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ECHIDNA (Emerging CHemIcals Database for National Awareness): a framework to prioritise contaminants of emerging concern in water

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ABSTRACT

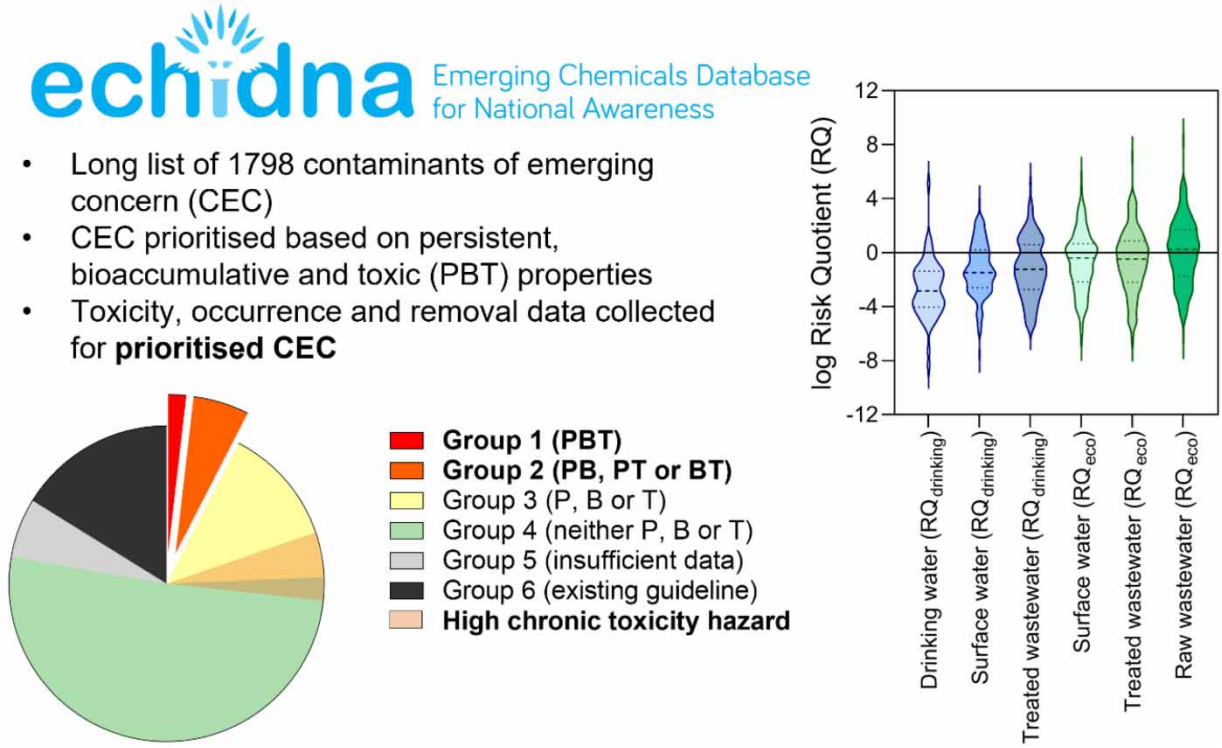
The widespread presence of contaminants of emerging concern (CEC) in surface waters, treated wastewater and drinking water is an ongoing issue for the water industry. The absence of regulatory guidance and limited occurrence, toxicity and removal data are defining criteria of CEC and make it difficult to prioritise which CEC pose the greatest risk. The online Emerging CHemIcals Database for National Awareness (ECHIDNA) aims to classify and prioritise CEC based on their potential risk, with the information presented in an easily accessible and intuitive manner. A candidate list of almost 1,800 potential CEC, including pesticides, pharmaceuticals and industrial compounds, was compiled using both Australian and international resources. These were ranked based on *in silico* assessment of their persistent, bioaccumulative and toxic (PBT) properties, as well as potential chronic toxicity hazard, yielding 247 CEC for further prioritisation. Risk Quotients (RQ) identified between 5 and 87 CEC posing a risk to human and ecosystem health, respectively, across drinking water, surface water, treated wastewater and raw wastewater. While the ability of the water industry to effectively prioritise CEC is limited by candidate identification and data availability, ECHIDNA can provide valuable information for better decision-making surrounding CEC management.

Key words: ecosystem health, human health, micropollutants, risk prioritisation, water industry

HIGHLIGHTS

- Contaminants of emerging concern (CEC) pose unique challenges to the water industry.
- ECHIDNA is a centralised data repository to help with decision-making around CEC.
- CEC are first prioritised based on their persistent, bioaccumulative and toxic (PBT) properties.
- Risk quotients are used to identify and rank CEC based on their potential risk in various water matrices.
- ECHIDNA can be curated to include newly identified CEC.

GRAPHICAL ABSTRACT



INTRODUCTION

Chemicals are pervasive in our everyday lives, with over 350,000 chemicals and mixtures registered for use globally (Wang *et al.* 2020). As a result of their widespread use, chemical contaminants including pesticides, pharmaceuticals and industrial chemicals, are commonly detected in water, sediment, soil and biota (e.g., Pico *et al.* 2019; Leon *et al.* 2020; Ben Mordechay *et al.* 2022; Wilkinson *et al.* 2022). Many of these chemicals are considered as contaminants of emerging concern (CEC), which is broadly defined as 'a chemical for which there are increasing concerns regarding its potential risks to humans and ecological systems' (Diamond *et al.* 2011). CEC can include both naturally occurring chemicals (e.g., algal toxins) and manufactured chemicals, as well as chemicals formed during treatment processes (i.e., disinfection by-products [DBP]) or via natural processes in the environment (i.e., transformation products) (Sauve & Desrosiers 2014).

As well as chemicals recently introduced into the environment from a new source, CEC include chemicals that may have been present in the environment for some time but for which new information about their toxicity or occurrence raises novel concerns about their potential risk. One such example is the antimicrobial triclocarban. Despite being a high-production chemical in use since the 1950s, there was limited information about the environmental occurrence of triclocarban until 2005 (Halden & Paull 2005). The development of a new analytical method with a lower detection limit meant that triclocarban could be detected at low ng/L concentrations and consequently was found in all river water samples downstream of wastewater treatment plants in one study (Sapkota *et al.* 2007). The subsequent detection of triclocarban in wastewater, surface water, biosolids, sediment and biota around the world identified it as a widespread contaminant and raised its profile to that of a CEC (Vimalkumar *et al.* 2019).

Guidelines and standards are available for only a fraction of the numerous chemicals present in the environment. For example, over 180 organic chemicals and chemical groups are included in the Australian Drinking Water Guidelines (ADWG) (NHMRC & NRMMC 2011), while around 70 organic chemicals and chemical groups are included in the World Health Organisation (WHO) Guidelines for Drinking water Quality (GDWQ) (WHO 2022). In contrast, CEC lack regulatory guidance (Sauve & Desrosiers 2014). Limited information about CEC toxicity and occurrence means that it is difficult to quantity the risk they pose to human health or the environment or to establish reasonable water quality targets. Yet

CEC are regularly detected in treated wastewater, as well as surface waters that serve as a source for drinking water treatment plants (e.g., Luo *et al.* 2014; Troger *et al.* 2018). Consequently, CEC are of concern for water utilities, but the lack of regulations combined with limited occurrence, removal and toxicity data make it difficult to assess the risks and prioritise CEC for further action. Indeed, a meta-analysis of 12 CEC found that, on average, peak concern about a CEC occurs around 14 years after the initial concern (Halden 2015). As the time between the onset of concern and regulatory action is long, there is a need for a proactive and science-based approach to help water utilities prioritise CEC.

In this article, we present the online data repository and risk prioritisation tool ECHIDNA, which aims to assist water utilities with prioritising CEC based on their potential risk, and to identify approaches that may help mitigate or reduce their risk to humans and the environment. This information is presented in an understandable format to assist uptake by the water industry. ECHIDNA currently prioritises close to 1,800 potential CEC covering common compound classes including DBPs, herbicides, pharmaceuticals, per- and polyfluoroalkyl compounds and transformation products. CEC are first prioritised based on *in silico* assessment of their persistent, bioaccumulative and toxic (PBT) properties, then based on toxicity, occurrence and removal data collected for prioritised chemicals. Risk Quotients (RQ) for both human health and ecosystem health are estimated to assist with management decision-making in the absence of regulatory guidance.

METHODS

Identifying the CEC candidate list

An overview of the ECHIDNA workflow is provided in Figure 1. A comprehensive CEC long-list was first compiled using various Australian and international resources. Australian resources included the ADWG (NHMRC & NRMMC 2011), Australian Guidelines for Water Recycling (AGWR) (NWQMS 2008) and the Queensland Public Health Regulation (Queensland Government 2018). Further, chemicals detected in water industry monitoring programmes (e.g., Western Corridor Recycled Water Scheme and Catchment and Drinking Water Quality Micro Pollutant Monitoring Programme) were included, as were chemicals in the DATATOX database developed in collaboration with Seqwater (Leusch *et al.* 2012). International resources such as the NORMAN List of Emerging Substances and the United States Environmental Protection Agency (USEPA) Contaminant Candidate List 4 were also used to identify potential CEC, as were recent academic CEC literature reviews (Richardson & Ternes 2018, 2022; Richardson & Kimura 2020). The current CEC long-list contains 1,798 chemicals and can be amended as new authoritative resources become available.

The Chemical Abstracts Service Registry Number (CASRN), simplified molecular-input line-entry system (SMILES) and DSSTox substance identifier (DTXSID) are collected for each chemical added to the long-list, along with the chemical class (e.g., herbicide, pharmaceutical, biocide). Further, available drinking water guideline values from ADWG, WHO GDWQ, European Union Drinking Water Directive (DWD), Drinking Water Standards for New Zealand, Health Canada Guidelines for Canadian Drinking Water Quality (CDWQ) and US National Primary Drinking Water Regulations (NPDWR) are collected. Environmental guideline values are also collected from Australian and New Zealand Guidelines for Fresh and Marine Water Quality (ANZECC & ARMCANZ), European Union Water Framework Directive (WFD) and USEPA National Recommended Water Quality Criteria.

Determining likely persistence, bioaccumulation and toxicity

The CEC are prioritised based on their PBT properties following guidance from Annex XIII of the REACH regulation (European Parliament & European Council 2006). REACH Annex XIII considers chemicals that have a half-life in fresh or estuarine water of >40 days as persistent (P), while chemicals that have bioconcentration factor (BCF) > 2000 are considered as bioaccumulative (B). Using the USEPA CompTox Chemicals Dashboard (Williams *et al.* 2017), OPEn structure–activity/property Relationship App (OPERA) modelled biodegradability half-life and BCF values are collected to represent P and B, respectively. For chemicals not present in the CompTox Chemicals Dashboard, P and B are predicted using the USEPA EPI Suite programme (USEPA 2012). Level III fugacity modelled half-life values are used for P and BCF values from regression-based methods are used for B.

Toxicity to both the environment and human health is considered in ECHIDNA. REACH Annex XIII considers chemicals with a chronic no-observed effect concentration (NOEC) or EC_{10} value of <0.01 mg/L for marine or freshwater organisms as toxic (T). The USEPA Toxicity Estimation Software Tool (TEST), which is within the CompTox Chemicals Dashboard, has modelled acute concentration causing 50% effect (EC_{50}) values for *Daphnia* (48 h) and Fathead Minnow (96 h) in molar units. The toxicity data are converted to mass units using the molecular weight and an acute to chronic ratio of 10 is applied

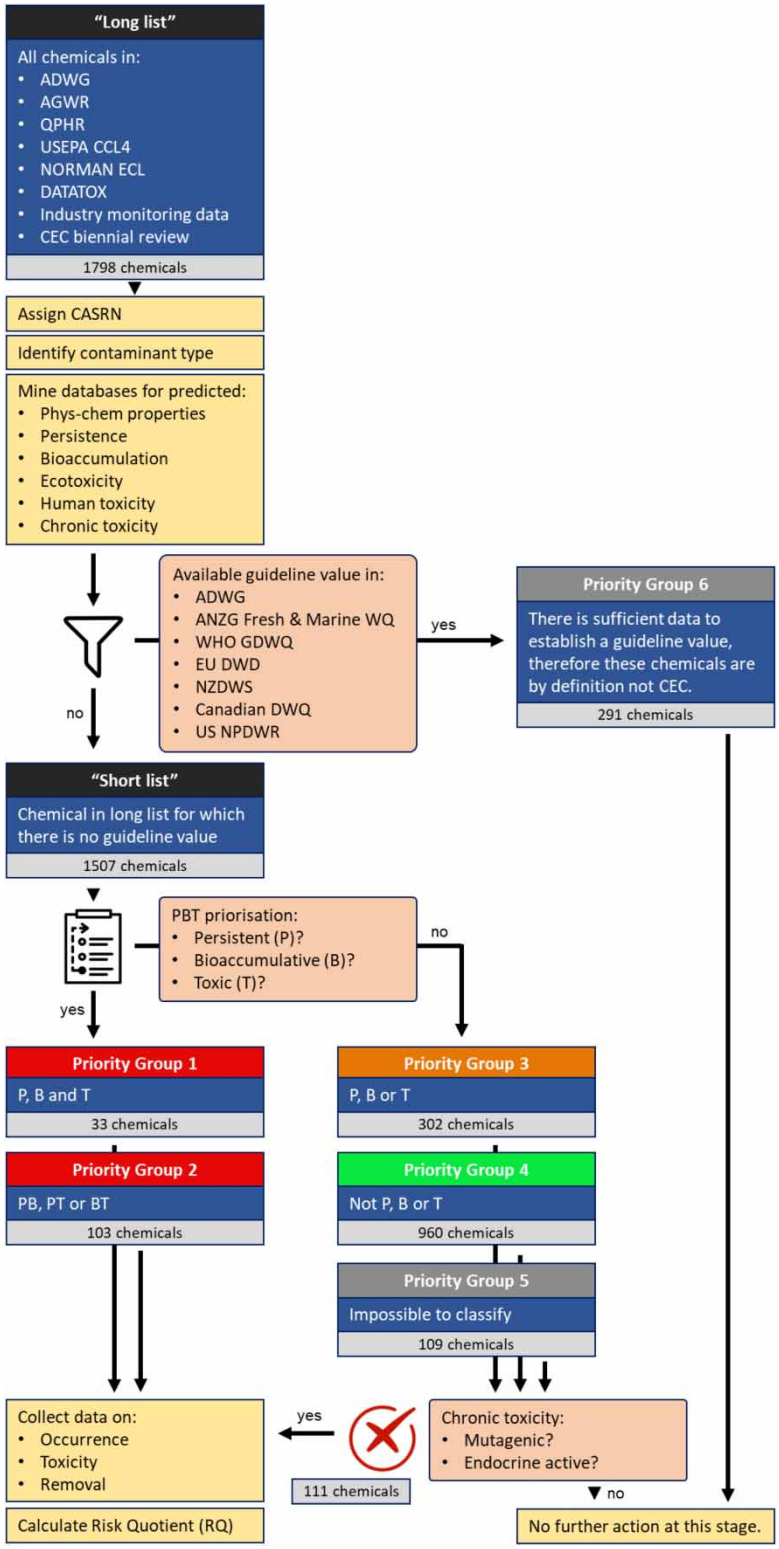


Figure 1 | Schematic of the workflow to produce data for ECHIDNA.

to estimate the chronic NOEC/EC_{10}. The acute to chronic ratio of 10 is based on the method for deriving Australian and New Zealand water quality guideline values for toxicants by Warne *et al.* (2018). In cases where a chemical is not present in TEST, the USEPA Ecological Structure Activity Relationships (ECOSAR) Predictive Model (USEPA 2016) is used to predict acute

toxicity values for *Daphnia* and fish. In addition, modelled rat oral 50% lethal dose (LD_{50}) values in units of mol/kg are available in the CompTox Chemicals Dashboard. LD_{50} is converted from mol/kg to mg/kg in order to classify them into the five acute toxicity hazard categories in the Globally Harmonised System (GHS) (United Nations 2023). Category I includes chemicals with $LD_{50} \leq 5$ mg/kg, Category II includes chemicals with $5 < LD_{50} \leq 50$ mg/kg, Category III includes chemicals with $50 < LD_{50} \leq 300$ mg/kg, Category IV includes chemicals with $300 < LD_{50} \leq 2000$ mg/kg and Category V includes chemicals with $LD_{50} > 2000$ mg/kg. Chemicals within Category I and Category II are considered T to humans.

The CEC are arranged into six Priority Groups based on the number of PBT characteristics that they trigger. Group 1, which is the highest priority, includes CEC that are classed as PBT. Group 2 includes CEC that trigger either PB, PT or BT, while Group 3 includes CEC that are either P, B or T. CEC classed as Group 4 are neither P, B or T, while CEC in Group 5 lack sufficient data to characterise them. Any chemical with a published guideline value is considered to not be a CEC, as sufficient data are available to allow regulatory bodies to derive a safe exposure threshold and water quality target. Therefore, chemicals with an existing guideline are designated Group 6.

Determining whether CEC pose a chronic health risk(s)

The toxicity assessment described above focuses on acute toxicity but does not consider chronic toxicity. Therefore, mutagenicity and estrogenicity are incorporated into the prioritisation as these are important factors that influence risk but may not be adequately captured by the acute toxicity data used for the PBT assessment. Predicted mutagenicity data are obtained from USEPA TEST using the prediction algorithm developed by Hansen *et al.* (2009), while predicted estrogenicity is obtained from the CompTox Chemicals Dashboard using the integrated pathway model for the estrogen receptor, developed by Judson *et al.* (2015). Chemicals with a predicted mutagenicity value of less than 0.5 are assigned a score of 0, while chemicals with a predicted mutagenicity value greater than 0.5 are assigned a score of 1. Any chemical without a mutagenicity value is assigned a score of 0.5. Predicted estrogenicity is indicated with either 'Y' or '-', with 'Y' assigned a score of 1 and '-' assigned a score of 0. Any CEC identified as being potentially mutagenic and estrogenic (score of 1.5 or greater) is flagged as posing a 'high chronic toxicity hazard' and considered in the full risk prioritisation, irrespective of their group ranking based on PBT.

Data collection

Toxicity, occurrence and removal data are collected for Priority Group 1 and 2 CEC, as well as any CEC identified as posing a 'high chronic toxicity hazard'. Whenever possible, the data are sourced by searching the peer-reviewed literature. The CEC name and CASRN, along with any common CEC acronyms, are searched in Web of Science and Google Scholar in combination with search terms including 'toxicity', 'ecotoxicity' 'removal', 'wastewater treatment', 'drinking water treatment', 'advanced water treatment', 'occurrence', 'wastewater', 'surface water', 'drinking water', 'recycled water' and 'monitoring'. However, established databases and repositories are used to supplement the CEC data, when necessary, to fill as many knowledge gaps as possible.

Data collection – ecotoxicology

After exhausting the literature search, experimental toxicity data for *Daphnia* and fish are also collected from the ECOTOXicology Knowledgebase (ECOTOX) (USEPA 2020), while modelled toxicity data from the CompTox Chemicals Dashboard or ECOSAR are used if experimental data are unavailable. Predicted no-effect concentrations (PNEC) are needed for risk prioritisation and these are collected from the NORMAN Ecotoxicology Database (Norman Network 2020). If no PNEC is available, it is calculated from the existing toxicity data by applying an assessment factor of 10 to NOEC values or an assessment factor of 100 to EC_{50} values.

Data collection – human health

Experimental mammalian toxicity data (e.g., no-observed adverse effect level [NOAEL] and/or acceptable daily intake [ADI]) are collected from the CompTox Chemicals Dashboard or from the Australian Pesticides and Veterinary Medicines Authority (APVMA 2022). Human data are used preferentially, followed by rat or mouse data. A provisional drinking water guideline is calculated according to the AGWR framework, where the body weight is 70 kg, the proportion of intake from water is 0.1, the safety factor is 1,000 and the volume consumed per day is 2 L. If experimental data are not available, a NOAEL is estimated from the modelled rat LD_{50} from the CompTox Chemicals Dashboard using an assessment factor of 17,000 based on Kramer *et al.* (1996).

Data collection – removal during (waste)water treatment

If removal data are not available in the peer-reviewed literature, modelled removal during wastewater treatment is obtained from the USEPA EPI Suite programme using the STPWIN model. This model predicts the elimination of a chemical via conventional activated sludge considering biodegradation, sorption to sludge and air stripping as the mechanisms of removal. The default sewage treatment plant settings are used. Predicted removal based on different drinking water treatment processes is estimated using simple indicative removal rules developed by Pronk *et al.* (2023). Removal efficiencies are estimated for conventional treatment (coagulation, flocculation), additional treatment (activated carbon, oxidation) and advanced treatment (reverse osmosis, advanced oxidation). An effort index (EI) based on conventional treatment, activated carbon and reverse osmosis was determined for each CEC using the equation provided in Pronk *et al.* (2023), with ease of removal (1-EI) calculated to help rank CEC.

Data collection – occurrence

In addition to the peer-reviewed literature, occurrence data are also collected from the NORMAN EMPODAT Database (Norman Network 2022). As occurrence data can be limited due to little active monitoring for CEC, values are extrapolated using available removal data when necessary. For example, the concentration of a chemical in wastewater effluent can be estimated based on the reported concentration in wastewater influent and percent removal.

Data collection – assignment of a reliability ranking

The reliability of the sourced data was scored as high, moderate or low. Using the example of removal, data sourced from the peer-reviewed literature were scored as 'high', while the reliability was scored as 'moderate' when the removal was calculated from a publication containing both influent and effluent concentrations. Finally, modelled removal data from the STPWIN model or based on Pronk *et al.* (2023) were scored as 'low' reliability.

RQ prioritisation

RQ are calculated for both ecosystem health (RQ_{eco}) and human health ($RQ_{drinking}$). RQ_{eco} are estimated for raw wastewater, treated wastewater and surface water by dividing the highest measured or predicted concentration in raw wastewater, treated wastewater or surface water, respectively, by the PNEC. $RQ_{drinking}$ are estimated by dividing the highest measured or predicted concentration in treated drinking water, surface water or treated wastewater, respectively, by the provisional drinking water guideline value. $RQ_{drinking}$ for treated wastewater is included as a worst-case scenario for potable reuse. Log RQ greater than 0 indicates a potential risk, and the higher the RQ the greater the potential risk. The CEC are ranked according to their calculated RQ, with the CEC with the highest RQ requiring immediate attention.

RESULTS AND DISCUSSION

Identification and prioritisation of CEC in ECHIDNA

The purpose of ECHIDNA is to provide an intuitive and accessible framework to prioritise CEC based on risk. This is to assist water utilities with management and decision-making about CEC. All 1,798 potential CEC identified in the long-list are included in ECHIDNA (https://www.echidnacec.com) (ECHIDNA 2023). Users can search for chemicals using either chemical name or CASRN or via chemical class (e.g., biocides, drugs of abuse, fungicides). The information available for all chemicals includes general information (e.g., SMILES, molecular weight, chemical structure and OPERA predicted physico-chemical properties), PBT prioritisation, chronic toxicity hazard assessment, reason for inclusion in ECHIDNA and any existing guidelines. When available, Google Trends data are included for each CEC as an indicator of public interest in a particular chemical. For chemicals that are identified as Group 1 (PBT) or Group 2 (PB, PT or BT) or chemicals with a high chronic toxicity hazard score, additional information regarding toxicity, occurrence and removal is included. Specifically, this includes ecotoxicity data and mammalian toxicity data, occurrence in different water matrices (e.g., wastewater influent, wastewater effluent, surface water, drinking water) and removal. While removal during wastewater treatment, advance water treatment, drinking water treatment and disinfection are considered, most of the available removal data included in ECHIDNA is for conventional activated sludge. RQ_{eco} and $RQ_{drinking}$ are also calculated, where available, with $\log RQ > 2$ indicating very high risk, $\log RQ$ −2 to 2 as moderate to low risk and $\log RQ < -2$ as very low risk. Screenshots of each section for an example chemical, the pharmaceutical fexofenadine, are shown in the Supplementary Material.

From the long-list of potential CEC, guideline values are available for 291 chemicals (Group 6), so these are excluded from further screening as these chemicals are not considered CEC given there is sufficient toxicity data available to derive reliable guideline values. After *in silico* assessment, 33 chemicals are classed as Group 1 and 103 chemicals are classed as Group 2, meaning that additional information about toxicity, occurrence and removal was sourced for these compounds. While prioritisation based on PBT is a widely accepted approach, it does have the limitation that hydrophobic CEC that are unlikely to be present in the water phase are prioritised (Diamond *et al.* 2011). This is indeed the case in ECHIDNA with many hydrophobic flame retardants included in Group 1. However, these are not filtered from the database to provide a comprehensive prioritisation (i.e., erring on the side of protection). While many Group 1 chemicals are likely to be well removed during treatment, experimental removal data are available for less than 50% of Group 1 chemicals, with variable removal efficiency of some Group 1 CEC, such as brominated flame retardants, reported (Kim *et al.* 2013). Further, some Group 1 chemicals have been detected in surface water at low μg/L concentrations (e.g., Alam *et al.* 2014; Kowalski & Mazur 2014), justifying the prioritisation of Group 1 and 2 CEC in ECHIDNA.

A further 302 chemicals are classed as Group 3 (P, B or T), with over 50% of the potential CEC, 960 chemicals, neither P, B or T (Group 4). Finally, there is insufficient *in silico* data to categorise 109 chemicals (Group 5). An additional 111 Group 3 and 4 chemicals are identified as potentially mutagenic and estrogenic (e.g., high chronic toxicity hazard), meaning toxicity, occurrence and removal data were collected for 247 CEC in total. The inclusion of CEC that are potentially estrogenic overcomes one of the limitations of PBT prioritisation approaches, specifically, that endocrine effects are not considered (Diamond *et al.* 2011).

Risk quotient ranking

To help prioritise CEC for further attention, RQ_{eco} for surface water, treated wastewater and raw wastewater and $RQ_{drinking}$ for drinking water, surface water and treated wastewater are calculated. Limited toxicity and occurrence data mean that $RQ_{drinking}$ for drinking water can only be calculated for 59 CEC, while RQ_{eco} for surface water can be calculated for 175 CEC (Figure 2). The median RQ decreases with level of treatment, with raw wastewater having the highest median RQ (RQ_{eco} 1.8) and treated drinking water having the lowest median RQ ($RQ_{drinking}$ 0.002). A log $RQ > 0$ indicates that a CEC poses a potential risk. In the case of treated drinking water, only five CEC have a log $RQ_{drinking} > 0$, which includes DBP (chloroacetaldehyde and N-nitrosodiethylamine), per- and polyfluoroalkyl compounds (perfluorononanoic acid, perfluorodecanoic acid) and a hormone (levonorgestrel) (Figure 3, Table S1). Only chloroacetaldehyde has a log $RQ_{drinking} > 2$, indicating it poses a very high potential risk.

Between 44 and 87 CEC have a log $RQ_{eco\ or}$ $RQ_{drinking} > 0$ in surface water, treated wastewater and raw wastewater (Tables S2–S6). CEC posing the highest potential risk to ecosystem health in both surface water and treated wastewater include the insecticides bifenthrin and imidacloprid, and the polycyclic aromatic hydrocarbon dibenzo(a,h)anthracene. Bifenthrin and dibenzo(a,h)anthracene also pose the highest potential risk in raw wastewater according to the ECHIDNA prioritisation. Other CEC with log $RQ_{eco} > 2$ in both surface water and treated wastewater include hormone ethinyl estradiol, flame retardants 1,2,5,6,9,10-hexabromocyclododecane and tris(chloroisopropyl)phosphate and insecticides spinosad and azinphos-ethyl. Further treatment may be required for CEC that are identified as posing a high risk, particularly if the source of the CEC cannot be minimised or it is an environmental transformation product.

How ECHIDNA compares to other prioritisation approaches

The aim of ECHIDNA is to help support evidence-based decision-making for the management and prioritisation of CEC in Australia. Since CEC are a concern for the water industry, several studies have previously developed CEC prioritisation approaches for wastewater and drinking water. For example, Kuskopf *et al.* (2020) described the decision-making process undertaken to prioritise CEC likely to pose a risk to ecosystem health in wastewater effluent discharged into the Great Barrier Reef. The study identified 600 potential CEC from the literature and available databases and considered factors such as occurrence in wastewater and receiving waters, physico-chemical properties, current regulations and availability of analytical methods to prioritise 150 CEC for analysis. The study identified five CEC with a hazard quotient above 1, including the flame retardant tris(2-chloroisopropyl)phosphate and personal care product galaxolide. Tris(2-chloroisopropyl)phosphate is Group 2 in ECHIDNA and has a RQ_{eco} of 2.64 for surface water and a RQ_{eco} of 2.83 for treated wastewater. In contrast, galaxolide is not prioritised in ECHIDNA as it is neither P, B or T and does not pose a high

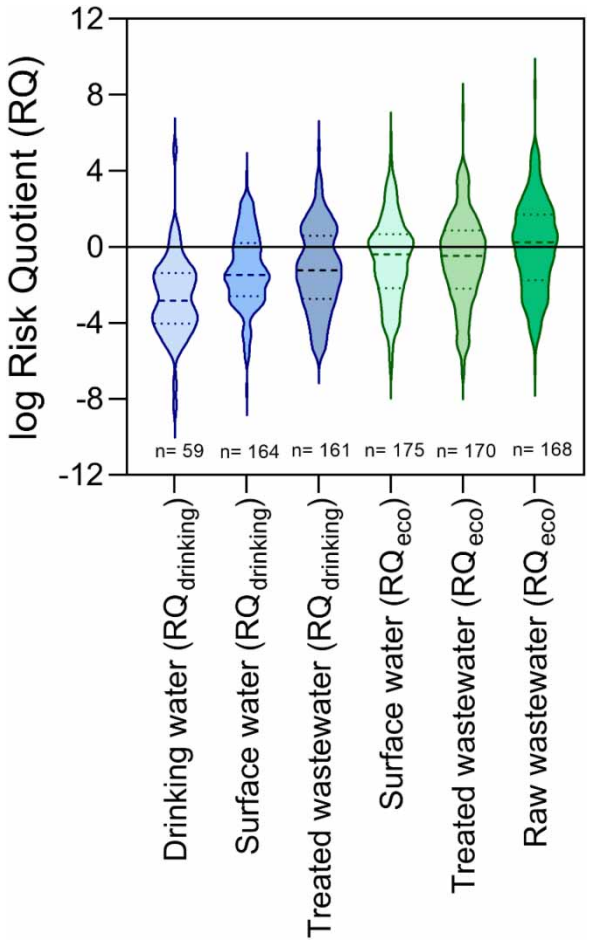


Figure 2 | Overview of all log risk quotient (RQ) for drinking water, surface water, treated wastewater and raw wastewater for both human health ($RQ_{drinking}$) and ecosystem health (RQ_{eco}). Log RQ > 0, which is shown by the solid line, indicates the CEC represents a potential risk. *n* indicates the number of CEC for each matrix.

chronic toxicity hazard. The discrepancy between Kuskopf *et al.* (2020) and ECHIDNA could be due to the inclusion of site-specific parameters in the CEC prioritisation, such as upstream catchment sources, as well as the detection in study site wastewater effluent.

In another example, the San Francisco Public Utilities Commission (SFPUC) prioritised CEC in drinking water based on groups of chemicals with similar properties or a common pathway to drinking water systems (e.g., algal toxins, leachates from materials, hormones), rather than individual chemicals (Olson *et al.* 2017). The CEC groups were screened using a series of evaluation questions covering general chemical information, the experience of SFPUC with the CEC group and toxicity, occurrence and removal of the CEC group. The screening evaluations were reviewed by both experts and stakeholders, with priority groups assigned to each CEC group. The CEC groups with high or medium priority were recommended for monitoring or mitigation, with microbial waterborne pathogens considered high priority and algal toxins, DBPs (nitrosamines) and DBPs (other than nitrosamines) assigned as medium priority for the 2016–2022 period.

Unlike these two examples, ECHIDNA does not focus on a particular treatment plant or a water type, but rather aims to be a useful tool for both wastewater and drinking water utilities, as well as regulators. Further, the approach taken in ECHIDNA is to identify as many potential CEC as possible using a range of sources, such as the peer-reviewed literature, water industry monitoring programmes and reputable CEC lists, rather than focusing on a smaller number of CEC or CEC groups. This is to limit the chance of missing CEC that may be relevant to water utilities.

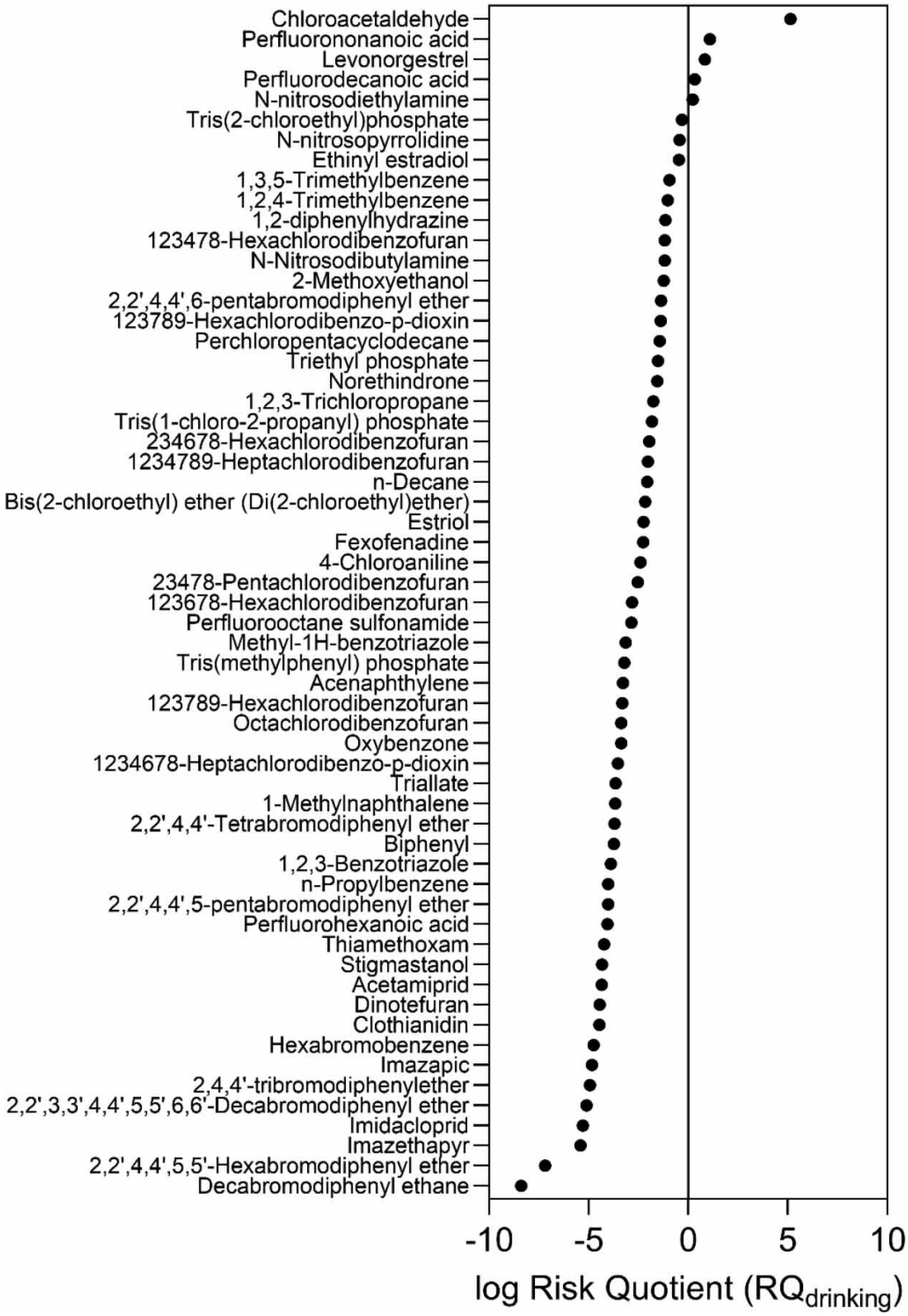


Figure 3 | Log Risk Quotient for human health ($RQ_{drinking}$) for treated drinking water. The solid line indicates log RQ > 0, with CEC with a log RQ > 0 posing a potential risk.

Limitations of ECHIDNA

The ability of ECHIDNA to prioritise CEC based on their risk to human and ecosystem health is limited by the initial identification of the candidate CEC long-list and by data availability. Potential CEC are identified from credible Australian and international sources, but as new chemicals are constantly being developed and released into the environment, ECHIDNA relies on ongoing curation to ensure that recently identified CEC are captured. An option therefore exists in ECHIDNA allowing users to submit update requests, such as for the inclusion of new chemicals in the CEC list or to contribute additional occurrence, toxicity or removal data for a particular chemical. The data used for PBT assessment and subsequent prioritisation in ECHIDNA are not based on experimental toxicity data but are instead modelled using quantitative structure–property relationship (QSPR) and quantitative structure–activity relationship (QSAR) models. This is an important limitation, but as the defining feature of CEC is precisely the lack of reliable data, this is a necessary compromise. Even so, the PBT properties of 109 chemicals could not be predicted.

The lack of occurrence and toxicity data in the literature for some CEC prevented the calculation of RQ_{eco} and $RQ_{drinking}$ for some chemicals. In fact, $RQ_{drinking}$ for treated drinking water can only be estimated for less than 25% of the Group 1, Group 2 and high chronic toxicity hazard CEC. However, identifying such knowledge gaps can help direct future research. As a result of the limited data, the estimated RQ_{eco} and $RQ_{drinking}$ represent a worst-case scenario, with the highest occurrence concentration used to calculate RQ. Further, much of the occurrence data is collected from international studies, so CEC concentrations may be higher than present in the Australian environment. The inclusion of more local monitoring data in ECHIDNA in the future can help make the risk prioritisation data more specific to Australia. Finally, ECHIDNA is limited to organic chemicals and does not consider the risks associated with microplastics, nanomaterials and other inorganic compounds or pathogens. This is because the tools used for PBT prioritisation are not suitable for these other classes of CEC.

CONCLUSIONS

CEC pose a challenge to the water industry as they lack guideline values and there is often limited knowledge about their occurrence, toxicity and removal, making it difficult to assess their risk. ECHIDNA addresses this issue by providing a framework to classify and prioritise CEC based on their potential risk. From a long-list of 1,798 CEC, 247 chemicals were prioritised for further evaluation based on their PBT properties or potential for high chronic toxicity hazards. Of the prioritised CEC, chloroacetaldehyde poses a very high risk in drinking water (log $RQ_{drinking}$ of 5.13), while 19 CEC pose a very high risk in surface water (log RQ_{eco} >2). While a lack of occurrence and toxicity data means that $RQ_{drinking}$ and RQ_{eco} cannot be calculated for all prioritised CEC, ECHIDNA can be updated with new removal, toxicity and occurrence data once available. There is also the potential to expand the scope of ECHIDNA beyond water to help prioritise CEC in other matrices, such as biosolids and soil, while the inclusion of CEC source in ECHIDNA could help with source control and mitigation. Future management of CEC requires flexible regulatory approaches and can benefit from using tools like ECHIDNA together with more complex and accurate QSPR and QSAR models.

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DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

CONFLICT OF INTEREST

The authors declare there is no conflict.

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