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MILESTONE REPORT 2
PROJECT 1166

Developing a Global Risk-based Tool for Prioritising Contaminants of Emerging Concern (CEC) for the Water Industry: Synthesis Report



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Developing a Global Risk-based Tool for Prioritising Contaminants of Emerging Concern (CEC) for the Water Industry: Synthesis Report

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About ECHIDNA

ECHIDNA (Emerging Contaminants for International Decision Analysis) is a science-based decision support tool developed to help the water industry assess and manage risks associated with contaminants of emerging concern (CECs). With hundreds of thousands of chemicals in use globally, many detected in water sources, ECHIDNA provides a consistent, evidence-based framework for informed decision-making. Developed through a WaterRA-supported initiative led by Griffith University, ECHIDNA is widely used across Australia and internationally, with ongoing collaboration ensuring the tool continues to evolve and support the sector in responding to emerging risks and maintaining confidence in water quality and safety.
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Table 1 Overview of peer-reviewed publications that have applied different approaches to prioritise CEC. Studies sorted in order of matrix. 9

Abbreviations

AAC	activity concentration at cutoff
CEC	contaminants of emerging concern
DBP	disinfection by-product
EAR	exposure−activity ratio
EC_{50}	concentration causing 50% effect
FR	flame retardant
ICRQ	Industrial Contaminant Risk Quotient
ICSS	Industrial Contaminant Screening Score
PAH	polycyclic aromatic hydrocarbon
PBT	persistent, bioaccumulative and toxic
PFAS	per- and polyfluoroalkyl substances
PMT	persistent, mobile and toxic
PNEC	predicted no-effect concentration
PCP	personal care product
QSAR	quantitative structure-activity relationship
SVHC	substances of very high concern
TDI	tolerable daily intake
ToxPi	Toxicological Priority Index
vPvM	very persistent and very mobile

1 Introduction

The Global CEC Risk Ranking Tool, which will be developed as part of Project 1166, is based on the existing contaminants of emerging concern (CEC) prioritisation tool ECHIDNA (Neale et al., 2023). However, there are a number of other CEC prioritisation approaches available worldwide that have been implemented to varying degrees. These range from simple screening based on predicted persistent, bioaccumulative and toxic (PBT) properties (e.g., Balakrishnan et al., 2024) to automated workflows that consider many different criteria (Isaacs et al., 2024). This report aims to provide an overview of the different approaches proposed to prioritise CEC in matrices relevant to the water industry (drinking water, surface water, groundwater, wastewater and biosolids), with any remaining gaps identified. Project partners were contacted on 17th February 2025 for their feedback on prioritisation tools they find useful. This included projects and publications detailing CEC prioritisation approaches, as well as web-based tools. Information from the project partners was complemented with a literature search to identify peer-reviewed studies on prioritisation tools. This report also aims to identify which aspects/functionalities would be appropriate to include in the Global CEC Risk Ranking Tool to meet the needs identified in Milestone 1.

2 Literature Review

In addition to studies identified by project partners, Web of Science and Scopus (two of the key databases of peer-reviewed scientific publications) were searched on 17th February 2025 to identify CEC prioritisation approaches applied in the literature. The terms *(prioritisation OR prioritization) AND (tool OR database) AND (micropollutant* OR "emerging contaminant*" OR "contaminant* of emerging concern" OR CEC) AND (water OR biosolid* OR sludge)* were searched in "All Fields" in Web of Science. The terms *prioritization OR prioritisation AND tool OR database AND micropollutant* OR "emerging contaminant*" OR "contaminant* of emerging concern" OR CEC AND water OR biosolid* OR sludge* were searched in "Article title, Abstract, Keywords" in Scopus. The search strings returned 53 hits for Web of Science and 46 hits for Scopus. Thirty-two of the studies appeared in both Web of Science and Scopus, with 21 studies only in Web of Science and 14 studies only in Scopus. This gave a total of 67 unique studies. The abstract of each paper was screened to ensure that only studies that prioritised CEC were included, with only original research studies considered. After screening, 19 studies relevant for Milestone 2 were identified.

3 Results

3.1 Published literature

Thirty studies were identified from both project partners (11 studies) and the literature search (19 studies), with the studies summarised in Table 1.

Most studies focused on water matrices, primarily surface water, wastewater and drinking water, including drinking water sources. Only one study, Newmeyer et al. (2024), focused on prioritising CEC in biosolids. Biosolids/wastewater sludge occurrence data were identified as a priority for the Global CEC Risk Ranking Tool in Milestone 1, with the lack of prioritisation approaches for this matrix clearly highlighting an important knowledge gap. Most of the reviewed studies are specific to a particular matrix, rather than considering multiple matrices, though the framework described in de Voogt et al. (2009), which was developed for prioritisation of specific pharmaceuticals, can be applied throughout the water cycle. Ideally, a CEC prioritisation tool for the water industry should consider multiple relevant matrices, though some publications do note that their workflow can be applied to other environmental matrices (Dulio et al., 2024). ECHIDNA currently includes occurrence data for wastewater influent, wastewater effluent, surface water including drinking water sources, drinking water and reclaimed water.

The candidate list of substances for prioritisation in some studies was simply based on what was monitored in the matrix (e.g., Choi et al., 2024; Deere et al., 2021; Villa et al., 2020). Other studies based the candidate list on regulatory databases (e.g., chemical products registered and approved for use) (Di Nica et al., 2015; Gago-Ferrero et al., 2018; Serasinghe et al., 2022) or existing compound lists (e.g., Water Framework Directive Watchlist, European Chemicals Agency Candidate list of substances of very high concern) (Been et al., 2021). The number of substances in the candidate lists ranged from 8 to >65,000. The candidate list in ECHIDNA (1820 chemicals and substances) was compiled based on both Australian and international sources including chemicals in regulation, chemical detected in water and existing compound lists (e.g. NORMAN Network emerging substances list and US EPA Contaminant Candidate List), as well as new CEC identified in academic reviews (e.g., Richardson and Kimura, 2020). Further, most of the studies considered a range of different chemical classes (e.g., pharmaceuticals, personal care products (PCPs), pesticides, disinfection by-products (DBPs), per- and polyfluoroalkyl substances (PFAS), flame retardants (FR), polycyclic aromatic hydrocarbons (PAHs)) (e.g., Alvarez et al., 2021; Baken et al., 2018; Lopez-Herguedas et al., 2023), though some only focused on a single class, such as pharmaceuticals (Di Nica et al., 2015; dos Santos and Nardocci, 2019). Rather than focusing on individual CEC, the San Francisco Public Utilities Commission prioritised CEC groups, such as algal

toxins and industrial and commercial chemicals, with expert review and customer interaction included in the prioritisation approach (Olson et al., 2017).

CEC that are PBT, persistent, mobile and toxic (PMT), or very persistent and very mobile (vPvM) are often prioritised for further investigation (e.g., dos Santos and Nardocci, 2019; Dulio et al., 2024; Hartmann et al., 2021). The lack of experimental data, particularly for CEC, means that these parameters are typically predicted, commonly using EPISuite and now CompTox Chemicals Dashboard (both US EPA) or online tools (RIVM PBT & PMT screening tool). Other proposed approaches include read-across based on structural similarity to group PMT and vPvM CEC (Chirsir et al., 2024), while coupling machine learning with models has been proposed to screen PMT and vPvM CEC (Zhao et al., 2022). Further, Hartmann et al. (2023) developed a continuous scoring system for P, M and T potential using modelled parameters, with an overall PMT score grouping chemicals as low to moderate, high or very high P, M and/or T. It should be noted that a limitation of these approaches and tools is that they are not compatible with inorganics, organometals and salts. PBT is used as the first screening level in ECHIDNA, though mobility is not considered. Mobility, which indicates the potential of a CEC to be transported in water and is typically assessed using the organic carbon-water partition coefficient, could be included in the Global CEC Risk Ranking Tool.

Occurrence was included as part of the prioritisation process in most studies, with CEC concentrations measured as part of the study (e.g., Kuskopf et al., 2020; Nikolopoulou et al., 2022) or existing databases utilised (e.g., Baken et al., 2018; Rosenblum et al., 2024). Some exceptions included Balakrishnan et al. (2024), where PCPs were prioritised based on hazard (PBT) only, which is in line with precautionary principles, and Serasinghe et al. (2022), where pesticides shortlisted for monitoring were identified based on approved use in the region of interest, toxicity and lack of routine monitoring. Any unapproved use was not considered in this study. While target chemical analysis is more frequently used, more recent studies now use non-target analysis and suspect screening for CEC prioritisation (e.g., Been et al., 2021; Ekpe et al., 2025; Newmeyer et al., 2024; Zhao et al., 2023). Parameters such as peak abundance, detection frequency and estimated concentration were used for prioritisation. The advantage of non-target analysis and suspect screening over targeted analysis is that prioritisation is not limited to only known, targeted chemicals, though it is less sensitive and often only a fraction of the detected features are identified to an acceptable confidence level (e.g., Level 1 (confirmed structure), Level 2a and 2b (probable structure) (Schymanski et al., 2014)). Non-target and suspect screening may be combined with bioanalytical tools to focus the identification and prioritization process on CEC with biological activity (Been et al., 2021).

Removal was also considered in studies that prioritised CEC in wastewater and drinking water (e.g., Gros et al., 2017; He et al., 2023; Lopez-Herguedas et al., 2023; Pronk et al., 2023). While removal was usually based on measured data, Pronk et al. (2023) developed indicative removal rules for the removal of CEC by conventional treatment, oxidation, activated carbon, reverse osmosis and advanced oxidation. These were combined to determine the "effort index" (i.e., how much effort is required to remove a particular chemical), which was used to prioritise CEC. Both experimental and predicted removal data are included in ECHIDNA, including predicted removal based on the approach in Pronk et al. (2023). As discussed in the Milestone 1 report, expanding the treatment function to calculate a risk quotient for the residual risk after the implementation of



a new treatment process in a treatment train was suggested as a new feature for Stage 2 of the project.

In addition to the toxicity data included in the PBT or PMT assessment, ecotoxicity (e.g., predicted no-effect concentration (PNEC), concentration causing 50% effect (EC_{50})) or toxicity (health reference levels, tolerable daily intake (TDI), drinking water guidelines) data are included in most CEC prioritisation tools (e.g., Baken et al., 2018; García-Vara et al., 2023; Osorio et al., 2016; Rosenblum et al., 2024; Sjerps et al., 2021). Together with the measured or predicted environmental concentrations, toxicity data are used to calculate risk quotients to rank CEC. Other terms used in the literature included benchmark quotient (Baken et al., 2018; Sjerps et al., 2021), hazard quotient (Kuskopf et al., 2020) and toxicity quotient (Alvarez et al., 2021), but the calculation is essentially the same. The current version of ECHIDNA includes both ecotoxicity risk quotients (calculated using PNEC) and drinking water risk quotients (calculated using drinking water guidelines). *In vitro* bioassay data from the CompTox Chemicals Dashboard were also used to prioritise CEC based on biological activity (Alvarez et al., 2021; Been et al., 2021; Ekpe et al., 2025). This was often done using exposure-activity ratios (EAR) based on the environmental concentration and activity concentration at cutoff (AAC) (i.e., defined response threshold) (Blackwell et al., 2017). Another approach to prioritise using toxicity data is the Toxicological Priority Index (ToxPi), where a score is derived for a CEC based on toxicity parameters, such as *in vitro*, *in vivo* and/or *in silico* data, as well as other fate and occurrence data (dos Santos and Nardocci, 2019; Ekpe et al., 2025; Zhao et al., 2023). The variables included in ToxPi differed between studies. Careful consideration is required to optimize variables and their corresponding weighting for a particular prioritisation purpose. Further, Newmeyer et al. (2024) used the Cheminformatics Hazard Comparison Module (US EPA) to prioritise CEC in biosolids, with a hazard profile and score generated for each chemical based on both experimental toxicity data and quantitative structure-activity relationship (QSAR) toxicity predictions.

Given the diversity of prioritisation studies, it is not surprising that different approaches are used to rank CEC. Some studies rank CEC based on the risk quotient or an equivalent approach (e.g., Alvarez et al., 2021; García-Vara et al., 2023; Villa et al., 2020). There is no single CEC ranking in ECHIDNA as several different matrices are included. However, users can access reports that rank CEC by ecological and human health risk quotients for the relevant matrices (e.g., ecological risk for raw wastewater, treated wastewater and surface water and human health risk for treated wastewater, surface water and drinking water). Other studies apply scoring systems where numbers are assigned based on different criteria including removal efficiency, persistence, bioaccumulation, detected concentration, detection frequency, risk quotient and/or toxicity (e.g., de Voogt et al., 2009; Deere et al., 2021; Gros et al., 2017). The scores are then summed to determine high priority CEC. Further, Isaacs et al. (2024) developed a scoring system for CEC in drinking water with 22 primary criteria covering environmental fate, occurrence in water and potential for release, as well as over 20 score adjustment factors, such as the potential for human exposure and detection frequency. This study developed an automated workflow, with much of the required data available in the CompTox Chemicals Dashboard and other public databases.

3.2 Other CEC prioritisation projects and tools

In addition to the published studies in Table 1, project partners also provided details of other CEC prioritisation projects and tools, which are outlined below.

TZW completed the "Selection of priority substances relevant to water supply and development of a substance list" research project, also known as "Hot Target", in 2018. A database of over 10,000 substances was screened based on PMT assessment, with removal by ozonation and activated carbon also considered. CEC that were PMT and unlikely to be removed by ozonation or activated carbon were deemed "hot targets". The project identified 89 hot targets, with 9 of these substances (1,4-dioxane, trichloroethylene, chloroform, 2,4-dinitrophenol, tris(2-chloroethyl)phosphate, 1,2-dichloropropane, trichloroacetic acid, 1,2-dichloroethane and 1,2-dimethoxyethane) assigned the highest exposure and hazard categories.

KWR undertook a project to identify priority drinking water relevant chemicals to test the robustness of purification plants (KWR 2016.005). From a long-list of substances from, among other sources, RIWA databases and research reports, chemical candidates were prioritised based on exceedance of standard or target values, with further screening based on toxicity, removal during drinking water treatment, physico-chemical properties and analysability. This resulted in a list of 23 priority pollutants, with gabapentin, ammonium and barbital having the highest score. The report is part of a 5-year cycle (2015-2020), with the most recent report still under embargo.

Kennisimpuls waterkwaliteit (KIWK) outlined an approach to prioritise biocides in groundwater and surface water for inclusion in monitoring programs (Meetstrategie Biociden: Overwegingen en criteria, 2022). The steps proposed in the prioritisation process included scoring based on use volume and product type, toxicity, availability of measurement method and use that would lead to emission of the biocide to surface water.

The "Decision-Making Framework for the Prioritization of Research into Constituents of Concern" research project, supported by GWRC and WRF, was completed in 2019 (Project Number WERF3C16/4889). The framework uses a Bayesian Network to help water utilities and other organisations prioritise CEC but does not in itself rank candidate lists of CEC. The web-based tool can be accessed at https://bncecs.wixsite.com/main. From a survey of the water industry, the project identified eleven criteria to be considered, including whether the contaminant is known or suspected to cause acute or chronic health risks and whether there are existing analytical techniques available with suitable limits of detection. Users score each criterion for each chemical, with uncertainty in the criteria scores and weighting of the importance of the criteria to the organisation considered in the final prioritisation. The current version of ECHIDNA incorporates a module to provide scores to use in the Bayesian prioritisation tool.

The "An Enhanced Source Control Framework for Industrial Contaminants in Potable Reuse" research project, supported by WRF and California State Water Resources Control Board, was completed in 2023 (WRF4960). The project focused on 262 industrial contaminants and identified priority contaminants for three conceptual advanced water treatment trains. An Industrial Contaminant Screening Score (ICSS) that considered both toxicity to human health and removal was used to prioritise the chemicals. Despite considering different treatment processes, NDMA, PFOA, PFOS and nitrosamine NMOR ranked highly in all three treatment trains. The project also

proposed an Industrial Contaminant Risk Quotient (ICRQ) using the ICSS and the detected chemical concentration, with specific actions triggered with ICRQ greater than 0.2 and greater than 1.

Some project partners indicated that they do not use any specific prioritisation tools, though PUB indicated that they regularly review CEC based on the framework presented in the 2008 GWRC report "Development of an International Priority List of Pharmaceuticals relevant for the Water Cycle". A publication based on this report, de Voogt et al. (2009), is included in Table 1.

Some water utilities have their own in-house prioritisation tools. As an example, Melbourne Water uses a quantitative risk assessment approach to identify CEC of concern in wastewater. Five models developed for Melbourne Water's wastewater treatment plants are used as part of the risk assessment, including a weight of evidence ranking tool, a fugacity model and food web bioaccumulation model (outlined in National Water Research Institute (2020)).

At the government level, Minnesota Department of Health (US) has an initiative to prioritise CEC with no or limited human risk information that are present or likely to be present in drinking water in Minnesota. The review considers exposure, such as typical use and potential for release, and toxicity. Members of the public can nominate a CEC for review. Minnesota Department of Health has recently partnered with US EPA to expediate the screening (outlined in Isaacs et al. (2024)). Further, while not specific to water, the Department of Climate Change, Energy, the Environment and Water (DCCEEW) (Australia) has developed a chemical informatics and analytics platform called ARChIE. It uses global inventories with over 240,000 chemicals (as of June 2024), with hazard profile, functional use and structural information included. Chemicals can be prioritised for regulatory purposes. ARChIE is not currently available to users outside the Australian Government.

4 Next Steps

This synthesis report has shown that there are many studies and projects that prioritise CEC. However, the majority are limited to a particular matrix, like drinking water or wastewater, with many restricted to a geographic area (e.g., Choi et al., 2024; Gros et al., 2017; Villa et al., 2020). This highlights the need for a global CEC prioritisation tool that covers the range of matrices relevant to the water industry. Of the functionalities identified in Milestone 1, addition of new matrices, specifically biosolids/wastewater sludge and reclaimed water, were identified as the highest priority. This synthesis review and feedback from project partners has helped to identify additional occurrence data sources that can be included in the Global CEC Risk Ranking Tool. This includes the US EPA Chemicals in Biosolids (2022) List, UKWIR Chemical Investigations Programme and US EPA Unregulated Contaminant Monitoring Rule (UCMR). While a single detected concentration is currently included for each matrix in ECHIDNA, it would be useful to provide country or region-specific occurrence data in the Global CEC Risk Ranking Tool. In addition to providing users with a better understanding of the relative risk in their region, this information can also indicate whether a particular CEC is a global CEC. Many of the resources used in other CEC prioritisation tools, such as the CompTox Chemicals Dashboard and the NORMAN Database System, are already utilized in the current version of ECHIDNA. However, information from other tools cited in the literature, such as the Cheminformatics Hazard Comparison Module, could also potentially be included in the Global CEC Risk Ranking Tool.

Expanding beyond Stage 1 of the project, this synthesis report has also identified other approaches and features that could be considered for the Global CEC Risk Ranking Tool. For example, the current version of ECHIDNA prioritises CEC based on PBT, but many recent studies and projects screen CEC based on PMT (e.g., TZW "Hot Target" project, Dulio et al., 2024). Therefore, screening based on mobility could be implemented. While the candidate list used in ECHIDNA covers both Australian and international lists and published literature reviews, we could expand the candidate list for the Global CEC Risk Ranking Tool to include any other CEC lists that project partners may be aware of. Further, chemical informatics and analytics platform ARChIE flags chemicals that are included in regulation, such as the Rotterdam Convention, the Stockholm Convention, REACH Annex XVII and REACH Candidate List of Substances of Very High Concern (SVHC). Presence in these and other regulatory lists (e.g., RIVM ZZS navigator) could also be indicated in the Global CEC Risk Ranking Tool. Additional functionalities to be added to the Global CEC Risk Ranking Tool in Stage 2 will be identified in Milestone 5.

Table 1 Overview of peer-reviewed publications that have applied different approaches to prioritise CEC. Studies sorted in order of matrix.

Study	Country	Matrix	Overview	# chemicals included	Chemical classes	Data sources	Outcomes
Newmeyer et al. (2024)	United States	Biosolids	Priority CEC in biosolids from US and Canada identified using non-target analysis and Cheminformatics Hazard Comparison Module	451 features, with 92 assigned confidence levels 1, 2a or 2b	Range of chemical classes	**Occurrence**: Current study **Sources**: CompTox Chemicals Dashboard (US EPA) **Toxicity**: Cheminformatics Hazard Comparison Module (US EPA) (prioritised based on human and ecological endpoints)	Top 5 prioritised chemicals for human health (both acute and chronic exposure) and ecological health identified, with both clorophene, ketoconazole and p-cresol relevant for both acute and chronic exposure. Fludioxonil and ketoconazole were highest priority for ecological endpoints
Baken et al. (2018)	The Netherlands	Drinking water	The risk of CEC relevant for drinking water assessed using benchmark quotients (BQ) (mean or maximum detected concentration/(provisional) guideline value)	686	Range of chemical classes	**Occurrence**: Various Dutch drinking water and surface water databases, as well as project data **Toxicity**: International guideline values, followed by provisional guidelines calculated using Tolerable Daily Intake (TDI), Acceptable Daily Intake (ADI), Reference Dose (RfD) etc (various sources)	163 chemicals relevant for drinking water were identified for toxicological assessment. Most chemicals did not pose a health risk, though vinylchloride, trichloroethene and bromodichloromethane had BQ > 1

Study	Country	Matrix	Overview	# chemicals included	Chemical classes	Data sources	Outcomes
dos Santos and Nardocci (2019)	Brazil	Drinking water	Environmental fate and toxicity data used to rank 39 pharmaceuticals using Toxicological Priority Index (ToxPi)	39	Pharmaceuticals	**Physico-chemical properties**: Published experimental data, EPISuite (US EPA) **Fate**: Published experimental data, PBT Profiler, TEST, EPISuite **Toxicity**: Published experimental data, QSAR Toolbox	Pharmaceuticals metronidazole, nitrofurantoin and ethinylestradiol had the highest fate and hazard-based ranking
Hartmann et al. (2021)	The Netherlands	Drinking water	Decision support tool to quantify the risk of CEC in drinking water developed based on assessment hierarchy. The main criteria were exposure, hazard potential and relevance to drinking water compared to other exposure routes	8	Pharmaceuticals, per- and polyfluoroalkyl substances (PFAS), industrial chemicals, microbial contaminants	Criteria was addressed based on literature review and consultation with experts (risk assessor, drinking water experts)	Approach only applied to 4 organic CEC. None of the CEC posed a high human health risk, with large uncertainty for 3-(4-Tert-Butylphenyl) propanal due to limited understanding of relevance of drinking water as exposure route
Isaacs et al. (2024)	United States	Drinking water	Priority CEC potentially in drinking water identified based on 27 data sources related to persistence and fate, occurrence and release potential, with score adjustments based on potential for human exposure, detection frequency, presence in regulatory lists	1867	Range of chemical classes	**Fate**: CompTox Chemicals Dashboard **Release**: Various state and national inventories **Occurrence**: US Geological Survey Water Quality Portal, state specific reports	Chemicals with the highest scores included beta-sitosterol, DEET, butachlor sulfonic acid, s-chloroaminoisopropylaminotriazine and atrazine

Study	Country	Matrix	Overview	# chemicals included	Chemical classes	Data sources	Outcomes
Olson et al. (2017)	United States	Drinking water	Unregulated compounds grouped into CEC classes, with priority assigned based on screening, expert and stakeholder reviewer. Monitoring and/or mitigation measures considered for high and medium priority CEC groups (San Francisco Public Utilities Commission, SFPUC)	No individual CEC, but 12 CEC groups	Groups include microbial waterborne pathogens, inorganics, hormones, disinfection by-products (DBPs) halogenated flame retardants (FR)	**General information:** Applicable health advisories, regulatory development status **Occurrence**: Presence in SFPUC supplies **Customer interaction**: General concern about CEC, media coverage	Microbial pathogens identified as high priority in 2016, with algal toxins, DBPs (nitrosamines) and DBPs (others) considered medium priority
Pronk et al. (2023)	The Netherlands	Drinking water	CEC in drinking water prioritised based on removal effort ("effort index"), which considers predicted removal by conventional treatment, oxidation, advanced oxidation, activated carbon and reverse osmosis	68	Range of chemical classes (chemicals selected based on exceedances in Dutch drinking water decree)	**Presence:** Exceedance of Dutch drinking water decree (RIWA-Rijn database) **Removal**: Effort index	18 of the chemicals had an effort index > 60, meaning low expected removal efficiency
Rosenblum et al. (2024)	United States	Drinking water	National drinking water data used to prioritise chemical classes and rank individual CEC based on hazard index (environmental concentration/health-based reference level)	139 (74 regulated, 65 unregulated)	Inorganic chemicals, DBPs, semi-volatile organic compounds, volatile organic compounds, non-volatile organic compounds	**Occurrence**: Six-Year Review of Drinking Water, Safe Drinking Water Information System, Unregulated Contaminant Monitoring Rule (US EPA) **Health Reference level**: Regional Screening Level (US EPA), plus other sources listed in paper	Inorganic compounds (e.g., chromium-6) and DBPs (e.g., bromodichloromethane, chloroform, dibromochloromethane, dichloroacetic acid) had the highest risk ranking. Top 50 risk ranked chemicals included 15 unregulated chemicals

Study	Country	Matrix	Overview	# chemicals included	Chemical classes	Data sources	Outcomes
Ekpe et al. (2025)	Republic of Korea	Groundwater	CEC in groundwater were prioritised using machine learning coupled with ToxPi. CEC were ranked based on 9 factors including suspect and non-target screening, toxicity data and environmental fate properties	252	18 classes including polycyclic aromatic hydrocarbons (PAHs), pesticides, pharmaceuticals, personal care products (PCPs)	**Occurrence**: Current study **Exposure**: CompTox Chemicals Dashboard **Toxicity**: CompTox Chemicals Dashboard **Fate**: CompTox Chemicals Dashboard	47 high priority chemicals were identified, which covered a range of classes (alkyl-PAHs, organophosphate FRs, parent PAHs, PCPs, pesticides, pharmaceuticals, phenols, plasticizers, transformation products, and other industrial use chemicals)
Sjerps et al. (2021)	The Netherlands	Groundwater	Target analysis and (preliminary) drinking water guideline values ((p)GLVs) were used to prioritise CEC in groundwater sources using BQ. Suspect screening was also used to prioritise chemicals for further identity confirmation	713 target chemicals, 12,294 features	Range of chemical classes	**Occurrence:** Monitoring data from Vitens drinking water laboratory (2010-2016) **Toxicity:** (p)GLVs, threshold of toxicological concern, *in vitro* data **Fate**: EPISuite **Removal:** calculated for target chemicals using monitoring data	153 target chemicals were detected at least once in source and drinking water, with p(GLV) available for 45 of the detected chemicals. All 45 chemicals had a BQ < 0.1, indicating no risk to human health
García-Vara et al. (2023)	Spain	Reclaimed water	CEC in reclaimed water and irrigation water prioritised using risk quotient (measured concentration/predicted no-effect concentration (PNEC)) based on non-target screening	158 CEC (confidence level 2)	Range of chemical classes, including pharmaceuticals, pesticides and industrial chemicals	**Occurrence**: semi-quantified concentration from current study **Toxicity**: PNEC (NORMAN Ecotoxicity or INERIS databases)	14 of the identified chemicals had a risk quotient greater than 1, indicating a potential risk. O-desmethyl-venlafaxine posed the highest risk, followed by venlafaxine and galaxolidone

Study	Country	Matrix	Overview	# chemicals included	Chemical classes	Data sources	Outcomes
Alvarez et al. (2021)	United States	Surface water	Risk-based prioritisation of CEC detected in Great Lakes Tributaries using exposure-activity ratios (EAR) (concentration/*in vitro* activity concentration at cutoff, based on Blackwell et al. 2017) and toxicity quotients (TQ) (concentration/ECOTOX endpoint)	185	19 classes including pesticides, PAHs, polychlorinated biphenyls, FR, pharmaceuticals	**Occurrence**: Passive sampler data from 2010-2014 **Toxicity**: ToxCast (EAR) and ECOTOX Knowledgebase (TQ) (both US EPA)	23 of the analysed chemicals, including atrazine and DEHP, exceeded EAR and TQ thresholds at a number of sites
Been et al. (2021)	The Netherlands	Surface water	Non-target analysis suspects in surface water were prioritised using a risk-based priority score (suspect concentration/5th percentile of activity concentration (AC_{50}))	Suspects selected from 21 lists	Range of chemical classes	**Occurrence**: Non-target screening from current study **Toxicity**: ToxCast, ToxAlerts, QSAR Toolbox	Priority scores ranged from 308 (1-ethyl-2-pyrrolidinone) to 1.6×10^{-6} (diphenylamine), with the estimated suspect concentration typically much lower than the 5th percentile of AC_{50}
Blackwell et al. (2017)	United States	Surface water	Risk-based prioritisation of CEC detected in Great Lakes Waters using EAR	96	Range of chemical classes	**Occurrence**: Current study **Toxicity**: ToxCast	Highest EAR for bisphenol A, followed by natural and synthetic hormones 17α-estradiol, 17β-estradiol, diethylstilbestrol, estriol, and estrone (all have EAR > 1)

Study	Country	Matrix	Overview	# chemicals included	Chemical classes	Data sources	Outcomes
Deere et al. (2021)	United States	Surface water	CEC in water assigned priority classes based on 6 questions covering persistence, potential to accumulate, toxicity, evidence of endocrine disruption, detection frequency and chemical charge	117	Primarily pharmaceuticals, but also industrial chemicals	**Occurrence**: Current study (passive sampling) **Fate**: EPISuite, CompTox Chemicals Dashboard **Toxicity**: ECOSAR (US EPA) **Endocrine disruption**: CompTox Chemicals Dashboard	Fifty of the 117 chemicals were classed as high priority in water, with two, estrone and diphenhydramine, meeting all 6 criteria
Di Nica et al. (2015).	Italy	Surface water	Veterinary pharmaceuticals were scored using an approach called RANKVET, which prioritises CEC based on risk to aquatic and terrestrial organisms using risk quotient (predicted concentration/PNEC). Also factors in metabolic rate in animals in prioritisation	48	Veterinary pharmaceuticals	**Use**: European Medicines Agency (EMA), Italian Ministry of Health **Fate**: Veterinary Substances DataBase (VSDB) **Toxicity**: VSDB **Metabolism**: Literature, VSDB **Exposure**: Predicted using EMA guidelines	CEC classed as very high risk in water include ivermectin, chlortetracycline, neomycin, gentamicin and streptomycin, with majority considered low risk
Nikolopoulou et al. (2022)	Ukraine	Surface water	Priority CEC in a river basin identified based on risk score calculated using detection frequency, exceedance of PNEC or environmental quality standard and magnitude of exceedance	83	Range of chemical classes	**Occurrence**: Current study **Toxicity**: PNEC (NORMAN Ecotoxicity database)	Bisphenol A, carbamazepine and imidacloprid were identified as site-specific CEC for surface water
Osorio et al. (2016)	Spain	Surface water	Priority pharmaceuticals in surface water in Spanish rivers identified based on toxic units (ratio of concentration to EC_{50} value)	76 (EC_{50} values only available for 55)	Pharmaceuticals	**Occurrence**: Current study **Toxicity:** EC_{50} values from literature, VSDB or ECOSAR or ECOTOX database	Highest priority compounds were sertraline, gemfibrozil and loratidine

Study	Country	Matrix	Overview	# chemicals included	Chemical classes	Data sources	Outcomes
Serasinghe et al. (2022)	Australia	Surface water	Approach proposed to identify new pesticides for inclusion in surface water monitoring programs based on regional use and toxicity	403	Pesticides	**Use**: Presence in Australian Pesticides and Veterinary Medicine Authority PubCris database **Toxicity**: Hazard statements from SafeWork Australia and PubChem, thresholds from Pesticide Properties Database (PPDB) **Routine analysis**: National Analytical Testing Authority database	While 403 pesticides from approximately 4,000 pesticide products were identified, 144 were shortlisted for inclusion in monitoring programs due to their use, toxicity and lack of routine testing
Villa et al. (2020)	Italy	Surface water	Pharmaceuticals in an alpine stream in area impacted by tourism were prioritised based on risk quotient	54	Pharmaceuticals	**Occurrence**: Current study **Toxicity**: PNEC from literature, followed by toxicity data from literature or ECOSAR	Amoxicillin, ibuprofen, diclofenac and clarithromycin posed the highest risk, particularly in winter months when concentrations were higher
Zhao et al. (2023)	China	Surface water	CEC in surface water screened using non-target analysis and prioritised using ToxPi, which was scaled to lowest PNEC, maximum peak abundance and detection rate	957 tentatively identified, with 96 assigned confidence levels 1 or 2	Range of chemical classes	**Occurrence**: Peak abundance and detection frequency (current study) **Toxicity**: PNEC (NORMAN Ecotoxicity database)	24 chemicals had high ToxPi scores, including 13-cis retinoic acid, 17β-estradiol, N,N-dimethyltetradecylamine and codecylbenzenesulfonic acid
Balakrishnan et al. (2024)	India	Wastewater	PCPs in commonly used products in Indian were prioritised based on their persistent, bioaccumulative and toxic (PBT) properties	102	PCPs	**Fate**: EPISuite **Toxicity**: ECOSAR	Methyl propional and octocrylene were considered highest risk as they were PBT

Study	Country	Matrix	Overview	# chemicals included	Chemical classes	Data sources	Outcomes
Choi et al. (2024)	Republic of Korea	Wastewater	CEC in wastewater effluent from 4 wastewater treatment plants (WWTP) were prioritised based on risk quotient and PBT prioritisation	43	Primarily pharmaceuticals, but also industrial chemicals and PFAS	**Occurrence**: Current study **Fate**: EPISuite **Toxicity**: Literature search, ECOSAR	Four different prioritisation approaches applied, with only DEET and benzotriazole identified as priority chemicals across all four approaches
Dulio et al. (2024)	EU	Wastewater	Prioritisation of CEC in 84 wastewater effluent samples based on exposure (using both target and suspect screening data), hazard and risk using the NORMAN Database System	65,690	Range of chemical classes	**Occurrence**: Target and suspect screening (EMPODAT, SusDat) **Fate**: Range of sources including literature, CompTox Chemicals Dashboard **Toxicity**: PNEC (NORMAN Ecotoxicity database), range of sources for "Carcinogenic, Mutagenic, or Toxic to Reproduction" and endocrine disruption	20 substances were identified as highest priority for target monitoring as they frequently exceeded PNEC (Cat S1), with a further 485 as high priority based on predicted effect data (Cat S3). Cat S1 substances included diclofenac, carbamazepine and bendiocarb
Gago-Ferrero et al. (2018)	Sweden	Wastewater	Priority chemicals were identified from the National Swedish Product Register database based on market availability, quantity used and likely environmental exposure during use. Suspect screening was applied to search for the priority chemicals in wastewater.	~23,000	Range of chemical classes	**Occurrence:** Current study **Exposure**: Exposure Index (Swedish Chemicals Agency) **Fate**: log K_{OW} (log K_{OW} >10 excluded) (source unclear)	160 chemicals priority identified, with 36 tentatively confirmed in wastewater effluent

Study	Country	Matrix	Overview	# chemicals included	Chemical classes	Data sources	Outcomes
Gros et al. (2017)	Sweden	Wastewater	Chemicals detected in wastewater were prioritised using a scoring system based on occurrence, removal efficacy and *in silico* based environmental fate and effect data	79	PFAS, pesticides, phosphorus-containing FRs, pharmaceuticals, PCPs	**Occurrence**: Current study **Removal**: Current study **Fate:** EPISuite **Toxicity**: ECOSAR	Pharmaceutical lamotrigine was identified as the top priority CEC, followed by pharmaceutical amitryptilline and FR TCIPP
He et al. (2023)	China	Wastewater	CEC in wastewater effluent around China were prioritised using an environmental health prioritization index (EHPi) that uses occurrence, removal and toxicity data	34	Primarily pharmaceuticals, but also industrial chemicals	**Occurrence**: Current study **Removal**: Current study **Toxicity**: Own data, CompTox Chemicals Dashboard, AQUIRE database (US EPA)	Ethynyl estradiol, 17β-estradiol, estrone, diclofenac and atrazine were the top 5 CEC based on their EHPi score
Kuskopf et al. (2020)	Australia	Wastewater	Seven factors, including previous detection in wastewater influent or effluent and available analytical method, were considered to identify potential CEC in wastewater. Prioritised CEC were analysed in wastewater and hazard quotient were calculated	>600	FR, illicit drugs, PAH, alkyl phenols, pharmaceuticals, PCP, pesticides, PFAS	**Screening**: Primarily literature review **Occurrence**: Current study **Toxicity**: PNEC (NORMAN Ecotoxicology database)	>600 chemicals were screened with 150 prioritised (though 301 chemicals analysed). Five CEC had a hazard quotient above 1, indicating a potential risk, with FR tris(2-chloroisopropyl) phosphate and PCP galaxolide posing the highest risk

Study	Country	Matrix	Overview	# chemicals included	Chemical classes	Data sources	Outcomes
Lopez-Herguedas et al. (2023)	Spain	Wastewater	Priority CEC identified in wastewater from two WWTPs based on removal efficiency, persistence, bioconcentration, mobility, risk quotient and detection frequency. Suspect screening was used to identify CEC in wastewater, then confirmed with targeted analysis in influent and effluent	88	Range of chemical classes	**Occurrence**: Current study **Removal**: Current study **Fate**: CompTox Chemicals Dashboard **Toxicity**: Range of sources including ECOTOX, ECOSAR, PPDB, literature	33 chemicals were identified as priority CEC, with pharmaceuticals amantadine, telmisartan, lopinavir and clarithromycin highly prioritised in both WWTPs
de Voogt et al. (2009)	EU	Any water type	Pharmaceuticals identified in the literature were screened based on seven criteria including regulation, consumption, toxicity, occurrence and resistance to treatment, with pharmaceuticals grouped into three priority classes based on the number of criteria met	153	Pharmaceuticals	Criteria used for screening came from 25 base documents that focused on prioritisation of pharmaceuticals	10 pharmaceuticals, including carbamazepine, sulfamethoxazole and diclofenac, were identified as high priority pharmaceuticals as they met at least 5 of the 7 criteria

Abbreviations: AC: activity concentration; ADI: acceptable daily intake; BQ: benchmark quotient; DBP: disinfection by-product; EAR: exposure-activity ratio; EHPi: environmental health prioritization index; EMA: European Medicines Agency; FR: Flame retardant; PAH: polycyclic aromatic hydrocarbon; PBT: persistent, bioaccumulative and toxic; PFAS: per- and polyfluoroalkyl substances; PNEC: predicted no-effect concentration; PCP: personal care product; (p)GLVs: (preliminary) drinking water guideline values; PPDB: Pesticide Properties Database; RfD: reference dose; SFPUC: San Francisco Public Utilities Commission; TDI: Tolerable Daily Intake; ToxPi: toxicological priority index; TQ: toxicity quotients; VSDB: Veterinary Substances Database; WWTP: Wastewater treatment plant

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