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MILESTONE REPORT 5
PROJECT 1166

Developing a Global Risk-based Tool for Prioritising Contaminants of Emerging Concern (CEC) for the Water Industry: Cost estimate for Stage 2



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Developing a Global Risk-based Tool for Prioritising Contaminants of Emerging Concern (CEC) for the Water Industry: Cost estimate for Stage 2

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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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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, developed as part of Project 1166, expanded the functionalities in the existing version of ECHIDNA. This included the addition of new matrices and the expansion of regional regulatory information, increasing the global relevance of the Tool for risk prioritisation of contaminants of emerging concern (CEC). However, several other potential functionalities were identified during the project. Therefore, the objective of Milestone 5 is to identify and prioritise potential enhancements to ECHIDNA as part of the proposed Stage 2 of the project and to create an indicative budget for each potential update. In the initial project plan, Milestone 5 also included identifying maintenance requirements (including regular updates) and confirming host arrangements and long term funding options, but this will now be determined by a research collaborative.

2 Options for new tool functionalities

The project team compiled a list of 15 potential tool functionality options for a proposed Stage 2. These include suggestions from project partners in the 2024 MiroBoard and features identified in the Milestone 2 synthesis report, as well as general feedback from project partners throughout this project. The list was shared in December 2025, with project partners asked to rank the options from highest priority to lowest priority, with 1 being the highest priority. The project team received responses from 6 project partners. For each response received, the rank was converted to a score e.g., a rank of 1 was assigned a score of 10, a rank of 2 was assigned a score of 9 and so on. The score for each option was summed to give a final score. The ranked list of options and their final scores is provided in Table 1. The revised treatment/removal function was by far the most popular proposed functionality.

Table 1 Ranked list of possible new tool functionalities, along with further information about each option, final score and indicative budget

Rank	Options for new tool functionalities	Further information	Score	Indicative budget*
1	Revised treatment/removal function	Align with WaterRA WaterVal projects (e.g. 3505), which assesses removal based on chemical class and assigns indicator chemicals. This functionality could allow users to combine different treatment processes to calculate overall removal during a treatment train	52	$23,726
2	Calculate risk quotient after new treatment process	Expand treatment function further to calculate a risk quotient for residual risk after a new treatment process is included in the treatment train	34	$5,226
3	Link to USEPA Drinking Water Treatability Database	The Drinking Water Treatability Database currently includes 69 entries, with information about removal by different treatment processes, as well as properties and fate and transport	33	$1,593

4	Link to existing literature	Link to existing published literature on the CEC by generating a search in Google Scholar and other databases	33	$2,613
5	Link to Products Use Categories from CompTox Chemicals Dashboard	Link to product and use categories from ChemExpo Knowledgebase, which assigns categories for chemicals, helping with source identification. This can help with catchment assessment and risk assessments	29	$3,475
6	Add "presence in regulatory lists" feature	Feature to indicate if a CEC is present in lists such as Stockholm Convention, Rotterdam Convention, REACH Candidate List of Substances of Very High Concern (SVHC) and IChEMS	13	$3,574
7	Present occurrence data graphically	This option would create a world map for each CEC to indicate where CEC have been detected and at what concentrations (e.g., indicated by colour scale). This would be in addition to current table form	12	$9,010
8	Integrate CHASM	CHASM or Chemical Hazard Assessment of Stormwater Micropollutants is currently a desktop tool to assess the suitability of stormwater for various potable and non-potable uses. It can generate a list of likely pollutants and could be integrated into ECHIDNA	12	$13,065
9	Expand occurrence, removal and toxicity data collection to CEC with moderate chronic toxicity	Currently CEC with highest chronic toxicity (estrogenic and mutagenic) and high chronic toxicity (estrogenic only) are prioritised for further data collection. This update would mean that CEC with moderate chronic toxicity (mutagenic only) would be included. This is an additional 232 CEC.	11	$57,188

10	Prioritise CEC based on persistent, mobile and toxic (PMT) properties	Currently CEC are prioritised based on persistent, bioaccumulative and toxic (PBT) properties, as well as predicted chronic toxicity, with recent projects also screening based on PMT. CEC that are PMT would be Priority Group 1, while CEC that are PM and MT would be Priority Group 2 *Note: PT already Priority Group 2*	10	$19,227
11	Include expert assessment	This would make ECHIDNA more user friendly by adding expert assessment (from the data in ECHIDNA) to provide a simple summary of the key points identified for each individual CEC in ECHIDNA, to facilitate communication	10	$37,057
12	Site-specific risk quotient calculation	Update interface to allow users to enter their own data, allowing them to calculate a risk quotient for their own site *Note: added data would not be saved*	7	$5,226
13	Link to bioassay data from CompTox Chemicals Dashboard	Link to ToxCast summary in CompTox Chemicals Dashboard, which indicates whether a CEC is active or inactive in tested bioassays	5	$853
14	Expand CEC candidate long list	The long list of CEC in ECHIDNA (currently ~1800) would be expanded based on project partner feedback (e.g., "Prioritised PMT/vPvM substances in the REACH registration database" report)	2	$4,252
15	Link to AMOS (Analytical Methods & Open Spectra)	The AMOS database, which is part of the Cheminformatics Module in the CompTox Chemicals Dashboard, include methods, spectra and chemical fact sheets for chemicals	0	$180

*Given in Australian dollars

3 Indicative budget

An indicative budget was prepared for each of the potential tool functionalities to be implemented in Stage 2. The estimated cost for each functionality is summarised in Table 1, with further information about cost factors outlined below. The tool functionalities are presented in ranked order. The indicative costs are given in Australian dollars (note: 1 Australian Dollar is 0.60 Euro and 0.70 US Dollar as of 19th February 2026).

1.1. Revised treatment/removal function

CEC removal, primarily based on literature data, is already included in ECHIDNA. The revised treatment/removal functionality would expand the current removal data section by aligning with the WaterRA WaterVal Projects. WaterVal aims to identify contaminant removal mechanisms for different treatment processes and identify appropriate indicator chemicals that can be monitored. This functionality could also allow users to combine different treatment processes to calculate overall removal during a treatment train. This functionality would require the collection of additional physico-chemical properties, such as molar volume for reverse osmosis (Pang et al., 2023). Predicted molar volume values, based on Percepta from ACD/Labs, are available in the USEPA CompTox Chemicals Dashboard. However, while many physico-chemical parameters can be extracted by the batch search function, molar volume is not one of them and would need to be searched individually for the 1804 CEC. Based on the time required to collect this parameter for all CEC in ECHIDNA, as well as time required to develop this functionality, we estimate $23,726 AUD would be required.

1.2. Calculate risk quotient after new treatment process

The risk quotient is currently calculated in ECHIDNA based on occurrence data from the literature and the predicted no-effect concentration (PNEC) for ecological impacts or the interim water quality value (IWQV) for human health. If available, occurrence data from the user's selected country or region is used, otherwise the highest concentration in a particular matrix is used. To explore how different treatment processes will alter the risk, the risk quotient for the residual risk could be calculated after a new treatment process is included. Percent removal is already provided in the Removal Data section of ECHIDNA, so users could select a treatment type and estimate the new risk quotient after treatment. We estimate $5,226 AUD would be required to add this new functionality.

1.3. Link to USEPA Drinking Water Treatability Database

The USEPA Drinking Water Treatability Database includes information on the removal of chemicals by up to 28 different drinking water treatment processes, as well as information about fate and transport. There are currently 69 chemicals in the Drinking Water Treatability Database. The chemicals in the Drinking Water Treatability Database would be crossed checked against CEC in ECHIDNA based on name, synonym or Chemical Abstracts Service (CAS) registry number, with a link for each relevant CEC added to the Tool. This would be added in the Removal Section in ECHIDNA. We estimate $1,593 AUD would be required to cross check the Drinking Water Treatability Database, extract the URL and update ECHIDNA.

1.4. Link to existing literature

To help users find additional information about a particular CEC, a new feature could be added to ECHIDNA to link to existing literature. For example, a link could be added to the General Information section of an individual chemical page that takes users to a Google Scholar search based on both chemical name and CAS registry number. We estimate $2,613 AUD would be required to add this functionality to ECHIDNA in Stage 2.

1.5. Link to Products Use Categories from CompTox Chemicals Dashboard

The USEPA CompTox Chemicals Dashboard lists Product Use Categories (e.g., personal care, home maintenance, cleaning products and household care, construction and building materials, batteries etc) for many chemicals. This is based on the ChemExpo Knowledgebase, which has Product Use Categories to over 40,000 chemicals. This information is useful for source identification and can help with catchment assessment and risk assessment. Product Use Category data can be downloaded from ChemExpo and the relevant data for many CEC can be extracted and imported into ECHIDNA. The inclusion of Product Use Categories in ECHIDNA would enable the creation of source reports. We would also include the link the Product and Use Categories page in the CompTox Chemicals Dashboard in ECHIDNA to ensure any updates in the Dashboard are captured. This would require adding the unique CEC DTXSID, which is already available in ECHIDNA, to the URL https://comptox.epa.gov/dashboard/chemical/product-use-categories. We estimate $3,475 AUD would be required to import the information from ChemExpo and add the link.

1.6. Add "presence in regulatory lists" feature

As discussed in the Milestone 2 report, the 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, such as project partner country relevant lists, as well as any relevant watchlists, could be added in Stage 2. After identifying relevant regulatory lists and watchlists, we would search for CEC in ECHIDNA based on name, synonym and CAS. We estimate $3,574 AUD would be required to add this feature to ECHIDNA.



1.7. Present occurrence data graphically

The updated version of ECHIDNA now includes occurrence data from 87 countries, with this data presented in a table form. Feedback on the Milestone 3 report suggested also presenting the occurrence data graphically. This could be achieved by creating a world map on each CEC page to highlight where a particular CEC has been detected and at what concentrations. Concentrations could be indicated by a colour scale. We estimate $9,010 AUD would be required to create this feature in ECHIDNA.

1.8. Integrate CHASM

CHASM or Chemical Hazard Assessment of Stormwater Pollutants is an online tool to help water professionals identify chemical hazards associated with land use and activities in stormwater catchments and provide guidance on approaches to effectivity identify CEC. It was designed to complement the Australian Guidelines for Water Recycling - Stormwater Harvesting and Reuse. CHASM was developed by WaterRA and could be integrated into ECHIDNA, aligning the two tools into one portal. The estimated cost of this is $13,065 AUD.

1.9. Expand occurrence, removal and toxicity data collection to CEC with moderate chronic toxicity

Only CEC that are predicted to be estrogenic and mutagenic (highest chronic toxicity, CT1) or estrogenic only (high chronic toxicity, CT2) are currently prioritised for occurrence, removal and toxicity data collection. Expanding data collection to CEC that are predicted to be mutagenic only (moderate chronic toxicity. CT3) would mean occurrence, removal and toxicity data would need to be collected for 232 additional CEC. Assuming one hour per CEC to search the peer reviewed literature for the required information, we estimate $57,188 AUD would be required for data collection.

1.10. Prioritise CEC based on persistent, mobile and toxic (PMT) properties

Currently, CEC are prioritised in ECHIDNA based on their potential persistent (P), bioaccumulative (B) and/or toxic (T) properties. However, there are increasing concerns about CEC that are persistent, mobile and toxic (PMT). Mobility (M) indicates the potential of a CEC to be transported in water and is typically assessed using the organic carbon-water partition coefficient (K_{OC}), which is already included in ECHIDNA. CEC with a log K_{OC} less than 3 are considered mobile, while CEC with a log K_{OC} less than 2 are very mobile (European Commission, 2022). This option would identify CEC that are predicted to be PMT. CEC that are PMT would be included in Priority Group 1 (currently PBT), while CEC that are PM or MT would be considered Priority Group 2 (currently PB, PT, BT). Excluding CEC that are already captured in Priority Group 1, Priority Group 2, CT1 or CT2, we would need to collect occurrence, removal and toxicity data for an additional 78 CEC that are predicted to be either PM or MT. Assuming one hour per CEC to search the peer reviewed literature for the required information, we estimate $19,227 AUD would be required for data collection.

1.11. Include expert assessment

The individual chemical page in ECHIDNA contains detailed information for each CEC. To help make ECHIDNA more user friendly, a short summary of the key points for each CEC in ECHIDNA could be added at the start of the individual chemical page to facilitate communication. If we estimate it takes 5 minutes per CEC to prepare the expert assessment text, this would be a total estimated cost of $37,057 AUD for the 1804 CEC currently in ECHIDNA. The cost could be reduced by focusing only on the priority CEC (e.g., Priority Group 1, Priority Group 2, CT1 and CT2). Excluding any proposed changes outlined in Section 3.9 and 3.10, this would be $12,900 AUD for expert assessment for priority CEC.

1.12. Site-specific risk quotient calculation

As discussed in Section 3.2, the risk quotient is calculated based on occurrence data from the literature. For this feature, the ECHIDNA interface would be updated to allow users to enter their own occurrence data to calculate an ecological or human health risk quotient for their site. The occurrence data would not be saved in ECHIDNA. We estimate $5,226 AUD would be required to add this new functionality.

1.13. Link to bioassay data from CompTox Chemicals Dashboard

The USEPA CompTox Chemicals Dashboard includes a bioactivity summary for many chemicals. This includes whether a chemical was active or inactive in different ToxCast assay, with up to 1570 assays run. For each chemical with ToxCast data, concentration-response plots are available, as well as the activity concentration at 50% of maximal activity (AC_{50}). A link to the ToxCast bioactivity summary could be added to the General Information section. As this only requires adding the unique CEC DTXSID, which is already available in ECHIDNA, to the URL https://comptox.epa.gov/dashboard/chemical/invitrodb, we estimate only $853 AUD would be required to complete this update.

1.14. Expand CEC candidate long list

The long list of CEC in ECHIDNA come from a range of sources including current guidelines, USEPA Contaminant Candidate Lists, NORMAN emerging contaminants lists and academic CEC reviews. The long list could be expanded based on project partner feedback. A CAS registry number would be assigned for each new CEC and the contaminant type would be identified. Predicted properties including physio-chemical properties, persistence, bioaccumulation and toxicity for all new CEC would be obtained by running a batch search in the CompTox Chemicals Dashboard. Some properties, such as predicted binding to the estrogen receptor, need to be searched manually for each CEC using Toxicity Estimation Software Tool (TEST), while USEPA resources like EPISuite or ECOSAR would need to be searched if predicted properties were not available in the CompTox Chemicals Dashboard. Priority Groups would be assigned based on PBT properties, as well as chronic toxicity. The list of new CEC would also be compared to existing guidelines as a chemical with sufficient toxicity data to derive a guideline value in a regulatory document is no longer a CEC and is considered Priority Group 6.



The estimated cost depends on the number of new CEC to be screened, as well as the number of CEC that would fall into Priority Group 1, Priority Group 2, CT1 or CT2 and would therefore require occurrence, removal and toxicity data collection (e.g., priority CEC). Assuming 100 new CEC were added to the Tool and 10 of these were priority CEC, we estimate a cost of $4,252 AUD.

1.15. Link to AMOS (Analytical Methods & Open Spectra)

The AMOS database, which is part of the Cheminformatics Module in the CompTox Chemicals Dashboard, includes methods, spectra and chemical fact sheets for chemicals. Addition of mass spectrometry (MS) fragmentation and spectral information was included in the 2024 Miro Board but was not considered a priority for Stage 1 of the project due to limited feedback. Again, this option was ranked the lowest priority based on feedback from the six project partners. The design of AMOS means that we could only link to the AMOS homepage, not individual CEC, meaning users would need to search for their CEC of interest. As this would mean only adding the same URL for each page, the cost associated with this option is minimal at $180 AUD.

4 Conclusion

The Milestone 5 report has presented and ranked 15 different options for new tool functionalities for a proposed Stage 2 of ECHIDNA, as well as the indicative cost of each option. As a next stage, a research collaborative will refine the budget for the new tool functionalities for Stage 2. The indicative budget presented in this report only covers the new features and does not include regular maintenance and hosting. These costs and options were identified in the Milestone 4 report and need to be confirmed through a research collaborative.

5 References

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