates depend on environmental parameters and biological activity [152, 153]. Wastewater treatment processes influence product formation and distribution. Incineration can degrade parent compounds but may generate secondary hazardous substances [152, 180]. Evaluation of treatment byproducts remains limited in many regulatory contexts. Emerging contaminants lack comprehensive oversight mechanisms. Regulatory frameworks frequently exclude newly identified TPs [136, 148, 150]. The absence of standardized monitoring reduces the capacity to mitigate risk. Integrated management strategies are necessary for effective pollution control. Coordinated policy development can address gaps in oversight.

2.4 PFAS and ultra-persistent transformation derivatives

Per- and polyfluoroalkyl substances exhibit exceptional environmental persistence. They comprise a broad and structurally diverse class that includes terminal perfluoroalkyl acids, perfluoroalkyl carboxylic acids, perfluoroalkyl sulfonates, fluorotelomer alcohols, fluorotelomer sulfonates, perfluoroalkyl sulfonamides, sulfonamidoethanols, ether PFAS, and other precursor or replacement compounds. These subclasses differ in environmental sources, transformation potential, mobility, bioaccumulation, analytical detectability, and toxicological relevance. Terminal perfluoroalkyl acids such as PFOA and PFOS are highly persistent, while many precursor compounds, including fluorotelomer alcohols and sulfonamide-based PFAS, may undergo microbial, oxidative, or abiotic transformation to form terminal perfluoroalkyl acids [79, 82]. This distinction is important because precursor-derived products can extend exposure duration, complicate remediation, and cause underestimation of total PFAS burden when monitoring focuses only on a limited number of target compounds [121, 191].These compounds resist degradation during conventional wastewater treatment [136, 149]. Transformation processes may produce derivatives with comparable or greater toxicity. Ultra-persistent metabolites complicate remediation efforts. Bioaccumulation of PFAS TPs has been documented in aquatic organisms [132, 136]. Trophic transfer can amplify exposure risks across food webs. Human health concerns arise from contaminated drinking water and seafood consumption. Conventional treatment technologies demonstrate limited removal efficiency. Emerging treatment methods show improved performance against PFAS contamination. Foam fractionation and electrochemical oxidation enhance removal compared to traditional approaches [148–150]. Continued research supports optimization of these technologies. Effective removal prior to environmental discharge remains a priority [148–150]. Regulatory measures increasingly address PFAS use and disposal. Stricter guidelines may reduce long-term environmental accumulation.

2.5 Transformation products generated during wastewater and drinking-water treatment

Treatment processes can generate additional TPs. Physical, chemical, and biological reactions alter contaminant structures [74, 180]. Treatment-generated TPs differ from parent compounds through structural changes such as oxidation, hydroxylation, halogenation, hydrolysis, ring opening, side-chain cleavage, dealkylation, demethylation, or conjugation. These modifications can change polarity, molecular weight, solubility, persistence, mobility, detectability, and toxicity. Thus, treatment should be viewed not only as contaminant removal but also as a transformation process that requires product-level monitoring.. Conventional treatment methods often fail to eliminate all contaminants [148, 150, 180]. Residual metabolites can persist in treated effluents and drinking water supplies. Advanced technologies such as membrane filtration and oxidation processes improve removal efficiencies [74, 148, 150]. Enhanced treatment reduces the environmental discharge of harmful byproducts. Characterization and monitoring of treatment-generated products remain essential. Untreated or partially removed metabolites may contribute to adverse health outcomes [148, 150]. Regulatory frameworks increasingly emphasize integrated monitoring of parent compounds and derivatives [85, 136]. Adoption of advanced treatment methods supports improved water quality protection.

Ongoing research strengthens the understanding of formation pathways and mitigation strategies.

Wastewater treatment plants are typically regulated according to influent acceptance criteria and final effluent discharge limits. However, such regulatory systems often do not fully assess the potential for accepted chemicals to transform during treatment processes, thereby generating secondary products that may not be captured in routine permitting or monitoring frameworks. This creates an important regulatory blind spot, as treatment itself may function not only as a removal system but also as a transformation environment for emerging contaminants and their derivatives [57, 73]. Similar challenges apply to atmospheric emissions, where permitted stack discharges may undergo post-release transformation through thermal mixing, plume interactions, and contact with emissions from nearby industrial processes, including cooling-tower systems. Disinfection by-products represent a major group of treatment-generated transformation products with direct public health implications. Classic DBPs, including trihalomethanes and haloacetic acids, form when disinfectants such as chlorine react with natural organic matter, bromide, iodide, or anthropogenic organic contaminants during drinking-water and wastewater treatment. These compounds are important because they demonstrate that treatment processes can reduce microbial risk while simultaneously generating secondary chemical hazards. Several DBPs have been associated with genotoxicity, carcinogenicity, reproductive concerns, and long-term human exposure through ingestion, inhalation, and dermal contact. Their inclusion strengthens transformation-product assessment by linking emerging-contaminant transformation with the established literature on treatment-derived chemical risk.

3 Formation pathways and transformation mechanisms of emerging contaminants

As the prevalence of emerging contaminants (ECs) in environmental systems increases, it is important to clarify the mechanisms through which parent compounds are converted into transformation products (TPs). TPs may form through microbial biotransformation, photolysis, hydrolysis, abiotic degradation, oxidation–reduction reactions, and engineered treatment processes such as ozonation, UV/H_2O_2, and other advanced oxidation processes [33, 34, 71, 78, 98, 103]. These mechanisms rarely occur in isolation,rather, parent compounds may undergo sequential or parallel reactions that generate interconnected transformation-product networks with different persistence, mobility, toxicity, and exposure relevance [15, 24, 189]. Figure 2 illustrates the major biotic and abiotic mechanisms responsible for TP formation from parent contaminants, including microbial metabolism, photolysis, hydrolysis, oxidation–reduction reactions, and treatment-associated transformations. Table 4 summarizes these mechanisms and highlights environmental conditions, such as pH, sunlight exposure, redox status, microbial activity, oxidant dose, organic matter, and temperature, that regulate reaction kinetics and product stability.

3.1 Microbial biotransformation processes

Microbial biotransformation represents a central mechanism in the degradation of emerging contaminants. Several bacterial genera and species have been associated with

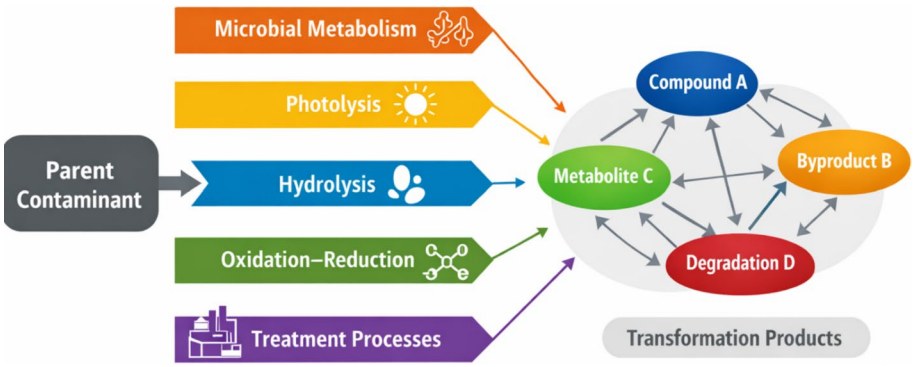

Fig. 2 Integrated biotic and abiotic transformation pathways. Key: The labels indicate the main transformation pathways: Compound A = microbial biotransformation; Byproduct B = photochemical transformation; Metabolite C = hydrolysis and other abiotic degradation reactions; and Degradation D = oxidation–reduction and treatment-associated transformation processes. These pathways are not isolated categories; they may occur sequentially or simultaneously in natural waters, soils, sediments, wastewater systems, and drinking-water treatment processes. Their interaction can generate interconnected transformation-product networks with different persistence, mobility, toxicity, and exposure relevance

the biotransformation of emerging contaminants and the formation of transformation products. Commonly reported examples include *Pseudomonas, Sphingomonas, Rhodococcus, Bacillus, Agrobacterium, Terrabacter, and other members of Proteobacteria, Actinobacteria,* and *Firmicutes*. For example, *Rhodococcus* strains have been linked to the transformation and dehalogenation of halogenated compounds, while *Sphingomonas, Agrobacterium, Terrabacter,* and *Pseudomonas* species have been reported to participate in the aerobic degradation of dioxin-like and aromatic contaminants [98, 205, 206]. *Bacillus* species have also been associated with aerobic transformation of nitroaromatic compounds [206]. These bacterial groups may contribute through enzymatic processes such as hydrolysis, dehalogenation, oxidation, reduction, hydroxylation, ring cleavage, demethylation, and conjugation. However, the specific bacterial taxa involved vary across contaminant classes, treatment systems, soils, sediments, and aquatic environments [98, 205, 206]. Microorganisms metabolize xenobiotic compounds through diverse enzymatic pathways. Gene products linked to these pathways reveal complex interactions between microbes and pollutants [4]. Expression patterns vary across environmental gradients and contaminant concentrations. Activated sludge systems illustrate these relationships in engineered environments. Associations between gene expression and micropollutant removal have been documented [3, 26]. Community composition influences degradation efficiency and metabolite formation. Functional redundancy within microbial consortia supports resilience under fluctuating conditions. Fungal species also contribute to contaminant transformation. Phanerochaete chrysosporium demonstrates the capacity to degrade 6:2 fluorotelomer alcohol [164]. Fungal enzymes mediate oxidative and reductive reactions that alter compound structure. These pathways expand understanding of ecological roles in pollutant turnover. Complex contaminant mixtures further shape microbial adaptation. Soils receiving agricultural runoff or industrial discharge contain diverse xenobiotics. Microbial communities adjust degradation pathways in synergistic manners [72, 177]. Such interactions influence bioremediation outcomes

Table 4 Mechanisms of transformation product formation

Transformation mechanism	Biotic / abiotic classification	Key controlling environmental factors	Typical contaminant groups affected	Relative persistence of resulting products	Typical product characteristics	Main analytical implication	Risk relevance
Microbial metabolism	Biotic	Microbial community composition, nutrient availability, temperature, oxygen status, and redox condition	Pharmaceuticals, pesticides, PFAS precursors, and industrial chemicals	Moderate to high	Metabolites may be more polar, mobile, bioactive, or further degradable	Requires pathway tracing, metabolite identification, and microbial-context interpretation	May reduce parent-compound toxicity but can also generate persistent or biologically active metabolites
Photolysis	Abiotic	Solar radiation intensity, wavelength, dissolved organic matter, water depth, turbidity, photosensitizers	Pesticides, pharmaceuticals, plastic additives, UV filters	Variable	Photo-products may be short-lived, reactive, or more toxic than parent compounds	Requires time-sensitive sampling and suspect/non-target screening	Important in sunlit surface waters, wetlands, and shallow aquatic systems
Hydrolysis	Abiotic	pH, temperature, water chemistry, functional groups, ionic strength	Industrial chemicals, pesticides, and pharmaceuticals	Low to moderate, but context-dependent	Products often reflect cleavage of ester, amide, lactam, or other hydrolyzable bonds	Requires pH-specific and temperature-specific interpretation	Can reduce persistence but may produce products with altered mobility or toxicity
Oxidation–reduction reactions	Abiotic/biotic	Redox potential, oxygen availability, electron donors/acceptors, metal catalysts, sediment chemistry	Chlorinated solvents, pesticides, PFAS precursors, industrial chemicals	Moderate to high	Products may be dehalogenated, oxidized, reduced, or converted into more mobile intermediates	Requires redox-sensitive sampling, pathway-specific identification, and comparison of oxidized and reduced products across environmental matrices	Can generate persistent, mobile, or more toxic intermediates, especially in sediments, groundwater, wastewater systems, and redox-variable environments

and metabolite profiles. Examination of microbial ecology can be used to inform management of contaminated environments.

3.2 Photochemical transformation reactions

Photochemical reactions strongly influence contaminant fate in sunlit environments. Aquatic ecosystems permit penetration of ultraviolet and visible radiation. Absorption of photons generates reactive species that initiate degradation pathways. Hydroxyl radicals often serve as primary oxidizing agents. Ozone is also an important and ubiquitous oxidant in environmental and engineered systems, where it can react directly with susceptible contaminants or indirectly generate reactive oxygen species that promote TP formation. Advanced oxidation processes employing UV light, ozone, and hydrogen peroxide enhance the breakdown of recalcitrant organics. Petre et al. [117] describe radical formation under combined irradiation and oxidant conditions. Reaction kinetics depend on spectral properties and activation energies [77, 138]. Product distribution varies according to contaminant structure and irradiation intensity. Interactions between photochemical and biological processes also occur. Engineered wetlands demonstrate light-enhanced microbial transformation of pharmaceuticals [165]. Photochemical reactions can increase substrate availability for microbial metabolism. Coupled dynamics improve overall contaminant removal efficiency. Consideration of these interactions refines predictive assessments of environmental fate.

3.3 Hydrolysis and abiotic chemical degradation

Hydrolysis constitutes a significant pathway for the transformation of many organic contaminants. Reaction rates depend on pH, temperature, and molecular structure. Aqueous conditions often facilitate cleavage of susceptible functional groups. Pharmaceuticals such as β-lactams undergo hydrolytic breakdown [23, 30]. Abiotic chemical degradation may yield products with altered toxicity. Structural modification does not guarantee reduced ecological impact. Dichloroacetamide herbicides illustrate this complexity. Microbial and abiotic pathways generate multiple byproducts requiring further characterization [98, 187, 188]. Comprehensive assessment of hydrolysis products remains necessary for accurate risk evaluation.

3.4 Oxidative and reductive environmental reactions

Oxidative and reductive reactions determine transformation pathways in diverse environments. Oxidative mechanisms often involve reactive oxygen species or chemical oxidants. Advanced oxidation techniques applied to chloronitrobenzenes demonstrate potential mineralization [8, 155]. Intermediate products, however, may persist and require further treatment.

Reductive processes frequently dominate in anaerobic settings. Anaerobic bacteria mediate reductive dehalogenation of halogenated organics [143]. Electron donor availability influences reaction efficiency and pathway selection. Iliakopoulou [60] emphasizes the relevance of these reactions in subsurface environments. Such processes contribute to detoxification and attenuation of persistent contaminants. Understanding redox dynamics enhances the design of remediation strategies.

3.5 Transformation during advanced oxidation and treatment processes

Advanced oxidation processes provide powerful tools for the remediation of persistent pollutants. Strong oxidants generate hydroxyl radicals that fragment complex molecules. Treatment efficacy depends partly on microbial community structure. Hernández et al. [51] report interactions between microbial populations and oxidation efficiency. Specific microbial groups can metabolize intermediate products formed during oxidation [10, 72]. Integration of biological and chemical pathways enhances the removal of both parent compounds and derivatives. Operational parameters such as oxidant dosage and contact time influence outcomes. Lyu et al. [94] highlight optimization strategies balancing biological and chemical processes. Kim et al. [75] also stress careful parameter adjustment for comprehensive degradation. Coordinated treatment design improves overall contaminant removal.

3.6 Coupled multi-pathway transformation networks

Environmental contamination rarely involves single transformation pathways. Interactions among microbial, photochemical, hydrolytic, and redox processes create complex networks. Systems biology and multi-omics approaches enable mapping of these interactions [65]. Integrated datasets reveal functional links among microbial communities and chemical reactions. Coupled pathways may generate synergistic degradation effects. Sequential aerobic and anaerobic stages enhance micropollutant removal [102, 184]. Aerobic metabolism can transform compounds into intermediates suitable for anaerobic degradation. Such staged processes support advanced bioremediation strategies. Kinetic interplay among pathways influences persistence and product formation. Jones et al. [67] emphasize predictive modeling frameworks incorporating multi-pathway data. Integrated models improve the assessment of environmental risk associated with emerging contaminants. Continued methodological advances support a refined understanding of transformation networks. These developments strengthen the capacity to manage complex contaminant mixtures across environmental systems.

3.7 Reversible transformation and back-conversion processes

Back-conversion is a critical but often overlooked process in transformation-product assessment because chemical transformation does not always proceed in a linear manner from the parent compound to a less active degradation product [41]. Some transformation products may revert to their parent compounds or form structurally related products with renewed biological activity under plant-mediated, microbial, photochemical, hydrolytic, or redox conditions [41, 58]. The methyl triclosan–triclosan system illustrates this concern because triclosan can undergo methylation to form methyl triclosan, a more hydrophobic and less photodegradable transformation product that may accumulate in aquatic organisms [122]. Plant-mediated back-conversion from methyl triclosan to triclosan has also been demonstrated, showing that a transformation product can regenerate the parent compound after uptake into biological systems [41]. This process is environmentally important because it can reintroduce a bioactive parent compound after apparent transformation, alter exposure timing, affect bioavailability, and complicate the interpretation of monitoring data

[41, 122]. Back-conversion also suggests that risk assessment should evaluate parent compounds and transformation products as interconnected chemical networks rather than as separate static endpoints [41, 58]. Incorporating reversible, sequential, and back-conversion transformations into monitoring and predictive models would improve estimates of persistence, exposure, and long-term ecological risk [41, 122].

4 Environmental fate, transport, and persistence

Environmental fate, transport, and persistence are central to transformation-product risk assessment because formation alone does not determine exposure. Once formed, TPs may degrade further, persist, bind to sediments, move through surface water or groundwater, pass through treatment systems, or become bioavailable to organisms [43, 145]. These outcomes are controlled by solubility, polarity, ionization, sorption, degradation half-life, pH, redox conditions, microbial activity, hydrology, and temperature. Understanding these processes is therefore necessary for identifying mobile, persistent, bioavailable, or regulatory-relevant transformation products [33, 34, 88]. Water solubility may indicate the aqueous mobility of TPs, but it is not sufficient on its own to measure environmental circulation. More soluble and polar TPs may remain in water and move through surface water, groundwater, wastewater effluent, and drinking-water systems. However, actual circulation depends on persistence, ionization state, sorption, degradation rate, hydrology, pH, organic matter, and treatment conditions [33, 34, 43, 145]. Figure 3 illustrates the environmental distribution pathways of TPs following their formation, highlighting partitioning and transport processes across major environmental compartments. Transformation products originating from a central pool disperse into water, soil, sediment, and atmospheric systems through processes such as sorption, volatilization, runoff, and atmospheric deposition. The conceptual framework (Fig. 3) emphasizes the interconnected nature of environmental compartments and demonstrates how physicochemical properties and environmental conditions jointly influence the mobility, persistence, and exposure potential of TPs within coupled environmental systems.

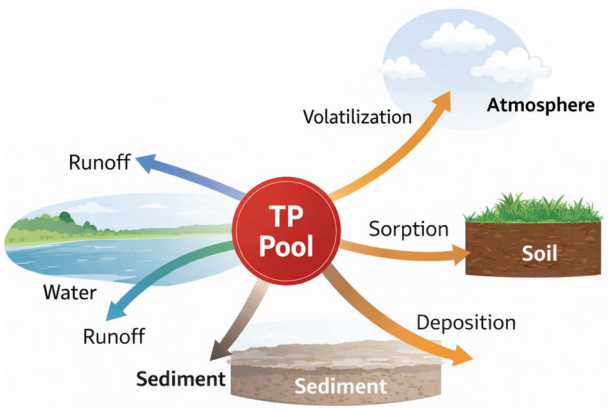

Fig. 3 Environmental fate and transport of transformation products

4.1 Physicochemical determinants of persistence and mobility

The persistence and mobility of emerging contaminants (ECs) are closely linked to their physicochemical properties, which govern their partitioning across various environmental matrices. Key properties include hydrophobicity, molecular weight, solubility, and volatility. Compounds with higher hydrophobicity often exhibit stronger sorption to organic matter in soils and sediments, thereby limiting their mobility and increasing their environmental persistence [11, 178, 179]. Conversely, more water-soluble contaminants tend to migrate more easily through soil and water systems [17, 48]. For instance, substances such as clomazone, an isoxazole herbicide, exhibit low sorption in sandy soils but higher sorption in organic-rich soils. This indicates that contaminants can behave differently depending on soil composition, thereby directly affecting their bioavailability and potential for long-range transport [48, 76]. Additionally, pollutants can undergo biotransformation, leading to the formation of metabolites that may possess different physicochemical properties, thereby further complicating their environmental behavior [14, 17, 42]. Table 5 presents the principal physicochemical parameters governing transformation-product persistence, mobility, partitioning behavior, and long-range environmental transport potential across environmental compartments.

4.2 Partitioning across environmental compartments

Partitioning across water, soil, sediment, and atmosphere determines contaminant fate. Distribution processes influence persistence, mobility, and exposure pathways. Contaminants interact with suspended particles, sediments, and biological tissues [17, 42, 158]. Sorption and desorption processes regulate movement between compartments. Hydrophobic compounds often associate with organic matter and sediments. Hydrophilic substances remain more mobile in aqueous phases. Partition coefficients provide estimates of environmental distribution tendencies. Variability in temperature, pH, and organic carbon content modifies these interactions. Environmental heterogeneity often shapes TPs' behavior.

Semi-permeable membrane devices have been used to assess partitioning in aquatic systems. These devices simulate passive uptake by organisms and sediments [25, 168]. Measurements from such tools reveal contaminant exchange between dissolved and particulate phases. Data derived from these methods support the modeling of exposure pathways. Acetochlor provides an example of context-dependent partitioning. Its behavior depends partly on interactions with soil microbial communities [25, 192, 193]. Microbial activity alters degradation rates and influences accumulation in nearby waters. Co-occurring contaminants and environmental conditions can shift partition equilibria. Such variability complicates predictions of transformation product distribution. Comprehensive assessment requires integration of chemical properties and ecological dynamics.

4.3 Bioavailability and trophic transfer potential

Bioavailability determines the extent to which contaminants can be absorbed by organisms. Absorption influences toxicity, metabolism, and ecological risk. Transformation products may differ substantially from parent compounds in uptake

Table 5 Transformation-product-specific physicochemical drivers of environmental fate and risk

Property	TP-specific relevance	Matrix/environmental modifiers	Effect on mobility and persistence	Risk implication
Water solubility	Many TPs are more polar and water-soluble than parent compounds	pH, salinity, dissolved organic matter, temperature	Can increase aqueous mobility and groundwater transport, but may reduce sediment sorption	Higher potential for drinking-water contamination and long-range aquatic exposure
Partition coefficient, Kow / Koc	Traditional Kow may poorly predict the fate of polar, ionizable, or charged TPs	Organic carbon, sediment type, black carbon, ionic strength, co-contaminants	Hydrophobic TPs may sorb to sediments; polar or ionized TPs may remain mobile despite low Kow	Possible underestimation of mobile TPs when parent-compound descriptors are used
Molecular stability	Determines whether TPs persist or undergo further transformation	Sunlight, redox status, microbial activity, pH, temperature	Stable TPs may persist after parent-compound degradation; unstable TPs may form secondary products	Long-term exposure risk and formation of secondary or tertiary TPs
Vapor pressure/volatility	Relevant for volatile or semi-volatile TPs formed from solvents, pesticides, and industrial chemicals	Temperature, air–water exchange, aerosols, indoor air chemistry	Can support atmospheric transport or redistribution between air, water, and surfaces	Regional or indoor exposure risk through inhalation and deposition
Ionization state, pKa	Critical for polar and charged TPs often missed by neutral-compound models	Environmental pH, mineral surfaces, dissolved ions, and organic matter	Controls pH-dependent sorption, membrane uptake, and transport across water, soil, and sediment	Site-specific risk, especially in groundwater, wastewater, and variable-pH systems

potential [84, 108]. Structural changes can increase polarity or alter membrane permeability. Atrazine metabolites illustrate variability in bioavailability. Differences in molecular structure influence organismal uptake and toxicity [14, 84, 108]. A study on common carp exposed to atrazine reported physiological alterations at sublethal levels [14]. Observed changes included shifts in blood parameters and histopathological effects. These findings indicate that TPs can remain biologically active. Trophic transfer amplifies ecological implications. Contaminants absorbed by primary producers or invertebrates can move through food webs. Lipophilic derivatives may bioaccumulate in higher trophic levels. Microbial degradation processes further influence bioavailability [100, 158]. Microbial activity can reduce toxicity by mineralizing compounds or increase exposure by forming reactive intermediates. Risk assessment must therefore consider dynamic interactions between degradation and uptake.

4.4 Long-range environmental transport

Long-range transport presents significant concerns for persistent contaminants. Volatile or low-molecular-weight compounds may undergo atmospheric dispersion [172, 178, 179]. Hydrophobic substances associate with particulate matter and are transported by water currents [158]. Transport processes expand contamination beyond original release sites. Agricultural runoff contributes to the regional dispersion of pesticides and derivatives. Modeling studies indicate persistence long after application [17, 70]. Long-range transport refers to the capacity of a chemical or transformation product to move far from its original source through atmospheric circulation, riverine transport, ocean currents, groundwater movement, or repeated deposition and remobilization across environmental compartments. It differs from general or extended transport, which may simply describe movement within a local or catchment-scale system. For transformation products, long-range transport is most relevant when compounds are sufficiently persistent, mobile, and resistant to degradation, thereby remaining detectable beyond the point of formation or release [13, 38, 137]. Seasonal precipitation and irrigation patterns influence the movement of water into surface and groundwater systems. Such processes enable exposure in distant ecosystems. PFAS represent a notable example of extended transport. These substances have been detected in groundwater and sediments years after their use ceased. Modeling efforts highlight the persistence and delayed attenuation of these effects [16, 129, 135]. Environmental conditions and transformation pathways affect mobility predictions. Comprehensive transport assessments must incorporate chemical properties and landscape characteristics. obile TPs may travel through surface runoff, groundwater recharge, river networks, wastewater effluent, irrigation return flows, and drinking-water abstraction systems. Over the long term, this transport can expand exposure beyond the original source area, complicate remediation, and increase risks to downstream communities and ecosystems. For policy-makers, mobility assessment supports decisions on monitoring priorities, drinking-water protection, catchment-scale regulation, source control, and inclusion of persistent and mobile TPs in risk-assessment frameworks [33, 34, 43, 145].

4.5 Indoor air transformation processes and health implications

Indoor environments represent an important but often underrepresented setting for the transformation of emerging contaminants. Unlike outdoor environments, indoor spaces contain complex mixtures of volatile and semi-volatile organic compounds released from cleaning agents, personal-care products, building materials, furnishings, pesticides, cooking emissions, and human occupants. These compounds may undergo gas-phase and surface-mediated reactions involving ozone, hydroxyl radicals, nitrate radicals, moisture, and indoor particles, producing secondary TPs with distinct exposure and toxicity profiles [174, 175]. For example, reactions of ozone with terpenes such as limonene, commonly emitted from fragranced cleaning and personal-care products, can generate aldehydes, organic acids, hydroperoxides, and secondary organic aerosols that may irritate the respiratory tract and contribute to asthma or allergy-related symptoms [106, 175].

Indoor surfaces also function as reactive reservoirs where semi-volatile compounds sorb, persist, and undergo delayed transformation. Surface films, settled dust, textiles, and human skin lipids can mediate chemical reactions and prolong exposure even after the original source has been removed [173, 174]. This is particularly relevant because people spend substantial time indoors, increasing the likelihood of inhalation, dermal contact, and incidental dust ingestion. The health implications of indoor TPs are therefore significant, especially for vulnerable groups such as children, older adults, and individuals with asthma or compromised respiratory health. Incorporating indoor air chemistry into transformation-product assessment broadens the review beyond wastewater, soil, and outdoor environmental matrices and highlights the need for integrated monitoring of indoor–outdoor exposure pathways. This concern is also relevant to indoor environments, where pollutant sources, ventilation, temperature, humidity, and indoor activities can influence contaminant concentrations, transformation processes, and human exposure risks, particularly through inhalation of volatile compounds and fine particles [5, 174].

4.6 Transformation-product accumulation and environmental reservoirs

Accumulation of TPs in environmental reservoirs poses sustained risks. Soils, sediments, and biota can act as long-term storage compartments. Persistent metabolites may remain detectable long after parent compound degradation [41, 76, 135]. Anaerobic conditions can alter transformation pathways and increase persistence. Certain contaminants become stable in deeper soil layers or aquifers [45, 86, 87]. Reduced oxygen availability modifies microbial metabolism and reaction kinetics. Accumulation in subsurface environments complicates remediation efforts. Sediment contamination provides an additional illustration. Fipronil residues detected in sediments have been linked to treated wastewater discharge [52, 170]. Elevated concentrations pose risks to benthic organisms and ecosystem integrity. Reservoir compartments may release stored contaminants under changing environmental conditions. A comprehensive risk assessment requires evaluating both parent compounds and TPs. Environmental reservoirs extend exposure duration and spatial reach. Understanding partitioning, bioavailability, transport, and accumulation strengthens predictive frameworks. Integrated monitoring and

modeling approaches support informed regulatory decisions and ecosystem protection. Several studies show that transformation products and related emerging contaminants occur at measurable concentrations in aquatic systems, groundwater, wastewater-impacted rivers, and biota [207]. For example, pharmaceutical parent compounds and transformation products have been detected in wastewater-receiving rivers at ng/L to µg/L levels, with concentrations depending on effluent dilution, river discharge, compound persistence, and in-stream attenuation. Li et al. [207] reported the presence of pharmaceuticals and selected TPs in four small European rivers receiving treated wastewater, showing that some compounds persisted downstream, while others attenuated through photolysis, sorption, or biotransformation. Stuart and Lapworth also summarized the groundwater and drinking-water relevance of TPs, including pesticide and pharmaceutical-related products detected at ng/L levels. These findings indicate that mobile and persistent TPs may contribute to long-term exposure through surface water, groundwater, bank filtrate, and drinking water.

Biological uptake is also relevant where TPs or related contaminants remain bioavailable. Aquatic plants, benthic invertebrates, aquatic insects, and fish may accumulate contaminants through direct water exposure, sediment contact, or dietary uptake. Such uptake can extend exposure beyond the water column and may support trophic transfer across aquatic and riparian food webs. Thus, concentration data should be interpreted alongside persistence, mobility, bioavailability, and uptake potential when assessing environmental and human health implications.

5 Ecotoxicological and human health implications of TPs of emerging contaminants

TPs of emerging contaminants present complex environmental and public health challenges. Many TPs originate from pharmaceuticals, industrial chemicals, and agricultural inputs. These derivatives may differ substantially from the parent compounds in terms of toxicity and persistence. Ecotoxicological evaluation increasingly recognizes their relevance to ecosystem integrity. Table 4 summarizes major toxicity mechanisms, exposure pathways, and documented ecological outcomes. Toxicological evidence for transformation products varies in strength and should not be interpreted uniformly. Some effects are supported by direct experimental evidence from in vivo, in vitro, or organism-level assays, while others are based on correlation analysis, environmental co-occurrence, QSAR prediction, or suspect/non-target screening prioritization. Direct experimental evidence is strongest when exposure concentration, organism response, and mechanistic endpoint are clearly linked. Correlation-based and predicted toxicity results are useful for prioritization but require confirmatory testing before regulatory interpretation. Transformation products may also differ from parent compounds in toxicity mechanisms because transformation can alter polarity, receptor binding, membrane permeability, persistence, metabolic activation, and bioavailability [33, 34, 208]. Toxicological assessment of TPs should distinguish acute endpoints such as LC50 and EC50 from chronic endpoints such as NOEC, LOEC, reproductive effects, developmental abnormalities, growth inhibition, and behavioral changes, while also considering mechanisms of action, including oxidative stress, endocrine disruption, genotoxicity, neurotoxicity, developmental toxicity, immunotoxicity, and microbial community disruption.

5.1 Mechanisms of toxicity of transformation products

Transformation products frequently retain biological activity following chemical modification. In some cases, toxicity increases relative to the parent compound. Methadone bio-TPs demonstrated ecotoxicological effects on freshwater algae [209]. Observed impacts suggest potential disruption of primary production in aquatic systems. Physicochemical characteristics influence toxic interactions with organisms. Hydrophobicity, polarity, and functional groups determine membrane permeability and receptor binding. Transformation products of selective serotonin reuptake inhibitors and beta-blockers illustrate this complexity. Laboratory studies suggested limited acute toxicity under controlled conditions [18]. Ecological concern persists due to exposure in effluent-dominated water bodies. Chronic exposure scenarios may yield different outcomes than short-term testing. Metabolic activation can further modify toxicity profiles. Biotransformation may generate reactive intermediates that can induce oxidative stress. Escher and Fenner [33, 34] emphasize inclusion of both acute and chronic endpoints in risk assessments. Comprehensive evaluation requires a mechanistic understanding of cellular and molecular interactions. Such approaches strengthen predictive frameworks for environmental safety.

5.2 Chronic and sub-lethal ecological effects across trophic levels

Chronic exposure to TPs can alter ecosystem structure and function. Sub-lethal concentrations may influence growth, reproduction, and behavior. Pesticide TPs have persisted in aquatic systems following agricultural application. Accumulation in sediments and biota contributes to long-term exposure. Persistent organic pollutants and associated derivatives may bioaccumulate in higher trophic levels. Fish consuming contaminated prey can exhibit elevated internal concentrations [181]. Such accumulation can impair immune function and reproductive success. Community-level effects may include shifts in species composition. Reduced abundance of sensitive taxa weakens ecosystem resilience. For example, 6PPD-quinone, a transformation product of the tire antioxidant 6PPD, has been linked to acute mortality in coho salmon, demonstrating how a product formed from environmental transformation can have severe population-level implications [169]. Pharmaceuticals, pesticides, PFAS, plastic additives, and other emerging contaminants have also been associated with reproductive impairment, behavioral changes, immune disruption, and endocrine-related effects in aquatic organisms. These sub-lethal effects may reduce reproductive success, alter predator–prey relationships, and weaken the abundance of sensitive taxa. At the community level, chronic exposure may shift species composition by favoring tolerant organisms while reducing sensitive taxa, thereby weakening ecosystem resilience. Trophic effects may also extend beyond aquatic systems. Aquatic insects and other organisms can transfer contaminants from water and sediment into riparian food webs, exposing terrestrial predators such as spiders and insectivorous organisms. These examples show that transformation-product risk assessment should consider not only acute toxicity but also sub-lethal effects, community change, trophic transfer, and long-term ecological monitoring [169]. Altered trophic interactions may extend beyond aquatic systems. Terrestrial predators relying on aquatic organisms can experience indirect exposure. Food web disruptions can have broader ecological implications. Long-term ecological monitoring remains essential for

detecting gradual population declines. Recognition of sub-lethal effects improves understanding of cumulative ecosystem stress.

5.3 Mixture toxicity and cumulative exposure risks

Environmental matrices typically contain mixtures of parent compounds and TPs. Interactions among contaminants may result in additive or synergistic toxicity. Lao et al. [83] and Guo et al. [49] report enhanced toxicity under mixture exposure conditions. Combined effects can exceed predictions based on single-compound testing. Activated sludge treatment processes sometimes generate TPs with elevated ecotoxicological risk [73]. Effluent discharges, therefore, introduce complex chemical mixtures into receiving waters. Continuous low-level exposure complicates traditional risk evaluation frameworks. Brown et al. [18] highlight concerns about chronic exposure to pharmaceuticals and their derivatives. Cumulative exposure may contribute to subtle health impacts over time. Behavioral, endocrine, or metabolic disruptions may not manifest immediately. Standard toxicity thresholds may underestimate mixture-driven risks. Integrated mixture assessment models are necessary for accurate environmental management. Such approaches enhance the protection of sensitive species and ecosystems.

5.4 Human exposure pathways and biomonitoring evidence

Human exposure to TPs occurs through multiple routes (Table 6). Drinking water contamination represents a primary pathway. Surface water influenced by wastewater discharge may contain persistent derivatives [181]. Inadequate treatment increases the potential for human ingestion. Biomonitoring studies provide direct evidence of exposure. Pharmaceutical TPs have been detected in urine and blood samples [81]. Detection confirms transfer from environmental matrices into human systems. Ghazi et al. [46] reported associations between certain transformation products and developmental or reproductive effects. This point is fundamental because transformation products may enter the human body through drinking water, food, inhalation, dermal contact, and consumer-product exposure, yet many remain poorly characterized toxicologically. Biomonitoring evidence from related contaminant groups, including phthalate metabolites, bisphenol analogs, and PFAS, demonstrates that human exposure can be detected in biological matrices and may be linked to endocrine, developmental, reproductive, or metabolic outcomes [171]. Such findings underscore the need for precautionary regulation. Advances in analytical chemistry improve detection in complex matrices, while high-resolution techniques enhance identification of trace-level contaminants [29]. Improved monitoring supports evaluation of exposure trends and risk mitigation strategies. Continued refinement of biomonitoring methods strengthens public health surveillance.

Case studies further illustrate ecological and health implications. Conazole antifungal TPs have demonstrated toxicity to sensitive fish species [96]. Glyphosate derivatives have been characterized as probable carcinogenic risks in environmental contexts [160]. Antimicrobial TPs may promote antibiotic resistance in aquatic microbial communities [199]. Antimicrobial transformation products may promote antibiotic resistance in aquatic and sediment microbial communities, particularly when legacy pollution, industrial residues, or conflict-related environmental detritus create selective pressures that favor resistant organisms and the persistence of

Table 6 Ecotoxicological and human health effects of transformation products

Transformation product type	Main exposure pathway	Dominant toxicity mechanism	Affected organisms/systems	Exposure concern	Relative evidence strength	Major uncertainty	Overall risk interpretation
Pharmaceutical metabolites and TPs	Drinking water, wastewater effluent, and aquatic food webs	Endocrine disruption, oxidative stress, behavioral alteration, and chronic toxicity	Fish, algae, invertebrates, amphibians, and humans	Continuous low-dose exposure in effluent-impacted waters	Moderate	Limited chronic toxicity data and incomplete mixture-risk assessment	Moderate to high concern, especially in wastewater-impacted aquatic systems
Pesticide and herbicide degradation products	Agricultural runoff, soil contact, food residues, and sediment exposure	Neurotoxicity, endocrine disruption, oxidative stress, and developmental toxicity	Aquatic organisms, pollinators, birds, soil biota, and humans	Episodic but potentially high exposure after application and rainfall events	High	Strong variation across pesticide type, soil chemistry, pH, sunlight, and species sensitivity	High concern where persistent or more toxic degradates form
PFAS terminal products	Drinking water, groundwater, food chains, and seafood consumption	Developmental toxicity, immunotoxicity, endocrine disruption, and metabolic effects	Humans, mammals, aquatic organisms, and wildlife	Long-term exposure due to persistence, mobility, and bioaccumulation	High	Incomplete precursor identification and uncertain toxicity of many replacement PFAS	Very high concern because of persistence, mobility, and chronic exposure potential
Plastic additive derivatives	Food packaging migration, landfill leachate, dust, and aquatic exposure	Hormonal interference, developmental toxicity, metabolic disruption, and oxidative stress	Humans, aquatic species, benthic organisms, and wildlife	Chronic exposure through consumer products, food contact materials, and environmental release	Moderate	Poorly characterized additive mixtures and limited data on degradation products	High concern, especially for endocrine-active additives and their derivatives
Industrial chemical transformation products	Industrial discharge, contaminated soil, sediments, air emissions, and occupational exposure	Carcinogenicity, cytotoxicity, organ toxicity, and oxidative stress	Humans, benthic organisms, microbial communities, and aquatic species	Site-specific exposure near industrial, waste, and remediation settings	Moderate	Diverse chemical structures and limited monitoring of secondary products	Moderate to high concern depending on persistence, toxicity, and exposure setting

resistance genes [133, 199]. Promotion of resistant strains introduces additional ecological and clinical concerns. Resistance genes can disseminate through environmental reservoirs. Such developments bridge environmental contamination and human health challenges. Comprehensive evaluation of TPs supports ecosystem protection and disease prevention.

A further concern is combined exposure to mixtures of parent compounds and multiple transformation products. In real environmental systems, organisms are rarely exposed to a single compound, and additive, synergistic, or antagonistic effects may occur. Novel transformation products detected through suspect and non-target screening are especially important because they may be structurally unknown, lack reference standards, and have limited toxicity data. These compounds should be treated as prioritization candidates for further testing rather than assumed to be harmless. This is particularly relevant for wastewater effluents, agricultural runoff, contaminated sediments, and treatment systems where transformation products may co-occur with parent compounds and other stressors.

6 Analytical detection and monitoring technologies for transformation products of emerging contaminants

Emerging contaminants, particularly pharmaceuticals and personal care products (PPCPs), present notable challenges for environmental monitoring due to their persistence and potential detrimental effects on ecosystems and human health. Understanding their TPs, detection methodologies, and regulatory responses is critical for effective management. Figure 4 presents a simplified analytical workflow used for the detection and identification of environmental TPs. The sequential process begins with

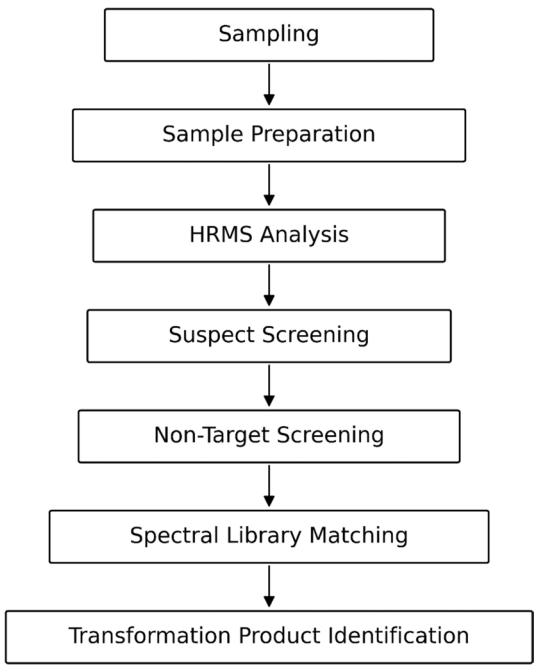

Fig. 4 Workflow for analytical detection and identification of transformation products using HRMS-based screening

environmental sampling and proceeds through high-resolution mass spectrometry (HRMS) analysis, suspect screening, non-target screening, spectral library matching, and final compound identification. The workflow highlights the integrated analytical steps required to systematically detect known and unknown TPs in complex environmental matrices.

6.1 High-resolution mass spectrometry approaches

High-resolution mass spectrometry has become central to the detection of TPs and emerging contaminants. This technique provides high mass accuracy and sensitivity at trace concentrations [178, 179, 196]. Precise mass measurements enable differentiation of compounds with similar nominal masses. Such resolution is critical when analyzing complex environmental matrices. HRMS supports quantification of highly persistent substances, including perfluoroalkyl and polyfluoroalkyl compounds. Hsu et al. [56] demonstrated its ability to detect PFAS migrating from food-contact materials. Many TPs arise from structurally simple precursors under varying environmental conditions. Accurate mass analysis facilitates the identification of subtle structural modifications.

Non-target detection represents a major strength of HRMS platforms. Tang et al. [159] and Erdal et al. [32] describe expanded contaminant coverage through full-scan acquisition. This approach captures signals beyond predefined compound lists. Tisler et al. [162] identified previously undetected polar micropollutants in wastewater effluents using HRMS. Such findings illustrate the role of advanced instrumentation in uncovering overlooked contaminants. Broader detection capabilities enhance environmental monitoring and exposure assessment.

6.2 Suspect and non-target screening workflows

Suspect and non-target screening workflows complement HRMS detection capabilities. These approaches allow identification of compounds not included in routine monitoring lists. Screening relies on accurate mass data, isotope patterns, and fragmentation spectra [32, 125, 157]. Compounds can be tentatively assigned without prior analytical standards. Suspect screening focuses on predefined lists of potential contaminants. Szabo et al. [157] advocate prioritizing this strategy to improve early detection of hazardous substances. Non-target workflows extend beyond suspect lists and evaluate all detectable features. Data mining algorithms rank signals according to intensity, frequency, or structural plausibility. Integration of screening results into regulatory contexts is increasingly discussed. Kronsbein (2025) presented a case study incorporating non-target findings into environmental oversight. Comprehensive chemical characterization supports evidence-based policymaking. Such workflows enhance identification of TPs that might otherwise remain undetected. Expanded screening improves proactive management of contaminants of emerging concern.

6.3 Stable-isotope and transformation-pathway tracing

Stable-isotope labeling provides detailed insight into contaminant transformation pathways. Isotopic tracers enable tracking of compounds through environmental and biological processes [27, 186]. Label incorporation clarifies degradation pathways

and the formation of intermediates. Creek et al. [27] demonstrated the use of isotopic approaches to elucidate biochemical mechanisms influencing contaminant fate. Isotope tracing reveals conversion efficiencies and metabolic branching patterns. Yin et al. [186] applied isotopic techniques to study engineered nanomaterials in environmental systems. Findings highlighted the dynamics and patterns of bioaccumulation. Stable-isotope methods strengthen the interpretation of HRMS data. Coupling isotopic labeling with high-resolution detection improves confidence in compound identification. Pathway tracing informs risk assessments by clarifying the formation of toxic intermediates. Such methodologies support regulatory evaluation and environmental modeling efforts.

6.4 Data processing, compound identification challenges, and spectral libraries

High-resolution mass spectrometry generates large and complex datasets. Effective data processing is essential for reliable compound identification. Automated feature extraction and alignment reduce analytical bias. Accurate identification often depends on comparison with spectral libraries [32, 141, 196].

Comprehensive spectral databases facilitate confirmation of TPs. Library expansion requires collaborative data sharing and standardization. Many emerging compounds lack reference spectra, complicating identification efforts. Advanced computational tools assist in structural prediction and annotation. Automation of data workflows enhances reproducibility and efficiency. López et al. [92] discussed analytical approaches adaptable to high-throughput interpretation. Similar strategies can streamline environmental HRMS data analysis. Addressing identification challenges improves the reliability of monitoring programs. A robust data infrastructure supports the integration of analytical findings into policy decisions.

6.5 Harmonization needs for global monitoring programs

Emerging contaminants require coordinated monitoring beyond national boundaries. Differences in analytical protocols limit the comparability of datasets. Wilkinson et al. [178, 179] highlight the impact of methodological variability on regulatory oversight. Standardization of sampling, analysis, and reporting enhances global surveillance. Scholars advocate development of harmonized frameworks for HRMS-based monitoring [125, 178, 179]. Consistent analytical parameters enable cross-regional data integration. Harmonization strengthens early warning systems for widespread contaminants. Integrated monitoring initiatives illustrate potential benefits of coordinated approaches. Standardized HRMS protocols for pesticide detection expand coverage of micropollutants. Shared databases and reporting standards support collaborative environmental assessment. Such frameworks enhance TP detection across diverse water systems. Global harmonization ensures effective management of emerging contaminants. Coordinated methodologies improve transparency and regulatory responsiveness. Table 7 compares major analytical technologies, emphasizing sensitivity and screening capabilities. Alignment of analytical practices strengthens environmental protection and public health safeguards.

Table 7 Analytical methods for detecting and characterizing transformation products

Analytical method	TP-specific detection role	Best suited TP type	Advantages	Key limitations
High-resolution mass spectrometry (HRMS)	Detects known and unknown TPs in complex matrices	Polar, mobile, unknown, and low-abundance TPs	High sensitivity; supports suspect and non-target screening; structural elucidation	Expensive; requires advanced data processing; many features remain tentatively identified
Liquid chromatography–tandem mass spectrometry (LC–MS/MS)	Confirms and quantifies known TPs	Targeted TPs with available standards	High sensitivity, specificity, and quantitative accuracy	Limited ability to detect unknown TPs; depends on reference standards
Gas chromatography–mass spectrometry (GC–MS)	Detects volatile or semi-volatile TPs	Volatile, thermally stable, and derivatized TPs	Established method; strong spectral-library support	Less suitable for polar, ionic, or thermally unstable TPs
Isotope-labeled tracing	Tracks transformation pathways and product formation	Mechanistically linked TPs formed from known parent compounds	Strong mechanistic insight; confirms parent–product relationships	Costly; complex experimental design; limited routine monitoring use

7 Predictive modeling tools for transformation-product identification and prioritization

Predictive modeling supports early identification, screening, and prioritization of transformation products when experimental data are limited. In this review, modeling is treated as a decision-support tool rather than a substitute for empirical monitoring or toxicological testing. This section focuses on four modeling approaches: QSAR and structure-based toxicity prediction, environmental pathway simulation, machine-learning-assisted prediction, and integrated exposure–toxicity pipelines. Their value lies in helping researchers and regulators identify likely transformation products, prioritize compounds for monitoring, and communicate uncertainty.

Predictive models differ in their appropriate use and evidentiary strength. QSAR models are useful for rapid toxicity screening and prioritization, but their reliability depends on whether transformation products fall within the model's chemical applicability domain. Pathway prediction models can identify likely reaction routes but remain less reliable for branched, sequential, and matrix-dependent transformation pathways. Machine-learning models can support pattern recognition across large chemical datasets, but their accuracy is limited by uneven training data, inconsistent reporting of transformation products, and limited representation of field conditions. Integrated exposure–effect models are useful for linking predicted occurrence to ecological or human-health relevance, but they require strong input data and transparent uncertainty reporting. Predictive models should therefore be used cautiously as prioritization tools rather than as substitutes for experimental confirmation [24, 103].

7.1 QSAR and structure-based toxicity prediction

Quantitative Structure–Activity Relationship models provide structured approaches for estimating toxicity and environmental behavior. These models correlate molecular descriptors with biological or physicochemical endpoints. QSAR techniques enable early screening of chemicals lacking experimental toxicity data. Abatan et al. [1] highlighted integrated simulation frameworks incorporating QSAR predictions for aquatic risk assessment. Their work emphasized predictive evaluation of ecological effects prior to environmental release. Structure-based models support prioritization of high-risk compounds for monitoring. Such tools assist regulators in identifying TPs with hazardous potential. Model refinement remains essential for reliability. Incorporation of updated experimental datasets improves predictive accuracy. Validation against observed toxicity endpoints enhances regulatory confidence. Continuous calibration ensures that QSAR outputs remain relevant as chemical usage patterns evolve. Integration of structural alerts and mechanistic descriptors strengthens the interpretation of model predictions.

7.2 Transformation-aware environmental pathway and reaction modeling

Environmental pathway models are useful for describing contaminant movement from sources through environmental media to receptors, but conventional source–pathway–receptor models often underrepresent transformation processes. For transformation products, this limitation is critical because chemical change may occur at any point along the pathway, including wastewater systems, surface water, groundwater, sediments, soils,

biota, and the atmosphere. Volatile organic compounds are especially important in this context because atmospheric transport, oxidation, photolysis, and plume mixing may generate secondary products after release. Transformation-aware pathway modeling therefore requires coupling transport models with reaction kinetics, compartment-specific degradation processes, and product-formation probabilities. Predictive assessment of transformation products can be strengthened by linking conceptual models to established screening tools. OECD QSAR Toolbox can support structural profiling, read-across, and endpoint prediction, while EPI Suite and ECOSAR can estimate physicochemical properties, environmental fate parameters, and aquatic toxicity endpoints for compounds with limited experimental data. enviPath and related pathway-prediction platforms can assist in identifying plausible biotransformation routes and intermediate products, while USEtox can support comparative toxicity and life-cycle impact assessment. These tools are most useful for early screening and prioritization, but their outputs should be interpreted with attention to applicability domain, data quality, structural uncertainty, and experimental validation needs.

Such models should account not only for where contaminants move, but also for how they change during movement. This requires integrating biotic and abiotic transformation parameters, including microbial metabolism, hydrolysis, photolysis, oxidation–reduction reactions, sorption-mediated transformation, and atmospheric reactions. Existing source–pathway–receptor models remain useful as screening tools, but they should be expanded into dynamic reaction–transport frameworks that can simulate parent-compound loss, transformation-product formation, persistence, and secondary exposure across multiple environmental compartments. This shift is essential for accurately predicting exposure and risk where transformation products may be more persistent, mobile, or biologically active than their precursor compounds.

7.3 Machine learning and AI-driven prediction of transformation products

Machine learning and artificial intelligence methods can support the prediction of transformation products by identifying patterns in large chemical, environmental, and toxicological datasets. These tools are useful for screening likely transformation pathways, prioritizing unknown compounds, and estimating environmental fate where experimental data are limited. However, their outputs should not be treated as substitutes for empirical evidence. Predictive performance depends strongly on the quality, representativeness, and completeness of training datasets, which remain uneven for many emerging contaminants and transformation products [6].

A major limitation is that many transformation-product datasets are biased toward well-studied contaminants, controlled laboratory conditions, and specific environmental matrices. As a result, machine-learning models may perform poorly when applied to poorly characterized chemicals, complex mixtures, or field conditions involving variable pH, temperature, microbial communities, light exposure, and redox status. Model interpretability is also a challenge because some algorithms can identify statistical associations without clearly explaining the underlying transformation mechanisms. For this reason, AI-driven predictions require verification through high-resolution mass spectrometry, pathway-tracing experiments, and independent field or laboratory datasets [91]. AI therefore has an important role in prioritization and hypothesis generation, but

transformation-product risk assessment still requires transparent validation, uncertainty reporting, and experimental confirmation before regulatory use.

7.4 Integrated exposure–toxicity predictive pipelines

Integrated exposure–toxicity pipelines combine predicted or measured concentrations with toxicity estimates to support screening-level prioritization. These approaches can help identify transformation products that require further monitoring or experimental testing. However, they should be interpreted cautiously because model outputs depend on input quality, endpoint selection, and the assumptions about uncertainty. Their main value is early prioritization rather than final regulatory decision-making.

Fork et al. [39] demonstrated the use of routine water quality data to estimate pharmaceutical levels. Such integration streamlines surveillance across aquatic ecosystems. Exposure predictions can be linked with toxicological benchmarks to estimate risk. Alignment with the Threshold of Toxicological Concern framework contextualizes concentration data [126]. Integrated pipelines may be used as decision-support tools to help identify contaminants that warrant further monitoring, prioritization, or regulatory attention. When applied with appropriate validation and uncertainty analysis, coupled exposure–effect modeling can support more efficient environmental risk assessment. These frameworks help agencies allocate monitoring resources effectively. Early detection of elevated risk facilitates timely intervention. Comprehensive predictive systems support transparent and evidence-based regulation.

7.5 Uncertainty analysis and model validation challenges

Variability in environmental conditions influences transformation pathways and transport rates. Data limitations may constrain model calibration. Sensitivity analysis helps identify influential parameters within simulation frameworks. Alharbi [6] emphasized continuous validation of machine learning models against empirical datasets. Predictive models for TPs remain constrained by incomplete training datasets, limited experimental confirmation, and uneven representation of environmental matrices. Prediction is especially difficult for branched, sequential, and matrix-dependent transformation pathways. Model outputs should therefore be accompanied by uncertainty reporting, applicability-domain assessment, and validation against laboratory or field data. These limitations are particularly important when models are used to support monitoring priorities or preliminary risk screening.

Predictive and analytical models remain useful for studying emerging contaminants and transformation products, but each has specific strengths and limitations [43, 99]. QSAR and related in silico models can estimate toxicity, persistence, mobility, and physicochemical properties where experimental data are unavailable, but they are less reliable for novel compounds, ionizable chemicals, PFAS, mixtures, and compounds outside the model training domain [43, 169]. Multimedia fate models help estimate persistence, partitioning, mobility, and long-range transport, but they depend heavily on input quality and may oversimplify local hydrology, degradation, and intermedia transfer [38]. Machine-learning-assisted suspect screening has improved prioritization of emerging contaminants in river water and passive sampler extracts, but it can generate false positives and depends on training data, database coverage, and feature quality. HRMS-based

non-target workflows have improved detection of transformation products in wastewater, particulate matter, and other complex matrices, but many identifications remain tentative and require confirmation with reference standards, MS/MS evidence, and retention-time matching [99]. Model selection should depend on the research question, chemical class, matrix, data availability, and need for validation rather than assuming that one model is suitable for all emerging contaminants [38, 99].

8 Integrating transformation products into environmental risk assessment

Incorporation of TPs into environmental risk assessment remains an urgent priority. Many regulatory systems were developed around parent compounds and single-substance evaluations. Transformation products introduce additional variability in persistence, toxicity, and exposure pathways. Effective integration requires conceptual, methodological, and regulatory adaptation. Current transformation-product risk assessment faces several technical bottlenecks. First, non-target and suspect screening workflows can detect large numbers of candidate compounds, but many remain at low structural-confidence levels, making it difficult to translate detection into quantitative exposure or risk estimates. Second, mixture toxicity remains difficult to assess because parent compounds and multiple transformation products may co-occur, interact additively or non-additively, and affect different biological endpoints. Third, prediction of bioaccumulation and trophic transfer remains uncertain because transformation products may differ from parent compounds in polarity, ionization, protein binding, metabolism, and environmental persistence. Finally, predictive models remain constrained by limited high-quality toxicity data, uneven training datasets, and weak validation under field conditions. These limitations show why transformation-product risk assessment requires tiered evidence, uncertainty reporting, and combined analytical, toxicological, and modeling approaches rather than reliance on any single method [24, 33, 34, 208].

To improve readability and strengthen risk interpretation, Table 8 summarizes representative transformation products across major contaminant classes, with emphasis on their parent compounds, relative toxicity or risk relevance, dominant environmental concerns, and current regulatory or monitoring status. This comparative structure highlights that transformation products are not uniformly less hazardous than their parent compounds; rather, some may be more persistent, mobile, bioaccumulative, or toxic, while others remain poorly characterized because of limited toxicity data and incomplete monitoring. Table 8 also clarifies an important regulatory gap: although several parent compounds are already monitored or restricted, many of their transformation products are not consistently included in routine risk-assessment or surveillance frameworks.

8.1 Limitations of current risk-assessment frameworks

Conventional risk-assessment frameworks emphasize parent compound toxicity and persistence. TPs are often considered only when data are readily available. Kern et al. [73], Escher and Fenner [33, 34], and Gasser et al. [43] highlight this imbalance. Bioactive derivatives may equal or exceed parent compound hazards [33, 34]. Limited evaluation of these products creates regulatory blind spots. Static modeling approaches further

Table 8 Representative transformation products, toxicity relative to parent compounds, and regulatory status

Parent compound/class	Representative TP	Toxicity/risk compared with parent compound	Key environmental concern	Regulatory status/monitoring relevance	References
6PPD, tire antioxidant	6PPD-quinone	More acutely toxic to some fish species; strongly associated with coho salmon mortality	Urban runoff, stormwater transport, and acute aquatic toxicity	Increasing monitoring and research attention; not yet fully integrated into many routine regulatory programs	Hiki et al. [54],Castan et al. [22],Wang et al. [169]
Triclosan	Methyl triclosan	More hydrophobic and less photodegradable than triclosan; may accumulate in aquatic organisms	Sediment accumulation, aquatic bioaccumulation, reversible transformation/back-conversion	Triclosan is regulated or restricted in some consumer uses; methyl triclosan is less consistently monitored	Pintado-Herrera et al. [122],Fu et al. [41],Huang et al. [58]
PFAS precursors	Terminal perfluoroalkyl acids, including PFAAs	Often more persistent and mobile than precursors; long-term exposure concern	Groundwater contamination, drinking-water exposure, bioaccumulation, and difficult remediation	Some terminal PFAS, such as PFOA and PFOS, are regulated or restricted, but many precursor-derived products remain under-monitored	Zhang et al. [191],Pickard et al. [121], Kreutz et al. [79], LaFond et al. [82]
Pesticides and herbicides	Pesticide degradates such as desethyl-atrazine, fipronil sulfone, and metolachlor ESA	Some pesticide TPs may be more persistent, mobile, or toxic than parent compounds	Agricultural runoff, groundwater contamination, aquatic toxicity, and seasonal exposure peaks	Parent pesticides are usually assessed more systematically than many degradates; TP requirements remain uneven across jurisdictions	Sinclair and Boxall [144], Krier et al. [80]
Carbamazepine	Carbamazepine epoxide and plant-associated metabolites	May retain biological activity; persistence and plant uptake raise exposure concerns	Wastewater effluent, reclaimed water irrigation, plant uptake, chronic exposure	Parent compound is frequently monitored; many metabolites are less routinely included	[33, 34, 124]
Phthalates	Monoester and oxidized phthalate metabolites	Some metabolites are biologically active and relevant for endocrine or developmental toxicity assessment	Food-contact materials, indoor dust, wastewater, human biomonitoring	Several parent phthalates are regulated, but environmental TP monitoring remains incomplete	[66, 171]
BADGE compounds	BADGE hydrolysis products	Hydrolysis products may retain toxicological and endocrine relevance	Epoxy resins, food-contact materials, wastewater, aquatic systems	Parent BADGE compounds are monitored in food-contact contexts; environmental TP monitoring remains limited	[166]
Pharmaceutical residues	Hydroxylated, dealkylated, or oxidized pharmaceutical metabolites	Toxicity varies; some products retain pharmacological activity or contribute to mixture risk	Wastewater effluent, surface water, chronic low-dose aquatic exposure	Parent pharmaceuticals are more commonly monitored than metabolites and TPs	[33, 34, 178, 179]

constrain assessment accuracy. Many frameworks assume fixed degradation rates and uniform environmental conditions. Transformation pathways vary across temperature, pH, microbial composition, and sunlight exposure. Such variability complicates predictions of long-term ecological impact. Kapo et al. [68] advocate the use of multimedia models that integrate biogeochemical processes across compartments. More dynamic simulations would better capture temporal and spatial variability. Model validation also presents challenges. Gaßmann noted that large-scale validation of pesticide fate models is insufficient. Scaling from laboratory conditions to catchment-level systems introduces uncertainty. Robust tiered assessment procedures are therefore necessary [68]. Sensitivity analyses and adaptive management components may improve regulatory confidence by identifying key uncertainties, testing model assumptions, and allowing risk-management decisions to be updated as new evidence becomes available.

Including TPs in exposure modeling requires advanced, context-sensitive approaches. Traditional models often omit complex interactions occurring in soils, sediments, and hyporheic zones. Li et al. [88] emphasize the hyporheic zone as a significant site of organic micropollutant attenuation. Biotransformation within this interface alters both parent compounds and derivatives. Models such as iSTREEM® can evaluate down-the-drain chemicals across hydrological settings [68]. Integration of empirical monitoring data improves predictive accuracy [115, 178, 179]. Field data allow calibration of concentration estimates and transformation rates. Evidence indicates that some TPs occur at concentrations higher than those of the parent compounds [18, 115]. Advanced computational tools expand exposure modeling capabilities. Machine learning and in silico simulations predict likely transformation pathways [91, 161]. These tools account for environmental variability and chemical interactions. Comprehensive frameworks integrating chemical fate, hydrology, and biological transformation enhance realism. Improved exposure modeling supports more accurate predictions of ecological and human health risks.

8.2 Cumulative and life-cycle risk assessment approaches

A cumulative risk assessment considers the combined impacts of multiple chemicals and their derivatives. Transformation products often contribute significantly to mixture toxicity. Brown et al. [18] conducted probabilistic ecological assessments of pharmaceutical derivatives. Findings suggested limited risk in certain effluent-dominated contexts. Risk magnitude, however, varies by environmental setting and exposure duration. Life-cycle assessment broadens perspective beyond point-of-discharge evaluations. Pharmaceuticals may enter agricultural soils through wastewater reuse and biosolid application [116]. Exposure can occur during production, use, disposal, and environmental redistribution. Brunning et al. [19] and Carter et al. [21] emphasize the integration of life-cycle stages into regulatory frameworks. Such approaches capture upstream and downstream risk dimensions.

Comprehensive life-cycle evaluation improves understanding of cumulative ecological burdens. Regulatory frameworks incorporating life-cycle perspectives can better anticipate long-term environmental consequences. Consideration of chemical group effects also strengthens prioritization efforts. Holistic risk assessment reduces underestimation of transformation product impacts. Exposure modeling can support risk assessment by

estimating where transformation products are likely to occur, how long they may persist, and which populations or ecosystems may be exposed [33, 34, 43]. For ecological risk assessment, predicted environmental concentrations can be compared with toxicity thresholds, species-sensitivity distributions, or predicted no-effect concentrations to identify compounds requiring monitoring or management attention [169]. For human-health risk assessment, exposure models can estimate intake through drinking water, food, wastewater reuse, inhalation, or dermal contact and can support hazard index, margin-of-exposure, or lifetime-risk calculations. These predictions can also help policymakers evaluate whether existing regulatory limits for parent compounds are adequate when persistent or mobile transformation products contribute additional exposure [33, 34, 145]. In the context of this review, exposure modeling is most useful for prioritizing transformation products for monitoring, identifying vulnerable exposure pathways, supporting provisional risk thresholds, and guiding future regulatory decisions where measured concentration and toxicity data remain incomplete [43, 169].

8.3 Decision-support tools for regulatory prioritization

Decision-support systems synthesize monitoring, modeling, and toxicity data for regulatory use. Liu et al. [89] advocate frameworks that prioritize chemicals requiring urgent attention. TPsIncluding TPs in these systems ensures comprehensive evaluation. Consideration of cumulative and synergistic effects strengthens prioritization accuracy. Adaptive management frameworks allow the incorporation of emerging scientific findings. Qu et al. [127] emphasize the importance of understanding the reversibility of certain TPs. Such knowledge directly influences regulatory decisions on compounds such as trenbolone acetate. Flexible decision-support tools accommodate evolving evidence. Continuous updates ensure responsiveness to new toxicity or exposure data. Transparent prioritization mechanisms enhance stakeholder confidence. Integration of TPs into regulatory systems ultimately improves environmental protection and public health outcomes. For risk characterization, transformation products can be prioritized using the risk quotient approach, where $RQ = PEC/PNEC$. PEC refers to the predicted or measured environmental concentration, while PNEC represents the predicted no-effect concentration derived from toxicity endpoints such as LC50, EC50, NOEC, or chronic values with appropriate assessment factors. An $RQ < 1$ generally indicates low expected ecological risk, while an $RQ \geq 1$ suggests potential concern and the need for further monitoring, toxicity testing, or management action. For transformation products detected through suspect or non-target screening, RQ values should be interpreted cautiously because concentration estimates, structural confidence, and toxicity data may be uncertain.

9 Policy, regulatory, and governance implications

TPs of emerging contaminants present complex governance challenges. Pesticides, pharmaceuticals, and personal care products generate derivatives that persist in environmental systems [93, 109, 110, 112]. These products may exhibit toxicity and mobility distinct from those of the parent compounds. Effective management requires adaptive regulatory frameworks and coordinated governance mechanisms.

9.1 Incorporation of transformation products within EU REACH, U.S. EPA, and international frameworks

Inclusion of TPs within major regulatory systems remains essential for comprehensive risk control. The European Union's REACH framework requires assessment of degradation products under certain conditions. Evidence indicates that some TPs pose risks comparable to those of the parent compounds [128]. Pharmaceuticals and personal care product derivatives have been detected in surface waters with retained bioactivity [128, 178, 179]. The United States Environmental Protection Agency has acknowledged the importance of evaluating TPs within chemical management programs [28, 178, 179]. Existing regulatory approaches, however, often focus on parent substances during approval stages. Dynamic formation processes and variable environmental conditions complicate comprehensive inclusion.

Guidelines may not fully capture the persistence, mobility, bioaccumulation, and secondary toxicity potential of transformation products, even when parent compounds are already regulated [178, 179]. This gap is fundamental because chemical risk assessment remains incomplete when transformation products are excluded from evaluation, particularly where degradation produces compounds that are more persistent, mobile, bioactive, or difficult to detect than their precursors [33, 34, 189]. Rhoads et al. [128] and Cwiertny et al. [28] emphasize the need for flexible regulatory strategies. Periodic updating of risk evaluations based on emerging analytical, toxicological, and exposure data can strengthen chemical oversight. Adaptive regulatory mechanisms may also improve responsiveness to evolving scientific evidence by allowing new transformation products, exposure pathways, and hazard endpoints to be incorporated into risk assessment frameworks.

Shared chemical databases have become important tools for identifying PFAS and possible PFAS transformation products in suspect and non-target screening workflows [44, 123]. The U.S. EPA CompTox Chemicals Dashboard hosts PFAS-related chemical lists, including PFASMASTER and PFASSTRUCT resources, which are widely used to build suspect lists for HRMS screening [44, 140]. NIST has coordinated the NIST Suspect List of Possible PFAS, which provides machine-readable PFAS structures and supports more consistent reporting of novel PFAS across laboratories [123, 140]. NIST also contributes spectral resources through the NIST/EPA/NIH Mass Spectral Library, which supports structural assignment and cross-laboratory comparison in suspect and non-target screening workflows [55]. Other open resources, including PubChem PFAS collections and the NORMAN Suspect List Exchange, expand global access to PFAS structures and improve harmonization in reporting novel PFAS [55, 140]. These shared databases help researchers identify candidate PFAS and transformation products, reduce duplicated effort, and improve the comparability of PFAS monitoring across laboratories and countries [123, 140].

9.2 Regulatory monitoring gaps and data-reporting limitations

Monitoring programs frequently prioritize known contaminants while overlooking TPs. Rhoads et al. [128] and Cwiertny et al. [28] highlight underreporting of derivatives occurring at elevated concentrations. Transformation products can enter aquatic systems through wastewater effluents [118, 119, 151, 178, 179]. Standard monitoring

protocols may not systematically target these compounds. Lack of harmonized reporting requirements limits cross-jurisdictional comparability. Snow et al. [151] and Petrie et al. [119] describe challenges in coordinating international assessments. Variability in sampling frequency, analytical techniques, and detection limits complicates data integration. Continuous enhancement of reporting standards is therefore necessary [43, 151].

Advanced analytical methodologies support improved detection. High-resolution mass spectrometry enhances identification of TPs [35, 59, 128]. Incorporation of such tools into regulatory monitoring frameworks strengthens exposure assessment. Reliable detection forms the basis for informed risk management decisions. Although several emerging contaminants are increasingly recognized as environmental risks, many are still not included in routine monitoring programs, and transformation products are even less systematically monitored. The EU Watch List mechanism under the Water Framework Directive provides an important model for tracking selected emerging contaminants, with substances such as diclofenac, steroid hormones, macrolide antibiotics, neonicotinoid insecticides, azole compounds, and selected pharmaceuticals included across different monitoring cycles since 2015. However, most transformation products remain outside these lists, highlighting the need for monitoring frameworks that include persistent, mobile, bioactive, or frequently detected transformation products.

9.3 Harmonized global standards for transformation-product assessment

Absence of unified global standards leads to inconsistent risk management outcomes. Regulatory regions often apply distinct criteria for evaluating TPs [118, 119, 128, 151, 154]. Divergent approaches may result in uneven levels of environmental protection. The development of harmonized guidelines would enhance the comparability of monitoring data. International collaboration among regulatory agencies and standardization bodies represents a constructive pathway. Snow et al. [151] and Petrie et al. [119] advocate coordinated assessment frameworks. Harmonization would support consistent identification, classification, and prioritization of TPs. Predictive modeling and in silico assessments offer tools for global alignment [28, 35, 128, 154]. Shared databases and standardized modeling protocols facilitate cooperative governance. Harmonized standards enhance transparency and strengthen global environmental stewardship.

9.4 Opportunities for precautionary regulatory approaches

Scientific uncertainty surrounding TPs justifies precautionary regulatory strategies. Many derivatives exhibit ecological and human health risks without complete toxicological characterization [28, 50, 138]. Precautionary measures may limit or suspend the use of chemicals pending a comprehensive evaluation. Hale et al. [50] emphasize relevance for persistent and mobile contaminants. Long-term environmental accumulation can lead to delayed, widespread impacts. Snow et al. [151] and Rhoads et al. [128] highlight regulatory gaps for such compounds. Löffler et al. [91] discuss predictive tools supporting early identification of hazardous derivatives. Application of precautionary principles strengthens proactive environmental governance. Regulatory systems incorporating uncertainty management can better protect ecosystems and public health. Early intervention reduces long-term remediation costs and ecological damage.

9.5 Policy-science interface and stakeholder engagement

Effective regulation of TPs depends on strong interaction between scientific research and policymaking. Gaßmann underscores the importance of translating scientific findings into regulatory practice. Engagement of researchers, industry representatives, and community stakeholders enhances policy legitimacy. Collaboration with industry can improve the development of safer chemical alternatives. Storck et al. [154] and Rhoads et al. [128] highlight the benefits of coordinated knowledge exchange. Public participation fosters transparency and builds trust in regulatory processes [118, 119, 151]. Cross-sectoral data sharing strengthens evidence bases for decision-making [59, 91]. Integrated governance approaches enhance the capacity to respond to emerging risks. Robust policy-science interfaces ensure that transformation-product management remains informed by evolving environmental evidence.

10 A predictive systems framework for transformation-product risk governance

Transformation products of emerging contaminants require governance systems that integrate science, monitoring, modeling, and regulation. Biotic and abiotic processes generate derivatives with distinct persistence, mobility, toxicity, and detectability profiles. These complexities require predictive and adaptive risk-management strategies. A systems-based framework can link transformation pathways to exposure dynamics, ecological effects, and policy outcomes. Although previous studies have emphasized the need to consider transformation products in environmental risk assessment, especially because they may be persistent, mobile, toxic, or analytically overlooked [24, 33, 34, 73, 189], fewer reviews have integrated formation mechanisms, environmental fate, detection workflows, predictive modeling, uncertainty analysis, and regulatory decision-making into a unified governance framework. This review addresses that gap by proposing a transformation-aware approach that evaluates parent compounds, intermediate products, secondary products, and environmental reservoirs as interconnected components of contaminant risk.

10.1 Conceptual pipeline linking transformation pathways to risk outcomes

A conceptual pipeline clarifies connections between chemical transformation and risk manifestation. Emerging contaminants undergo degradation through microbial, photochemical, and chemical processes. Resulting TPs may differ significantly from parent compounds in structure and activity. Risk governance also requires anticipatory modeling tools. Quantitative structure–activity relationship models support the estimation of toxicity and environmental behavior. Computational chemistry techniques complement QSAR predictions for new or unidentified derivatives [69, 172]. These approaches enable early identification of high-risk TPs. Studies examining pesticide derivatives illustrate this need. TPs of tebuconazole have been evaluated for ecological effects [40]. Certain derivatives exhibited toxicity levels comparable to those of the parent compounds. Löffler et al. [91] and Xiong et al. [182, 183] emphasize inclusion of such findings in predictive risk frameworks. Comprehensive toxicity screening improves prioritization and regulatory preparedness. A structured pipeline integrates

transformation identification, exposure modeling, toxicity prediction, and risk characterization. Such integration supports transparent and evidence-based governance decisions.

10.2 Integrated monitoring–modeling–policy decision loop

An effective governance framework requires continuous feedback between monitoring and modeling systems. Laboratory-derived transformation rates often diverge from field observations [47, 53, 176]. Environmental variability influences degradation kinetics and metabolite persistence. Field data strengthen the calibration of environmental fate models. Gaßmann demonstrated simulation frameworks TPsthat predict pesticide TPs at plot and catchment scales. Integration of empirical monitoring data enhances predictive reliability. Such approaches improve estimation of concentrations under realistic exposure scenarios [47]. A monitoring–modeling–policy loop allows adaptive regulation. Observed discrepancies between predicted and measured concentrations trigger model refinement. Updated outputs inform revised management strategies. Continuous iteration improves risk governance over time. This loop also supports transparency in regulatory processes. Stakeholders gain access to updated assessments based on empirical evidence. Integration of laboratory and field data strengthens the scientific credibility of policy decisions.

Integration of monitoring data into predictive models enhances assessment accuracy. Real-time and high-resolution datasets improve the representation of environmental variability. Advances in remote sensing and low-cost sensors enable expanded monitoring coverage [7, 187, 188]. These technologies facilitate the detection of spatial hotspots and temporal trends. Satellite-based observations complement ground-based measurements. Álvarez-Romero et al. [7] describe the value of satellite data for broad spatial assessments. Integration of diverse data streams strengthens model calibration. Continuous feedback between monitoring and modeling improves predictive performance. Such integration also supports adaptive regulatory management. Updated monitoring results refine exposure and toxicity estimates. Dynamic adjustment of risk thresholds becomes possible under this framework. Monitoring-to-model integration enhances transparency and responsiveness within environmental governance systems.

10.3 Priority-setting frameworks for emerging contaminants

Effective governance requires structured prioritization of contaminants and derivatives. Tiered screening frameworks assess the potential toxicity and the likelihood of exposure [2, 199]. Initial screening identifies compounds requiring detailed evaluation.

Pharmaceutical TPs provide relevant examples. Carbamazepine and diclofenac derivatives have been detected across environmental matrices [12, 53]. Multimedia fate modeling clarifies their distribution and persistence [2], (Authority 2017). Priority-setting frameworks integrate toxicity predictions with transport modeling. Combined evaluation improves identification of high-risk TPs. Such approaches guide allocation of monitoring resources and regulatory attention. Incorporation of multimedia models strengthens cross-compartment assessments. Soil, water, sediment, and atmospheric

pathways can be evaluated simultaneously. Comprehensive screening enhances preventive environmental management.

10.4 Implementation pathways for environmental management agencies

Environmental agencies require operational tools translating predictive insights into policy actions. Advances in computational modeling support automated exploration of reaction pathways [120]. Such tools identify likely TPs before widespread detection. Comprehensive modeling frameworks for persistent contaminants, such as PFAS, illustrate their practical application [47, 194]. These models integrate chemical properties, transport processes, and degradation dynamics. Agencies can apply outputs to set monitoring priorities and regulatory thresholds. Machine-learning-enhanced databases facilitate communication of biotransformation data [129]. Centralized repositories allow real-time updates as new evidence emerges. Regulatory practices become more adaptive and responsive under this system. Implementation pathways should emphasize cross-sector collaboration and capacity building. Integration of predictive modeling, monitoring, and stakeholder engagement ensures informed governance. A predictive systems framework strengthens anticipation of environmental risks associated with TPs. Adaptive, data-driven management supports the long-term protection of ecosystems and public health.

To support adaptive environmental governance, transformation-product assessment requires integration of source identification, mechanistic understanding, analytical detection, exposure–toxicity evaluation, and regulatory prioritization within a continuous monitoring–modeling feedback system. The framework presented in Fig. 5 synthesizes these interconnected processes into a predictive governance structure that links scientific evidence generation with regulatory decision-making. By integrating transformation pathways, analytical workflows, exposure assessment, and prioritization criteria, the framework provides a systems-oriented approach to identify high-risk transformation products and to improve proactive environmental management under evolving contamination scenarios.

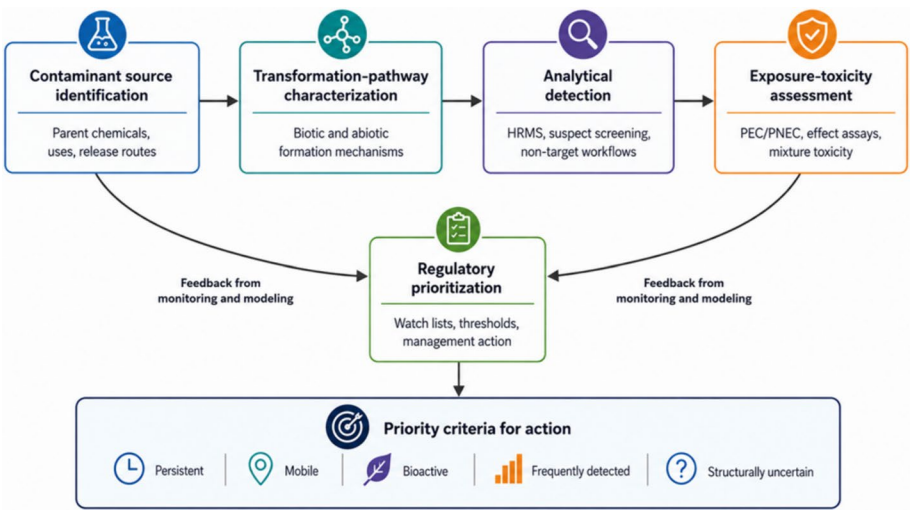

Fig. 5 Integrated predictive framework for transformation-product risk governance

The framework (Fig. 5) illustrates the sequential integration of contaminant-source identification, transformation-pathway characterization, analytical detection, exposure–toxicity assessment, and regulatory prioritization within an adaptive monitoring–modeling feedback system. The model emphasizes continuous refinement of regulatory thresholds and prioritization criteria based on emerging scientific evidence, environmental monitoring, and predictive modeling outputs. Priority actions focus on transformation products exhibiting persistence, mobility, bioactivity, frequent detection, or structural uncertainty.

11 Research priorities and future directions

Future research on transformation products should move beyond general calls for improved detection and regulation toward implementable research pathways that connect analytical chemistry, toxicology, modeling, and governance. Future transformation-product research and governance should prioritize five interconnected actions: advancing HRMS-based detection of known and unknown products, integrating monitoring with toxicity and effect-based assessments, improving predictive models for formation, persistence, mobility, and toxicity, incorporating transformation products into regulatory risk assessment and prioritization, and developing interoperable databases linking chemical identity, occurrence, toxicity, and modeling outputs. Other priority areas include high-confidence non-target screening combined with rapid toxicity testing, cross-scale prediction of transformation pathways from laboratory systems to field settings, standardized monitoring protocols for global comparability, and regulatory workflows that translate uncertain detection evidence into tiered risk-assessment decisions.

11.1 High-confidence non-target screening linked to rapid toxicity assessment

Continued advancement in analytical technologies remains essential for detecting TPs in complex matrices. Ultra-high-performance liquid chromatography coupled with high-resolution mass spectrometry has significantly expanded detection capabilities [107, 156]. These platforms allow identification of trace-level compounds across diverse environmental compartments. Non-target screening approaches broaden analytical scope beyond predefined contaminant lists. Such methods reveal previously unrecognized TPs. Expanded detection improves understanding of cumulative environmental burdens. Molecular techniques further enhance insight into transformation mechanisms. Metagenomics and transcriptomics enable in situ examination of microbial communities involved in contaminant degradation [91]. These tools clarify links between microbial gene expression and transformation pathways. Tratnyek et al. [163] demonstrated integration of molecular approaches with ecological assessments to evaluate pharmaceutical impacts. Despite progress, methodological challenges persist. Transformation products may form transiently or degrade rapidly under changing conditions. Analytical protocols must therefore accommodate variability in stability and concentration. Standardization of sampling and processing procedures is critical [104]. Harmonized methodologies improve comparability across regions and studies. Future analytical innovation should emphasize miniaturized sensors, improved spectral libraries, and automated

annotation workflows. Enhanced detection precision strengthens environmental surveillance and regulatory response.

11.2 Data integration and FAIR transformation-product databases

Comprehensive global databases are essential for consolidating knowledge on the formation of TPs and their toxicity. Initiatives such as the NORMAN Suspect List Exchange provide foundational infrastructure [53]. Expanded integration across chemical classes and geographic regions remains necessary. Interoperable database frameworks facilitate data exchange between laboratories and regulatory agencies [192]. Standardized metadata formats improve usability and transparency. Shared repositories accelerate the identification of recurring TPs across ecosystems. Artificial intelligence and machine learning can enhance the utility of databases. Automated pattern recognition supports real-time interpretation of monitoring results. Xiong et al. [182, 183] highlight the role of predictive analytics in anticipating environmental impacts. Integration of monitoring data, toxicological endpoints, and modeling outputs strengthens risk assessment pipelines. International data-sharing agreements are central to effective collaboration. Coordinated information exchange reduces duplication of effort and improves response time. The development of comprehensive transformation-product registries will enhance global environmental governance.

11.3 Multiscale fate, exposure, and ecological risk studies

Ecological risk assessment must address spatial and temporal variability. Acute toxicity endpoints alone fail to capture chronic and cumulative impacts [185]. Long-term exposure and bioaccumulation require detailed evaluation across trophic levels. Multiscale frameworks examine the impacts of cellular responses on ecosystem dynamics. Liu et al. [90] documented bioaccumulation of pharmaceuticals within aquatic food webs. Such findings inform understanding of trophic transfer and ecological amplification. Risk assessments should incorporate species-specific vulnerabilities, life-stage differences, and reproductive effects. Consideration of gender-related susceptibility enhances precision. Integrating land-use change and socio-ecological dynamics enriches environmental modeling [199]. Spatial heterogeneity also influences exposure pathways. Catchment-level modeling combined with local monitoring improves ecological interpretation. Multiscale approaches align environmental science with ecosystem-based management principles.

11.4 Global monitoring standards and cross-disciplinary collaboration

Complex transformation-product dynamics require interdisciplinary collaboration. Chemists, toxicologists, ecologists, engineers, and social scientists contribute complementary expertise. Partnerships integrating environmental chemistry with engineering have improved wastewater treatment design. Collaborative frameworks encourage holistic problem-solving. Integration of ecotoxicology with public health perspectives broadens understanding of cumulative risk. Engagement with policymakers enhances the translation of research findings into regulation. Community stakeholder participation strengthens legitimacy and contextual relevance. Inclusion of affected populations improves alignment between research priorities and societal concerns. Dedicated

funding streams for interdisciplinary initiatives support sustained collaboration. Establishing centers of excellence focused on transformation-product research would promote innovation. Such structures facilitate shared infrastructure, training, and data exchange.

11.5 Predictive toxicology and tiered regulatory prioritization

Predictive environmental toxicology continues to evolve with computational and experimental innovation. QSAR models remain central to structure-based toxicity estimation. Integration of advanced modeling techniques enhances predictive reliability. Emerging technologies such as organ-on-a-chip systems and three-dimensional bioprinting improve the simulation of biological responses. These platforms provide ethically responsible alternatives to traditional animal testing. Enhanced physiological relevance improves extrapolation to environmental scenarios. Understanding molecular mechanisms of toxicity remains a research priority. Mechanistic studies clarify pathways linking chemical structure to adverse outcomes. Improved mechanistic knowledge strengthens model parameterization and regulatory interpretation. Coupling computational predictions with experimental validation enhances confidence in risk assessments. Integration of toxicogenomics and high-throughput screening can refine hazard identification. Future progress depends on coordinated investment in predictive tools and experimental platforms. Advancing predictive environmental toxicology will support proactive governance of TPs. Strengthened modeling, monitoring, and interdisciplinary collaboration will enhance the protection of ecosystems and human health.

12 Conclusion

This review identifies five priority recommendations for transformation-product research and governance: improving high-confidence HRMS-based detection of known and unknown products; linking monitoring results with toxicity testing and effect-based assays; expanding predictive tools for formation pathways, persistence, mobility, and toxicity; including transformation products in risk assessment, watchlist monitoring, and regulatory prioritization; and developing interoperable databases that connect chemical identity, occurrence, toxicity, and model outputs. Transformation products of emerging contaminants constitute a pivotal frontier in environmental chemistry, toxicology, and regulatory science. This review demonstrates that the environmental risks associated with chemical pollution cannot be adequately characterized without systematic consideration of the dynamic processes that convert parent compounds into structurally and toxicologically distinct derivatives. Across environmental matrices, microbial, photochemical, hydrolytic, and oxidative processes generate complex transformation networks that frequently produce compounds with altered persistence, mobility, and biological activity. These transformation dynamics reshape exposure pathways, ecological interactions, and long-term contaminant behavior, often leading to risk profiles that diverge substantially from those predicted based solely on parent compounds.

Advances in analytical technologies, particularly high-resolution mass spectrometry, suspect and non-target screening workflows, and isotope-assisted pathway tracing, have improved the capacity to detect and characterize previously overlooked transformation

products. Concurrently, predictive tools, including QSAR models, environmental fate simulations, and machine-learning-based transformation prediction, are enabling earlier identification of high-risk compounds and supporting more proactive environmental risk governance. Nevertheless, substantial challenges remain, including incomplete knowledge of transformation pathways, uncertainty in predictive models, limited spectral libraries, and insufficient harmonization of global monitoring practices. Regulatory frameworks continue to lag behind scientific understanding, with many risk-assessment systems still prioritizing parent-compound evaluation while overlooking the cumulative risks associated with transformation products. Integrating transformation products into exposure modeling, cumulative risk assessment, life-cycle evaluation, watch-list monitoring, and regulatory prioritization is essential for achieving more realistic chemical safety evaluations. A systems-oriented monitoring–modeling–policy feedback loop, supported by interoperable global databases and decision-support tools, offers a practical pathway for strengthening adaptive environmental management. Future progress will depend on interdisciplinary collaboration across environmental chemistry, toxicology, data science, engineering, and policy domains to develop predictive, transformation-aware environmental governance frameworks. Expanding global transformation-product databases, advancing multiscale ecological risk studies, and embedding precautionary principles into regulatory decision-making will be central to addressing the increasing complexity of chemical contamination. Transitioning from static parent-compound assessments to dynamic, transformation-informed risk evaluations represents a necessary paradigm shift to protect environmental and public health in the era of emerging contaminants.

Acknowledgements
Not applicable.

Author contributions
Matthew Chidozie Ogwu and Sylvester Chibueze Izah conceived and designed the review, wrote the original draft of the manuscript, and supervised the entire project. Olugbemiga Ojo Aliu, Ayebapreye Kari, and Esther Ugo Alum contributed to the systematic literature review, supported the theoretical development and methodological structuring of the manuscript, and provided critical intellectual inputs. Matthew Chidozie Ogwu, Sylvester Chibueze Izah, Olugbemiga Ojo Aliu, Ayebapreye Kari, and Esther Ugo Alum all participated in manuscript revision, conceptual refinement, validation of key arguments, and critical editing. All authors reviewed, edited, and approved the final version of the manuscript for publication.

Funding
No funding was received for this work.

Data availability
No datasets were generated or analysed during the current study.

Declarations

Ethics approval and consent to participate
Not applicable.

Consent for publication
Not applicable.

Competing interests
The authors declare no competing interests.

Received: 22 February 2026 Accepted: 15 June 2026
Published online: 01 July 2026

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