New praxis for assessment and management of risks with unwanted chemicals in water

In Swedish: Ny praxis för bedömning och hantering av risker med oönskade kemiska ämnen i vatten

Project scope, structure and organization

Chemicals in water pose a significant environmental and public health risk. To provide safe drinking water and enable effective reuse of wastewater, while also protecting aquatic ecosystems and human health, potential risks from unwanted chemicals must be addressed. Current water regulations cover only a limited number of substances and offer no guidance on how to handle new or unknown chemicals and mixture effects, creating major challenges for the water sector. Despite advances in analytical techniques and risk assessment, effective tools for interpreting screening data and developing mitigation measures are lacking. A more comprehensive framework for assessing chemical risks in water is needed at both national and international levels. Our long-term vision is to establish a new effective praxis for the assessment and management of chemical risks in water to better protect the environment and human health.

This project, conducted from November 2024 to May 2025, initiated cross-sectoral dialogue to map the current landscape and envision future developments for chemical risk assessment in both natural and engineered water systems. The project was structured around four workshops, bringing together experts, decision-makers, and practitioners. These workshops helped identify key knowledge gaps and barriers, leading to proposed next steps toward a new praxis for assessing and managing chemical risks. The work included internal meetings to prepare for the workshops, facilitation of the workshops themselves, and the synthesis of outcomes. The project began with a digital information meeting, followed by three in-person workshops focused on thematic discussions of analytical methods, risk assessment approaches, legislation, and communication. These workshops targeted stakeholders from different sectors and featured invited speakers with international expertise. The following stakeholder groups were represented in the workshops: water producers, municipalities, private companies, researchers, the Swedish Water and Wastewater Association (Svenskt Vatten), and national authorities such as the Swedish Environmental Protection Agency (Naturvårdsverket), Swedish Chemicals Agency (Kemikalieinspektionen), Swedish Agency for Marine and Water Management (Havs- och vattenmyndigheten), Geological Survey of Sweden (Sveriges geologiska undersökning), National Food Agency (Livsmedelsverket), National Veterinary Institute (Statens veterinärmedicinska anstalt), and County Administrative Boards (Länsstyrelserna). A final in-person workshop integrated and synthesized all project outcomes, which were subsequently presented in a digital meeting open to all interested parties.

Given the extensive production and use of chemicals in the society leading to the potential presence of hazardous chemicals in water, as well as the complexity and challenges associated with analytical methods, risk assessment, legislation, and communication, this project focused on identifying key areas for improvement and fostering collaboration among stakeholders. The objectives of this project were to:

- assess the usability and readiness of current analytical methods for detecting hazardous chemicals and mixtures in water systems and identify gaps for future research and development;
- identify key barriers and propose improvements to chemical risk assessment methods;

- discuss gaps in current chemical legislation and evaluate practices of regulatory authorities and water companies in safeguarding public health and the aquatic environment;
- highlight challenges in informing the public about chemical risks while maintaining trust in water safety;
- identify key stakeholders, bridge gaps between stakeholders, and engage individuals with key expertise to contribute to future project applications and foster collaboration in upcoming projects.

Report structure

This report begins by presenting the **complex challenge** of the multitude of unwanted chemicals in our water, covering issues like analytical detection difficulties, risk assessment limitations, fragmented legislation, and communication challenges. We then outline the **desired future state**, discussing associated opportunities, barriers, and potential future scenarios. Hypotheses for system change and involved stakeholders are also presented. Finally, we **propose the next steps**, among them the formation of relevant stakeholder groups, necessary to reach this desired future state.

Complex challenge analysis

A growing spectrum of unwanted chemicals in our water

Humans produce tens of thousands of different chemicals each year, and new ones are developed every day. Currently, 350 000 different chemicals and mixtures are registered in national and international inventories (Wang et al., 2020), and the European Environment Agency (2020) estimates that approximately 100,000 chemicals are presently on the market. The chemosphere is expanding exponentially, with synthesis pathways for more than 500 000 new chemicals being determined annually (Llanos et al., 2019). The volume of chemical use is also vast; in the European Union (EU), an average of 210 million tons of chemicals hazardous to human health and 80 million tons hazardous to the environment are consumed annually (EUROSTAT, 2023). Many of these chemicals and their degradation products end up in natural waters, forming complex mixtures in which individual compounds may be present in very low concentrations (Ferraro & Prasse, 2021).

Water bodies are under increasing pollution pressure from a wide range of both point and diffuse sources. These include industrial and household chemicals, pollution from affected sites, leakage of chemicals during product use, stormwater runoff, wastewater, agricultural releases of nutrients and pesticides, and accidental spills. Additionally, water bodies are impacted by biological stressors, including algal blooms, viruses, parasites, and bacteria. Climate change is expected to exacerbate these challenges, as a higher frequency of extreme rainfall events may result in greater volumes of chemicals entering water systems from agriculture, wastewater, landfills, and contaminated sites (Olafsdottir et al., 2021). Chemical risks can arise suddenly through accidents or intentional actions, or develop gradually due to long-term, low-level discharges. Consequently, the timeframe for threats posed by unwanted chemicals in water ranges from immediate to decades, adding considerable complexity to chemical risk assessments.

Targeted monitoring studies by the NORMAN network[1] have identified more than 4,500 chemicals in various water bodies, including freshwater, marine water, groundwater, and

[1] https://www.norman-network.net/

wastewater effluents (Dulio et al., 2024; NORMAN, 2025). This contrasts with findings from non-targeted analytical methods, which detect approximately 37,000 chemical features – both known and unknown (Manz et al., 2023). The detected chemicals represent a wide array of chemical classes, originating from diverse sources, such as industrial and consumer use, pesticides, pharmaceuticals, abiotic and biotic transformation products, and natural toxins. These chemicals also differ in their properties and potential biological effects.

Recent headlines[2] and public debates[3] frequently highlight alarming incidents of chemical pollution, underscoring the urgent challenges we face in safeguarding water quality. These events often catch even water managers unprepared, revealing a critical lack of expert support needed to manage risks proactively and make informed decisions for sustainable water use. To protect the environment and human health from exposure to hazardous chemicals, we must assess their presence holistically. This calls for the advancement of existing and new analytical methods, improved risk assessment approaches, and the development of appropriate policies and legislation. Many tools that could facilitate such holistic assessments are already available in the scientific domain but have yet to be widely implemented in practice. This implementation gap is largely due to the lack of user-friendly tools and sufficient legislative support for their use. Making these tools accessible and providing necessary support would enable all water managers – regardless of their internal expertise – to successfully apply these methods in practice.

Detection methods are complex and under development

Many analytical methods, such as effect-based methods and mass spectrometry analyses (including target, suspect, and non-target screening), are available for characterizing chemicals and their effects in water. Each method has a different purpose, with its own advantages and disadvantages. Navigating the most appropriate methods or workflows for specific challenges is not an easy task. For instance, there are many options within each technique – some are suitable for quantitative determinations, while others can function as early warning systems for new or unknown chemicals and mixtures. Moreover, to gain deep insight into water quality, a combination or tiered application of methods may be needed. A significant challenge lies in the sheer complexity of the chemicals. The vast array of potentially hazardous chemicals exhibits diverse physicochemical properties, necessitating a wide range of analytical methods for effective detection. This diversity impacts every stage of analysis, from sampling and sample preparation to final instrumental detection, such as choosing between liquid chromatography (LC) and gas chromatography (GC) coupled with mass spectrometry (MS). While LC-MS is suitable for water-soluble chemicals, many regulated compounds are better analyzed by GC-MS.

Micropollutants include both inorganic and organic compounds, with the complexity of organic compounds being far greater than that of inorganic ones. Current practice predominantly relies on targeted MS analysis to quantify known organic micropollutants, using either low- or high-resolution MS. The resulting data provide concentrations of micropollutants in water (or other matrices), which can then be used for risk assessment and mass balance modeling. However, most of the targeted analyses routinely performed in the water sector are restricted to a limited set of regulated compounds. This is a significant

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[2] https://www.mitti.se/nyheter/unika-fororeningar-hittade-i-stockholmarnas-blod-6.3.287294.a8862f3ba9
[3] https://www.dn.se/debatt/standiga-giftlarm-skrammer-upp-oss-i-onodan/ and https://www.aktuellhallbarhet.se/opinion/debatt/pfas-larmen-ar-inte-overdrivna-de-ar-valgrundade/

drawback, as it is uncertain whether these compounds truly represent the most important chemical hazards present in water.

To address the limitations of the targeted analysis, suspect and non-target screening MS are valuable techniques. In suspect screening, a comprehensive list of chemicals is investigated, most of which lack available reference compounds. Non-target screening is even broader in scope, employing an unbiased approach to answer questions such as “What is in the sample?” or “What are the differences between samples?” Both these screening techniques require high-resolution MS and are designed to identify contaminants of emerging concern, including little-known or previously unreported pollutants. While these techniques are very powerful, they also have notable limitations, i.e., they are labor-intensive, require expertise, and, due to the lack of analytical standards, the resulting data are typically qualitative or semi-quantitative. This lack of quantitative concentration data makes it difficult to perform risk assessments, leaving water companies unable to easily interpret the hazard information of identified chemicals. Additionally, the general sample preparation methods required to capture a broad range of chemicals in non-target analysis can result in detection limits that are too high to detect compounds present at very low concentrations. If well-known pollutants cannot be reliably detected with these tools, trust in non-target screening results can diminish. Consequently, these broader screening techniques are not yet suitable for routine use; they remain infrequent and are primarily conducted within the context of research projects.

When the goal of analysis is to determine the toxicological effects that chemicals in water might trigger, effect-based methods, such as bioassays, are particularly useful. These methods detect the combined biological activity of all compounds present, including those that are unknown or not specifically measured. By assessing actual biological effects, such as endocrine disruption, genotoxicity, or oxidative stress, effect-based methods offer a complementary perspective on water quality. Effect-based methods are generally divided into two main approaches: *in vitro* and *in vivo*. *In vitro* methods are cell-based assays that measure specific biological responses at the molecular or cellular level. Using cultured cells or biochemical systems, *in vitro* tests can detect effects like hormone receptor activation, oxidative stress, or DNA damage. These tests are highly sensitive and provide mechanistic insight by targeting specific modes of action. In contrast, *in vivo* methods involve exposing whole organisms (such as fish, algae, or crustaceans) to environmental samples under controlled conditions. These tests measure integrated biological responses, including growth inhibition, reproductive impairment, developmental effects, or behavioral changes. *In vivo* assays capture the full complexity of living organisms, including metabolism and bioavailability of pollutants. Together, *in vitro* and *in vivo* effect-based methods provide complementary perspectives: *in vitro* assays reveal potential modes of action, while *in vivo* methods demonstrate ecological relevance and organism-level outcomes. However, both the EU and the international community are increasingly moving away from *in vivo* approaches in order to reduce animal testing, and are placing greater emphasis on the use of *in vitro* methods.

Together, chemical analysis and effect-based methods provide a holistic assessment: chemical analysis identifies what is present in the water, while bioassays reveal what these chemicals do. This integrated approach strengthens risk assessment and supports better protection of aquatic ecosystems and human health. However, a challenge remains that chemical analysis rarely identifies which specific chemicals are responsible for the effects detected using *in vitro* methods. Additionally, *in vitro* effect-based methods indicate hazard but not exposure risk, making it difficult for water managers to assess actual risks without established threshold values.

Risk assessment is limited by the lack of data and critical thresholds

Chemical risk assessment helps protect aquatic and human health by evaluating the likelihood and severity of adverse effects resulting from harmful chemicals in water. Two main risk assessment approaches are in use: qualitative and quantitative. Qualitative risk assessment relies on descriptive or categorical judgments of risk in the absence of data, whereas quantitative risk assessment compares estimated or measured chemical concentrations with critical thresholds established to prevent adverse health or environmental effects. Notably, risk assessments for human health and the aquatic environment are conducted within different regulatory frameworks, each with its own terminology, data requirements, protection goals, and methodological challenges. In practice, risk assessment for both human health and the aquatic environment employs a mix of qualitative and quantitative methods.

Qualitative risk assessment is often the starting point for evaluating risk when data are scarce and rapid decision-making is required. This approach uses descriptive risk matrices, such as "low," "moderate," and "high" risk (e.g., following Water Safety Plan principles according to the World Health Organization). Classification is typically based on expert judgment of event occurrence and the resulting likelihood and severity of adverse health effects. Mass-balance calculations and transport models are often used to estimate the fate of chemicals from the source to the evaluation site. This risk assessment approach is commonly employed in early-stage screening, site-specific scenarios, and for data-poor chemicals. However, it is limited by subjectivity and uncertainty, which can result in inconsistent outcomes.

Quantitative risk assessment is a data-based approach used to evaluate the potential adverse health impacts of individual chemicals in water by comparing their concentrations to established critical thresholds. Importantly, the protection goals for human health and the aquatic environment differ according to regulatory frameworks. For aquatic health, critical thresholds are typically based on effects such as growth, mortality, reproduction, and immobilization. In contrast, human health assessments focus on endpoints including effects on organ systems (such as hepatotoxicity, renal effects, neurotoxicity, immunotoxicity, and endocrine disruption), developmental effects, and carcinogenicity, among others.

Risks to the aquatic environment can be assessed for individual chemicals using thresholds such as Predicted No Effect Concentrations (PNEC) or Derived No Effect Levels (DNEL), as documented in the registration dossiers mandated under REACH, or using Water Quality Objectives defined by the Water Framework Directive. Probabilistic methods can also be applied, where distributions of potential chemical concentrations are compared to distributions of species sensitivities, such as through Species Sensitivity Distributions (SSDs) (Posthuma et al., 2002). Additionally, risks can be assessed for mixtures of chemicals, typically using the concentration addition method as an initial approach (Backhaus & Faust, 2012).

Risks to humans are evaluated by comparing chemical levels in, for example, drinking water to health-based guidance values, such as tolerable daily intakes, reference values, and acceptable daily intakes. These critical thresholds are based on animal studies or epidemiologically derived associations with a health endpoint. Sand et al. (2015) developed the "risk thermometer" tool, which modified the risk assessment approach by accounting for the effect severity of the critical threshold used (e.g., enzyme activation has a low severity, while cancer has the highest severity). The "risk thermometer" was recently applied to categorize effects from "no concern" to "high risk" for quantified chemical concentrations in drinking water measured at three Swedish drinking water facilities (Glynn et al., 2024), showing that risk could be estimated for only 25% of all measured chemicals due to missing detection levels and/or critical thresholds. Moreover, humans are exposed to the same chemical from multiple sources, raising uncertainties in the translation of the critical thresholds to maximum water limits that would be directly comparable with measured exposure levels.

Despite methodological differences, most risk assessment methods share the basic approach of comparing exposure concentrations to critical thresholds for human or environmental health. However, for the majority of chemicals, data on both exposure levels and critical thresholds are lacking. The European Environmental Agency (2020) estimates that only about 500 chemicals are well-characterized in terms of their exposures and hazards, while over 100 000 chemicals are on the market. Additionally, scientific research covers only a small fraction of the chemosphere, with a disproportionate focus on individual metals (Kristiansson et al., 2021).

Real-time monitoring as well as long-term monitoring of chemicals in water are largely lacking. Given limited resources, monitoring should be a collaborative effort involving multiple stakeholders, particularly in densely populated areas, and could include joint screening initiatives in less populated regions. The monitoring of micropollutants under the ‘Rhine 2040’ program serves as a positive example in this context (International Commission for the Protection of the Rhine, 2022). Water managers typically rely on analogue alarm signals to enable risk assessments of antagonistic threats, accidental spills, or firefighting operations, all of which may cause intentional pollution or the unintentional formation of toxic chemicals in water. However, currently available sensors are generally too insensitive to provide sufficient early warning, unless they are used for a specific chemical or a relevant indicator parameter. Crucially, clear guidelines for risk-based monitoring programs are lacking, including guidance on where and how often to sample, which methods to use, what parameters to measure, and how to interpret results. Furthermore, studies have shown that a large portion of chemicals detected in drinking water or the broader environment cannot be adequately assessed for risk, because analytical detection limits are often too high for accurate quantification (Glynn et al., 2024).

Critical threshold values, below which no harmful effects are expected, for both humans and the environment are lacking for most chemicals. One way to address these data gaps is through risk indication, a screening approach that identifies potential chemical risks across a large number of substances. This method relies on measured or estimated physicochemical properties (such as persistence and water solubility), available data on chemical occurrence, and hazard classifications based on effect estimates (such as *in vitro* data for various endpoints). While the risk indication method can help highlight chemicals that warrant further scrutiny, monitoring, or regulation, it faces significant uncertainty due to limited knowledge of actual exposure levels and the frequent absence of critical thresholds. To supplement threshold data, it is often necessary to use modelled data, such as Quantitative Structure-Activity Relationship (QSAR) or other types of read-across data from similar chemicals. However, traditional QSAR methods and thresholds derived from the best available toxicological data can vary by several orders of magnitude (Gustavsson et al., 2023; van Dijk et al., 2021). Furthermore, even when toxicological data are available, endpoints often focus on acute, high-dose exposures, which poorly reflect the reality of chronic, low-level exposures. The translation of toxicological data into critical thresholds thus further complicates the risk assessment process, resulting in a lack of clear risk indicators and action plans for many chemicals.

In summary, risk assessments are typically conducted only for a limited set of well-studied, legacy chemicals that have established measurement methods and extensive toxicological data spanning multiple endpoints. These assessments are often retrospective and chemical-specific, overlooking uncertainties in population-level exposures and health effects for both aquatic life and humans. This retrospective approach can delay necessary actions in response to emerging chemical risks. Importantly, the risks arising from chemical mixtures are frequently overlooked, which likely results in a substantial underestimation of overall risk. This is particularly concerning, as studies have shown that while low levels of individual chemicals may not pose a threat, their combined effects could be significant.

Fragmented legislation hinders effective risk management

The legislation governing the management of chemical risks is fragmented, slow and reactive. Several chemicals are addressed in different policies relating to drinking water, wastewater reuse, and environmental protection. Well-known, regulated, and frequently analyzed compounds, such as priority chemicals and river basin-specific pollutants (RBSPs), represent only a small fraction of the chemicals that may be present in natural waters. Notably, threshold values for PFAS are still not regulated under the Swedish Drinking Water Directive (LIVSFS 2022:12) until 1 January 2026. The EU Drinking Water Directive 2020/2184 fails to incorporate EFSA's recommended tolerable intake for the four most concerning PFAS compounds, reflecting the slow legislative process for addressing chemical risks. Meanwhile, water companies have been held liable for providing water as a product that must be free from toxic chemicals. In a landmark ruling, the water utility Ronneby Miljö och Teknik was found liable for personal harm due to elevated PFAS levels in the drinking water in Kallinge (Swedish Supreme Court verdict, 5 December 2023, case T 486-23). Water companies therefore require faster expert support to enable earlier warnings of emerging chemicals of concern.

Moreover, the management of risks arising from chemical mixtures is generally insufficient. Although chemicals are recognized as posing threats to freshwater ecosystems on a continental scale (Malaj et al., 2014; Posthuma et al., 2020, 2019), only 45 substances are currently prioritized under the Water Framework Directive. Even when environmental thresholds, such as PNEC and DNEL from the REACH regulation, are exceeded, mandatory actions are often not required. Additionally, inconsistencies in threshold values across different EU legislations further exacerbate this issue (Gustavsson et al., 2023; van Dijk et al., 2021). Similarly, failing to achieve "good chemical status" under the Water Framework Directive does not automatically trigger specific measures, making it difficult for authorities to justify interventions to external stakeholders. Some regulations, such as EU Regulation 2020/741 on the use of reclaimed water for irrigation, do not set limits for known hazardous chemicals, including PFAS and heavy metals. As new chemicals are continuously introduced to the market, keeping legal documents updated remains a persistent challenge. This makes it difficult for the water sector, such as drinking water providers, to consistently meet the legal requirement to supply 'wholesome and clean' water and further complicates the safe reuse of treated wastewater. It is important to note that while EU directives set minimum standards for assessment, the specifics of implementation are often left to national governments. This can lead to inconsistencies in application but also provides opportunities for countries to adopt more advanced strategies.

A major hurdle in the regulatory implementation of advanced analytical techniques, including effect-based methods and comprehensive chemical screening, is the lack of standardized protocols, proficiency testing programs, and consensus on how to interpret and utilize the generated results. Both scientists and regulators need a thorough understanding of the limitations of these techniques to ensure correct interpretation. However, authorities and practitioners often struggle to utilize and apply information from the scientific community due to time constraints and a lack of specialized expertise. As a result, the adoption of novel methods is frequently hindered by the absence of clear guidance for decision-making. Decision-support tools that aid in interpreting qualitative chemical data, such as the likely presence of a chemical in a sample, and in deriving threshold values for uncontaminated water may be crucial for the successful implementation of these advanced approaches.

The slow pace at which regulations and monitoring practices adapt to new scientific findings and emerging threats has significant consequences. Monitoring campaigns often rely on centrally established priority lists, which leads to slow adaptation and prolonged periods of hazardous releases and exposures before action is taken (European Environment Agency, 2013). The case of PFAS, where more than three decades passed between their detection in humans and the establishment of regulatory limits in drinking water, highlights this dangerous lag, facilitated by industry influence and a lack of transparency (Grandjean & Clapp, 2015).

Promisingly, advancements in qualitative (Hollender et al., 2023) and quantitative (Finckh et al., 2022, 2024) screening techniques are facilitating their regulatory use. The regulatory application of effect-based methods is also being evaluated (Wernersson et al., 2015; Carere et al., 2021), with progress in harmonizing methods for endocrine disruption and ongoing evaluations for genotoxic effects. Other *in vitro* methods can identify a range of health-based endpoints (such as immunotoxicity, oxidative stress, thyroid effects, and other biological responses) in water samples, offering alternatives to traditional animal testing (ECHA, 2023; Brack et al., 2019). The interpretability of observed effects varies, with endocrine disruption and genotoxicity being more direct than more complex endpoints like oxidative stress. In the proposal for a directive amending the Water Framework Directive, the Groundwater Directive, and the Environmental Quality Standards Directive, it is suggested that the monitoring of estrogenic compounds using *in vitro* effect-based methods should be mandatory in all member states (COM2022 540 final).[4] However, while effect-based methods can detect a broad range of potential health-related cellular impacts from water mixtures, there is still a lack of knowledge on how to extrapolate results from such studies into meaningful hazard characterizations relevant for human and ecosystem health. Techniques employing enrichment methods (Schulze et al., 2015; Lunde Hermansson et al., 2025) offer valuable insights into the overall toxicity of complex mixtures but still face challenges in translating results directly to individual chemical concentrations.

[4] Proposal for a Directive of the European Parliament and of the Council amending Directive 2000/60/EC establishing a framework for Community action in the field of water policy, Directive 2006/118/EC on the protection of groundwater against pollution and deterioration and Directive 2008/105/EC on environmental quality standards in the field of water policy. https://eur-lex.europa.eu/resource.html?uri=cellar:d0c11ba6-55f8-11ed-92ed-01aa75ed71a1.0001.02/DOC_1&format=PDF

Effective communication is essential for risk management

Communication barriers exist both between individual organizations and across different sectors. A key challenge is the effective dissemination of water quality information and action plans across relevant authorities, underscoring the interconnectedness of the water cycle. For example, the significant costs associated with PFAS removal from drinking water (estimated at €18 billion annually if PFAS use continues unabated (EurEau, 2025)) contrast with the narrow focus of wastewater treatment plants on specific pollutants like pharmaceuticals. This highlights a lack of integrated approaches and results in cost-inefficiencies in addressing chemical pollution. Communicating chemical risks presents another challenge. Risk assessment, chemical analysis, and toxicological effects are complex topics, not only for the public but sometimes for water managers themselves. According to the EU Drinking Water Directive 2020/2184, drinking water producers are responsible for timely communication and providing information about water quality. A central aim of the directive is to strengthen transparency by ensuring public access to water quality data both under normal conditions and in the event of non-compliance. This creates a need for support in effectively communicating chemical risks to both the public and decision-makers. Conveying results from chemical screening studies or effect-based methods is particularly challenging in the absence of established thresholds. Tentative identification of a potentially harmful chemical at a single time point could trigger costly investigations in the absence of proper guidelines. Similarly, a detected effect in a sensitive bioassay may not directly indicate harm to humans or larger organisms but could still be relevant for more vulnerable species under chronic exposure.

Contribution to the mission of Water Wise Societies

This project contributes to the mission of Water Wise Societies – sustainable water for all by 2050 – addressing primarily water quality as well as indirectly water quantity across the three formulated sub-goals and specific assignments:[5]

- **Resilient supply and management of water in society**: Ensuring the safety of water through robust detection and risk assessment methods for hazardous chemicals and their mixtures (primarily, assignment Ensure good drinking water quality).
- **Wise water use:** Improving the wise use of water by promoting quality-based reuse of treated wastewater, thereby minimizing chemical risks to aquatic and human health and ensuring efficient management of water resources (primarily, assignment Recycle and reuse water and its resources).
- **Thriving lakes, streams, and groundwater:** Providing the necessary tools to monitor, prevent, and mitigate the spread of hazardous chemicals in surface and groundwater (primarily, assignment Prevent and reduce the spread of hazardous substances).

Ultimately, this work lays the foundation for a systemic shift in water quality management, moving from reactive, fragmented approaches to proactive and holistic strategies. It paves the way for the creation of a national function that will foster collaboration between science, policy, and various sectors. By supporting advances in methodology, risk assessment, and data interpretation for the water industry and environmental monitoring, this function will also help enable regulations that are more adapted to real-time scenarios – crucial steps toward a water-wise and health-protective future.

[5] https://waterwisesocieties.se/delmal/

Desired future state

Vision

Our vision for the future is a sustainable and holistic water management system that encompasses the entire water cycle – from catchment to tap water and wastewater – ensuring safe and sustainable water for all, with respect to chemical hazards. Rooted in a One Health perspective, this vision recognizes the interconnectedness of human, animal, and environmental health. Future chemical risk assessments are envisioned to be proactive, preventive, and transparent, evaluating potential risks from both known and emerging chemicals in near real-time, while also considering the long-term effects of chemical mixtures. A widely implemented proactive water monitoring system will enable the early detection of chemicals and their biological effects in water sources by integrating advanced analytical techniques - both chemical and bioanalytical – for a comprehensive understanding of water quality. Interoperable databases and computational tools will facilitate data-driven, proactive, and harmonized risk assessments, drawing on information such as usage patterns, emission data, chemical monitoring results, chemical-specific properties, and toxicity or effect-based data as key risk indicators. Regulations and monitoring practices will evolve to address the increasing complexity and diversity of chemicals in real-world water systems. This will include the adoption of action-driven threshold levels and clear risk communication tools to support rapid mitigation efforts. Mitigation should occur at the source whenever possible; however, based on risk assessments, additional treatment at water plants may be required to ensure water safety. Early warning systems, guided by the precautionary principle, will provide timely information about potential risks in all water bodies before they threaten the environment or human health.

Our ambition is to establish a national function, such as a competence platform/center, that can provide support in the adaptation and use of existing state-of-the-art tools for conducting and developing risk assessments of chemical risks in water.

Opportunities

The transition toward a sustainable, healthy, and well-protected water system is a complex challenge that also brings significant opportunities for innovation and policy advancement. Strategic initiatives such as the EU Green Deal, the Zero Pollution Action Plan, and the Chemicals Strategy for Sustainability have created a critical window for adopting holistic, precaution-based risk assessments that protect all water resources. Efforts to implement and harmonize legislation and best practices for managing chemical risks in water can benefit substantially from the activities in other EU member states, particularly those supported by EurEau[6] and the Joint Research Centre.[7] International initiatives and projects provide valuable opportunities to integrate cutting-edge research and innovative solutions. Notable examples include SOLUTIONS,[8] PARC,[9] ZeroPM,[10] the NORMAN Network,[11] and IRISS,[12] all of which are at the forefront of global efforts to address chemical risks in the environment.

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[6] https://www.eureau.org/
[7] https://commission.europa.eu/about-european-commission/departments-and-executive-agencies/joint-research-centre_en
[8] https://www.solutions-project.eu/
[9] https://www.eu-parc.eu/projects
[10] https://zeropm.eu/about/
[11] https://www.norman-network.net/
[12] https://iriss-ssbd.eu/iriss/about-iriss

National collaboration among researchers, authorities, and the water industry is a key opportunity to shape legislation and regulatory frameworks while promoting the adoption of innovative approaches. Engaging with national organizations such as the Swedish Water and Wastewater Association (Svenskt Vatten) and national research clusters national research clusters (DRICKS,[13] VA-kluster Mälardalen,[14] VA-teknik Södra,[15] Dag & Nät)[16], the Toxicological Council (Toxikologiska rådet)[17] can amplify this impact.

Significant opportunities exist in leveraging technological advancements to improve chemical detection, monitoring, and modeling for timely exposure information. High-throughput *in vitro* toxicity testing across various health endpoints, combined with advances in translating effects between *in vitro* and *in vivo* systems and the use of predictive computational tools, paves the way for more robust hazard assessments. Harmonizing methods to derive biologically meaningful *in vitro* thresholds will facilitate rapid decision-making and shifting from single-chemical to mixture risk assessment. Another critical opportunity lies in developing regulatory maximum thresholds for prioritized risk drivers using effect-based and other toxicological data, while accounting for population variability and lifetime protection. The development and integration of advanced computational methods, including AI-powered predictive models, transport models, toxicokinetic models, read-across approaches, and text mining, will underpin the creation of proactive, data-driven risk assessment frameworks. Encouraging adherence to FAIR (Findable, Accessible, Interoperable, Reusable) data principles (Wilkinson et al., 2016) among authorities and stakeholders is a crucial opportunity. Establishing comprehensive, interoperable, and transparent databases for chemical information which is currently scattered, chemical/product use and emission data, and hazard characterizations will significantly enhance proactive risk assessment capabilities by developing risk indications for many chemicals.

Providing guidance on advanced tools for proactive decision-making and rapid risk mitigation offers significant opportunities for water managers. Effective risk communication can also help draw policy attention to emerging chemicals. Establishing a national support function for water managers would help address knowledge gaps and promote effective implementation.

Barriers

Despite the promising opportunities, several significant barriers need to be addressed to achieve meaningful progress. Fragmented legislative responsibilities across multiple governmental agencies, combined with slow policy responses, contribute to delays in regulating emerging chemical threats and evaluating unknown substances and mixtures. This is further compounded by the absence of clear guidance for action and the perceived high burden of proof required to regulate individual chemicals.

The lack of data on exposure, use, production, degradation, and human/environmental toxicity for most chemicals represents a major barrier. Critical knowledge gaps regarding long-term, low-dose effects on critical endpoints (endocrine, immune, neurological functions, etc.) also hinder comprehensive risk assessment. The scattered nature of existing data and its frequent mismanagement (not following FAIR principles) further exacerbate this problem.

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[13] https://www.chalmers.se/institutioner/ace/centrum-och-infrastrukturer/dricks/
[14] https://www.va-malardalen.se/va-kluster-malardalen
[15] https://va-tekniksodra.se/
[16] https://www.ltu.se/forskning/forskningsamnen/va-teknik/dagnat
[17] https://www.kemi.se/en/about-the-swedish-chemicals-agency/organisation/the-toxicological-council

Current models for hazardous properties are neither accurate enough nor have a large enough applicability domain to be useful. A preference for potentially less effective mechanistic models over data-driven "black-box" approaches can also constitute a barrier. Another significant barrier is the lack of standardization in both analytical methods and risk assessment practices. Interpreting chemical signals from suspect and non-target analysis (semi-quantitative and qualitative data) and biological signals from effect-based methods into applicable risk assessment measures remains challenging.

The absence of established thresholds for high-risk chemicals significantly hinders the implementation of effective preventative measures. Moreover, existing limits are often based on current detection capabilities rather than long-term health impacts. In many cases, analytical detection limits are too high to effectively monitor harmful concentrations of certain chemicals, making it difficult to enforce more stringent and health-relevant thresholds. Inconsistent thresholds due to differing methodologies across uses and regions further complicate the regulatory landscape. In addition, commercial laboratories are unable to offer analyses of emerging chemicals unless there is sufficient demand from paying customers. As a result, research-developed methods may fail to reach public use.

A lack of resources (knowledge, economic, personnel) among many water managers, particularly smaller ones with staff having multiple responsibilities, limits their capacity to adopt new, non-legislated analyses like advanced analytical methods and effect-based methods. Furthermore, there is a lack of effective business models to translate research into practical tools that are accessible and supported for use by practitioners. As a result, valuable research findings often remain scattered across publications and are not fully utilized to their potential.

Future scenarios

From the discussions during the project, several potential future scenarios for addressing the complex challenges of chemical risk assessment in water emerged. These scenarios range from incremental improvements to more transformative and integrated approaches. The focus shifts between the following scenarios, with scenario 1 continuing on the current path, 2 focusing on data-driven approaches, 3 focusing on effect-based methods, and 4 integrating all methods for a more holistic approach.

Scenario 1: Evolutionary adaptation - risk assessment 2.0 (slow adaptation)
This scenario envisions a future where improvements in chemical risk assessment occur gradually, primarily relying on traditional chemical-by-chemical analysis and existing lists of priority chemicals. Regulatory actions for emerging chemicals remain delayed and reactive. Mixture effects are largely overlooked, and responsibilities across different entities remain fragmented. While analytical methods may see incremental advancements, their integration into a holistic risk assessment framework is slow. This trajectory enables continued exposure to unknown chemicals, placing the burden of remediation and associated costs on the state and water utilities, and misses opportunities for proactive risk mitigation.

Scenario 2: Data-driven early warning and rapid response
This future prioritizes the establishment of sophisticated, data-driven early warning systems. By integrating cross-sectoral data from product registers, patents, water samples, and chemical usage with advanced computational technologies (AI-driven prediction models, read-across, machine learning), timely alerts for potential chemical risks are generated. This enables rapid implementation of risk mitigation measures. However, this scenario may

struggle to establish clear, biologically relevant threshold limits for environmental and human health, and its success is heavily dependent on political and institutional support for data sharing and utilization.

Scenario 3: Integrated One Health for proactive prevention
This vision embraces the One Health concept, recognizing the interconnectedness of environmental, aquatic life, and human health. The focus is on holistic risk assessment, utilizing effect-based monitoring tools to address mixture effects. Strong cross-sectoral collaboration safeguards water quality from source to tap, fostering shared responsibility and unified risk assessment methods aimed at preventing chemical exposure before harm occurs. While this scenario prioritizes prevention and ecological health, it may not fully leverage the potential for automated data analysis and early warning systems, leading to delayed actions and higher clean-up costs in some instances.

Scenario 4: Proactive and preventive risk assessment through integrated intelligence
This scenario represents a convergence of the strengths of the previous scenarios. It combines advanced data surveillance using advanced computational methods with comprehensive chemical and biological monitoring technologies to challenge traditional risk assessment paradigms. The implementation of biologically meaningful thresholds enables rapid and targeted actions. Crucially, this future emphasizes the identification of key risk drivers to facilitate proactive political interventions aimed at reducing chemical emissions at their source. Achieving this requires a significant acceleration in the derivation of regulatory thresholds based on *in vivo*, *in vitro*, *in silico* and (eco)epidemiological data.

Emerging themes

Overall, several cross-cutting themes have emerged as key to advancing future chemical risk assessment in water systems. These include the integration of advanced analytical techniques and effect-based methods, the development of early warning systems, and the application of FAIR data principles to enable predictive and holistic risk assessment approaches. Addressing gaps in existing legislation and developing clear regulatory frameworks, including biologically relevant thresholds and action guidelines for new monitoring approaches, are identified as key priorities. Effective risk assessment in the future necessitates strong cross-sector collaboration. This, establishing mechanisms for knowledge sharing, expert support, and coordinated action is vital. Overcoming the lack of resources and expertise is crucial for widespread adoption of advanced monitoring and risk assessment practices. The establishment of national support and guidance structures can help address this.

Hypotheses for system change

The following **hypotheses for system change** have been identified to achieve our future state vision:

- To increase the adoption and trust in **new monitoring approaches,** collaboration among researchers, policymakers, and water managers on data sharing, method development, and validation is essential. Sustained investment in method development and harmonization, supported by funding and policy, will improve the sensitivity, robustness, and comparability of advanced analytical methods, leading to a more comprehensive and actionable monitoring system.
- **Integrating analytical methods**, i.e., effect-based methods, suspect and non-target screening alongside targeted chemical analyses will enhance the detection of potentially

hazardous, unknown, or unregulated chemicals and complex mixtures in water. Standardized methods and workflows should define which initial effect-based parameters to measure, and subsequent analytical steps based on preliminary findings. Guidance on interpreting chemical and biological signals will support a precautionary approach for potentially hazardous chemicals and mixtures with unknown long-term effects.

- Creating **a register of hazardous chemical uses and emission data**, organized by water basin, could provide water managers with crucial information to identify potential chemical threats.
- Different **computational models** constitute valuable extrapolation tools for evaluating the biological effects of substance mixtures and emerging contaminants. Coupling detailed chemical use data with new state-of-the-art models for hazardous properties will allow for early identification of chemicals of emerging concern.
- Establishing **early-warning systems** at critical control points (e.g., water intakes, upstream of drinking water treatment plants, discharge points, or downstream of treated wastewaters or industrial waters) will enable the proactive detection and management of hazardous events before they impact the environment and water consumers.
- **Updating** water quality **regulations** to encompass a broader range of chemicals and prioritized biological effects will align monitoring programs more effectively with actual environmental risks. This shift necessitates clear, science-based directives that move beyond focusing on specific chemicals to considering total effects. More research is needed to define acceptable thresholds, and standardized methods are crucial for establishing relevant baselines and threshold values across different water types. Identifying and prioritizing key toxic effects and linking substance groups to these effects will also improve risk assessment.
- **Communicating** results from effect-based methods presents unique challenges due to the abstract nature of toxic effects compared to already accepted regulatory thresholds (such as PNEC, maximum water limits, etc.). Effective communication of chemical risks requires subject matter expertise, a clear message, avoidance of overly technical language, and transparency about current knowledge and uncertainties. Utilizing national authorities for communication can enhance credibility and ensure consistent messaging, and many water organizations may benefit from support in this area.
- A **national function** (e.g., a competence platform/center**)** providing expert support to regulating authorities and practitioners will help close the gap from research to application. Such a function can provide support regarding monitoring and risk assessment, perform horizon scanning and effectively communicate information on coming policy changes to scientists, facilitate meetings between scientists and policy makers, and foster collaboration between different sectors.

Stakeholder mapping

National regulatory agencies: Swedish authorities including the Swedish Environmental Protection Agency (Naturvårdsverket), Swedish Chemicals Agency (Kemikalieinspektionen), Swedish Agency for Marine and Water Management (Havs- och vattenmyndigheten), Geological Survey of Sweden (Sveriges geologiska undersökning), and the National Food Agency (Livsmedelsverket). Their relevance lies in coordinating chemical monitoring programs, maintaining databases, and facilitating dialogue on water quality and limits across different parts of the water cycle. Securing consistent representation from national authorities was difficult in the project due to their substantial workloads and limited resources.

Additionally, the distribution of water-related responsibilities across numerous governmental bodies complicated engagement efforts.

International agencies: European agencies such as the European Chemicals Agency (ECHA), European Food Safety Authority (EFSA), and the European Environment Agency (EEA). Their relevance is in providing risk assessment frameworks and supporting data sharing initiatives. Other national agencies in EU and institutes like RIVM (National Institute for Public Health and the Environment, Netherlands), KWR Water Research Institute (the Netherlands), Eawag (Swiss Federal Institute of Aquatic Science and Technology, Switzerland), UFZ (Helmholtz Centre for Environmental Research, Germany) and similar organizations offer potential for knowledge exchange on relevant methods and tools.

Water sector organizations and funding bodies: Water Wise Society is a potential source of initial funding. The Swedish Water and Wastewater Association (Svenskt Vatten) is a potential funding source and a national collaboration platform with the capacity to advocate for the sector, facilitate collaboration, and potentially influence policy.

Water managers: Drinking water producers have a central role in defining challenges and prioritizing directions. Their involvement is relevant for managing risk objects, communicating with industries, monitoring water quality from source to tap, participating in case studies, applying developed risk assessment tools, engaging with authorities and the public, and deciding on proactive prevention measures. Wastewater treatment plants monitor the quality of treated wastewater effluents; their participation is relevant for case studies, applying risk assessment tools, and deciding on actions to prevent chemical release. Municipalities are relevant for managing risk objects and communicating with industries. County Boards and Water Conservation Associations have an important role in environmental monitoring of hazardous chemicals.

Scientific community: Researchers from various disciplines are relevant for developing computational tools, sensitive and broad analytical detection methods (target, suspect, non-target screening), and effect-based approaches (*in vitro* and *in vivo* methods). Their contributions are relevant for creating interpretation tools, establishing monitoring case studies, developing harmonized risk assessment frameworks, determining thresholds, and building expert networks across various scientific fields. Universities have the potential to develop decision support for new methods, such as suspect and non-target screening.

Companies: Companies have an important role in commercializing relevant scientific findings, making them available for continuous use.

IT Experts: Database and technology providers are relevant for providing the necessary infrastructure for online database platforms and assessing the feasibility of different technologies.

Industry: Chemical manufacturers and other industries are relevant due to their need to engage in transparent data-sharing regarding chemical use and patent information, as well as participating in cooperative actions to mitigate risks.

Policy makers and government: Politicians and government officials are the implicit target audience for communication regarding the importance of new methods like effect-based analysis to drive legislative implementation. EU program representatives are potential collaboration partners and sources of funding through initiatives like the EU Green Deal, the Zero Pollution Action Plan, and the Chemicals Strategy for Sustainability. Leveraging EU channels is also a key strategy for disseminating knowledge and influencing policy, particularly when Swedish expertise in specific areas can contribute to broader European discussions.

Proposed next steps

Based on our analysis of the complex challenge and the envisioned future state, we have identified a series of steps necessary to achieve that vision. These steps vary in both scope and time horizon. To bring clarity and coherence to the path forward, we have arranged the steps in a logical, sequential order, as indicated by numbers. Each step is also categorized by its level of importance, as indicated by A or B, with A representing the highest priority. The estimated time required for successful implementation of each step is roughly represented by three categories: short-term (1–3 years), medium-term (3–10 years), and long-term (more than 10 years).

Fostering collaboration and knowledge exchange

1. Open dialogue and joint projects: Promote communication and collaboration among water managers, producers, agencies, researchers, and industry through workshops, training, and joint data projects. Priority A, short-term.
2. Cross-sector collaboration platforms: Establish mechanisms and networks to facilitate data sharing, harmonized terminology, knowledge exchange and joint initiatives across different regulatory sectors and stakeholders. Priority A, medium-term.
3. Long-term national function: Create a long-term national function (platform or center) for horizon scanning, method support, data interpretation, training, and innovation. Priority A, long-term.

Creating and updating monitoring methods, developing integrated monitoring and early warning systems

1. Method mapping and gap analysis: Systematically review and classify existing chemical and effect-based methods, assess their coverage of the current chemical and toxicological space, assess their accessibility, and identify critical knowledge and technology gaps. Priority A, short-term.
2. Develop and validate holistic monitoring frameworks through pilot projects: Implement real-world testing of integrated chemical (target, suspect and non-target screening) and effect-based monitoring frameworks in various water systems for comprehensive water quality assessment. Priority A, short-term.
3. Create fact sheets and guidelines for practitioners: Propose recommendations on the selection of analytical methods, sampling strategies, and interpretation of data and results, for different contexts and water systems. Priority A, short-term.
4. Further optimization, development, and standardization of methods: Optimize existing target methods to reach lower detection limits when needed from a regulatory perspective, develop new target methods for novel (not yet studied) hazardous micropollutants, develop suspect screening lists for specific needs (catchment specific, water-type specific), and standardize advanced analytical methods, including non-target screening and effect-based analysis. Priority A, medium-term.
5. National coordination of laboratory analyses: Ensure effective national coordination of methods and analytical resources for detecting micropollutants and assessing their effects in water. Priority A, long-term.

6. Modelling and detection methods integration: Combine advanced transport models with detection methods for comprehensive water quality assessment and source tracking. Priority B, medium-term.

Adopting and developing new computational tools and infrastructure

1. Implementation of existing hazard prediction tools: Collect, evaluate, and combine existing hazard prediction tools into an easily accessible software platform or website. Several *in vivo* prediction tools are already available, and new AI-based solutions are currently in development (see, e.g., Gustavsson et al., 2024). Tools for *in vitro* predictions are also available via the US EPA ToxCast program. By combining these resources, water managers will be able to predict the hazardous properties of chemicals with missing data, thereby expanding the number of chemicals for which quantitative risk assessments can be conducted. Priority A, short-term.
2. Develop or adopt new AI-based models for hazard prediction: Further expand the range of hazardous properties that can be predicted with high accuracy by developing and/or adopting new models, particularly for properties where current performance is limited, such as human toxicity, persistence, and mobility. Priority A, medium-term.
3. Use toxicokinetic modelling: Apply mathematical models that describe the absorption, distribution, metabolism, and excretion of chemicals, in order to extrapolate *in vitro* effect concentrations to equivalent internal concentrations in aquatic organisms and humans for high-risk chemicals. Priority A, short-term.
4. Develop AI-based models for *in vitro* to *in vivo* extrapolations: Provide tools which help water managers predict *in vivo* results from *in vitro* assays. Most guidance for risk assessment is currently written for *in vivo* data. By providing accurate extrapolations between *in vivo* and *in vitro* data, future guidelines on effect-based methods could be better grounded in current practices. Priority B, medium-term.
5. Gathering and sharing information to interoperable data platforms: Information on chemical hazards and use is currently scattered across various agencies, firms, research projects, etc. Gathering and sharing information on, e.g., chemical use, contaminated areas, and human activities would allow identification of potential exposure scenarios. This would, in turn, allow for more focused monitoring campaigns and more informed decisions. Depending on the type, data could be shared either via centralized databases or via external partners (e.g., the NORMAN network). Priority A, medium-term.
6. Text mining for emerging risks: Identify, test, adapt, and implement existing relevant tools to scan patents, scientific literature and use databases for early identification of new problematic chemicals (see, e.g., Hartmann et al., 2019). Priority B, medium-term.
7. Computational tools for data interpretation: Establish tools to interpret complex chemical and biological datasets, e.g., signals in the monitoring data obtained from suspect/non-target screening and multiple assay results from effect-based methods. By collecting both non-target data and results from effect-based methods, it will become possible to predict effect-based results from non-target screening data. Priority B, long-term.

Enhancing risk assessment

1. Method mapping and method gap analysis: Systematically review and classify existing methods for risk assessment, their accessibility, and identify critical knowledge gaps. Priority A, short-term.
2. Create fact sheets and guidelines for practitioners: Develop a simple guide for conducting risk assessments for various water uses, including information on the required data, where to find it, and the maximum allowable levels of chemicals in water. Priority A, short-term.
3. Development of user-friendly risk assessment tools: Create and develop user-friendly tools for water managers (see, Risk thermometer and QCRA for current examples) to facilitate rapid quantitative risk assessment and decision-making. These tools should be accessible through software applications and/or web interfaces to ensure easy and efficient use by water managers. Priority A, short-term.
4. Development of next-generation mixture risk assessment methods: Create guidance for translating biological effects from effect-based methods to risk and for implementing biological thresholds for mixture effects in regulatory frameworks. Finally, harmonize approaches that integrate biological thresholds from effect-based methods and maximum health-based water limits for priority risk drivers. Priority A, medium-term.
5. Incorporating exposure scenarios and uncertainties: Account for varying exposure scenarios (e.g., seasonal and climate change) and uncertainties in risk assessment processes. Priority B, medium-term.

Informing policy and regulation

1. Working towards harmonization: Promote the harmonization of monitoring and risk assessment methods. Priority A, short-term.
2. Defining baselines and thresholds for effect-based methods: Focus research on identifying the most relevant biological effects for regulatory consideration (Priority A, short-term). Research and establish baseline values for effect-based methods in different water types and define relevant thresholds and trigger values for their application. Priority A, medium-term.
3. Watchlist updates and derivation of thresholds for emerging chemicals: Develop praxis to rapidly identify emerging chemicals and establish thresholds for high-risk chemicals in water bodies, considering health and environmental data. Priority B, short-term.
4. Guidelines and protocol development for operators and regulators: Create actionable guidance for method selection, sampling strategies, and data interpretation to facilitate practical application of new approaches. Priority A, medium-term.

To effectively advance the risk assessment and management of unwanted chemicals in water, we envision transitions across five system dimensions, as shown in Figure 1. As a key effort, we propose establishing a national support function. This function should include coordinating stakeholder efforts and cross-sector collaboration; enhancing water quality monitoring and analysis; integrating data and developing computational tools; harmonizing risk assessment methodologies and developing thresholds for hazardous chemicals; and bridging the gap between scientific advancements and policy development.

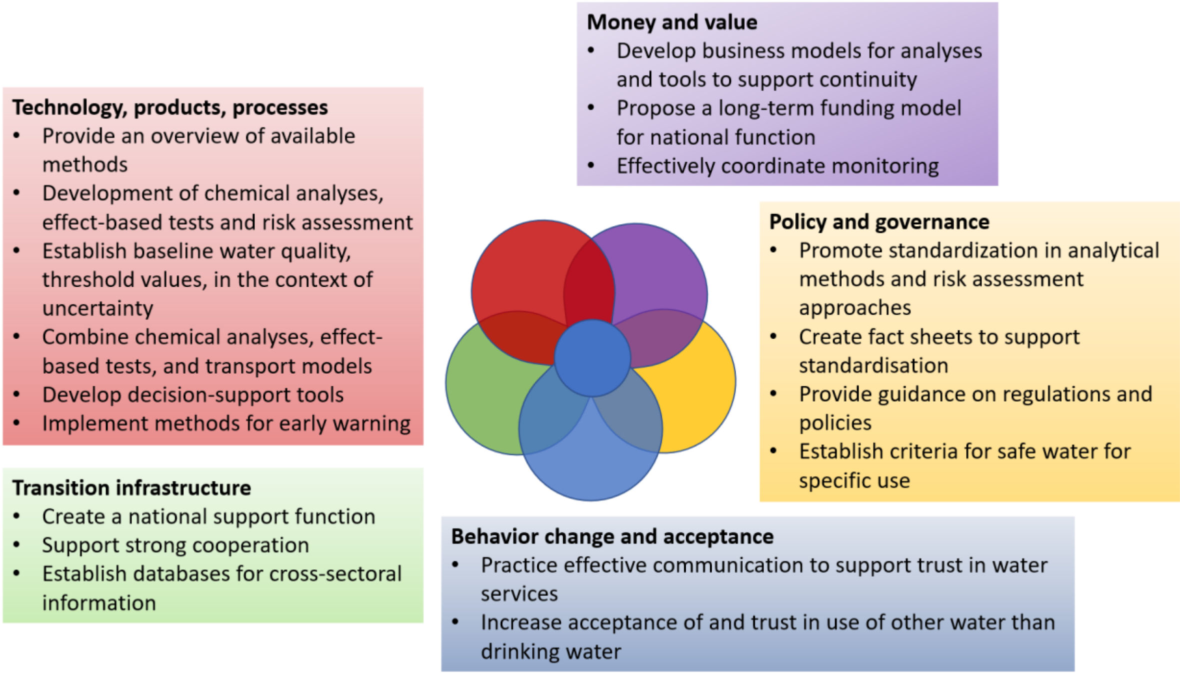

Figure 1 Envisioned transitions across five system dimensions in response to the complex challenge of assessing and managing risks from unwanted chemicals in water.

Project group

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Declaration of generative AI use

During the preparation of this report ChatGPT (GPT-3.5 and GPT-4) by OpenAI and Gemini by Google were used in order to improve readability and flow of the text. After using these tools/services, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

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