Water Research AUSTRALIA

echidna

MILESTONE REPORT 3
PROJECT 1166

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



waterra.com.au

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

AUTHOR/S

Peta Neale
Griffith University

Steve Melvin
Griffith University

Fred Leusch
Griffith University

WATERRA RESEARCH MANAGER

Marty Hancock
Research Manager

DATE OF PUBLICATION

2026

FUNDING CONTRIBUTOR

Water Research AUSTRALIA

echidna

Global Water Research Coalition

About WaterRA

Water Research Australia is the leading independent, member-driven hub that turns collaboration into impact—advancing research, translating insights, and building capability across Australia's water sector. Our purpose is simple: help our members solve the sector's most pressing challenges—together. We do this in ways that are simple, effective, and deliver great value research outcomes for our members and the communities they serve. Founded in the CRC for Water Quality & Treatment in 1995, we've maintained an unbroken focus on member-based research and measurable impact, turning collective intent into shared solutions for a resilient, safe, and sustainable water future.

For more information visit www.waterra.com.au

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.

For more information visit www.waterra.com.au/echidna

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

Milestone Report 3

ISBN: 978-1-921732-43-0 Project number: 1166

Citation

Water Research Australia 2026, Developing a Global Risk-based Tool for Prioritizing Contaminants of Emerging Concern (CEC) for the Water Industry: Addition of new functionalities, Water Research Australia Limited, Adelaide.

Date of publication

October 2026

Publisher

Water Research Australia Limited
250 Victoria Square, Adelaide SA 5000
ABN: 32 127 974 261
www.waterra.com.au
research@waterra.com.au

© Water Research Australia Limited 2026

This work is copyright. Apart from any use permitted under the Copyright Act 1968, no part of it may be reproduced for any purpose without written permission from the publisher. Requests and inquiries concerning reproduction rights should be directed to the publisher.

WaterRA and individual contributors are not responsible for the outcomes of any actions taken on the basis of information in this research report, nor for any errors or omissions. WaterRA and individual contributors disclaim all and any liability to any person in respect of anything, and the consequences of anything, done or omitted to be done by a person in reliance upon the whole or any part of this research report. This research report does not purport to be a comprehensive statement and analysis of its subject matter, and if further expert advice is required; the services of a competent professional should be sought.

Contents

Contents iv
Figures iv
Abbreviations v
1 Introduction 1
2 Revision of chronic toxicity hazard 2
3 Addition of new matrices 4
4 Risk quotient for biosolids/WWTP sludge 6
5 Regional regulatory information 8
References 9
Appendix 1: Equations used to estimate predicted environmental concentrations in soil 10
Appendix 2: Equations used to estimate human intake 16

Figures

Figure 1 Example of "Estrogen Receptor Binding" TEST prediction for CEC mefenamic acid in the USEPA CompTox Chemicals Dashboard 2

Abbreviations

ADI	acceptable daily intake
BW	body weight
CAS	Chemical Abstracts Service
CIP	Chemical Investigations Programme
CEC	contaminants of emerging concern
CT	chronic toxicity
IWQV	interim water quality values
$K_{soil\text{-}water}$	soil-water partition coefficient
LD_{50}	median lethal dose
NOAEL	no observable adverse effects level
PEC	predicted environmental concentration
PNEC	predicted no-effect concentration
RfD	reference dose
RHO_{soil}	bulk density of wet soil
RQ	risk quotient
TEST	Toxicity Estimation Software Tool
TDI	tolerable daily intake
WWTP	wastewater treatment plant

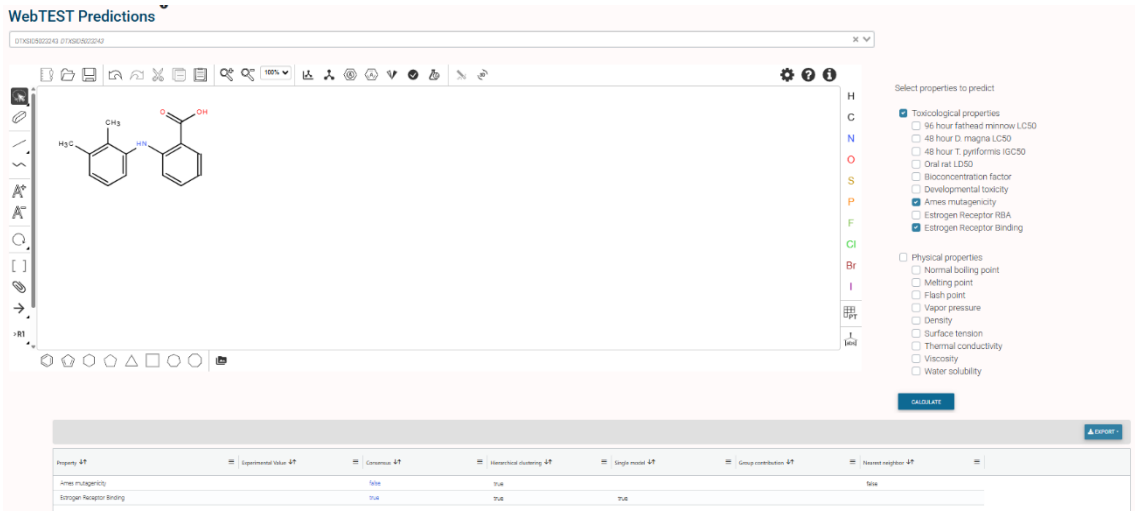
1 Introduction

The primary objective of Project 1166 is to expand the current Australian version of ECHIDNA to become a user-friendly risk-based prioritization tool for contaminants of emerging concern (CEC) for the global water industry. The objective of Milestone 3 was to add at least one new functionality into the Global CEC Risk Ranking Tool. The new functionalities, addition of new matrices and expansion of regional regulatory information, were identified in the Milestone 1 prioritisation report. This report provides an overview of the new data included in the Global CEC Risk Ranking Tool. The chronic toxicity hazard assessment used to identify priority CEC has also been refined in the Tool and this is discussed in Section 2. The Global CEC Risk Ranking Tool is expected to be online by October, with end users able to test and provide feedback to the project team.

2

Revision of chronic toxicity hazard

The project team reviewed the existing version of ECHIDNA prior to adding new occurrence data and regional regulatory information. During this review, we discovered an error with the estrogenicity predictions used as part of the chronic toxicity hazard assessment. We had previously screened for estrogenicity using the ERMODEL based on Judson et al. (2015) in the CompTox Chemicals Dashboard, with chemicals with a "Y" considered estrogenic. However, on closer inspection, we have realised that "Y" means that that a chemical is included in the list of 1812 chemicals in Judson et al. (2015) and does not indicate whether a chemical is estrogenic or not. Therefore, estrogenicity is now predicted using the "Estrogen Receptor Binding" Toxicity Estimation Software Tool (TEST) in the USEPA CompTox Chemicals Dashboard (example in Figure 1). A chemical was considered estrogenic if it had a predicted value greater than or equal to 0.5. Chemicals with a value of less than 0.5 were considered not estrogenic. This is the same approach previously used for the mutagenicity predictions.



Predicted Estrogen Receptor Binding for O=C(O)C=1C=CC=CC1NC2=CC=CC(=C2C)C from Consensus method

Prediction results

Endpoint	Experimental value	Predicted value
Estrogen Receptor Binding value	N/A	0.71
Estrogen Receptor Binding result	N/A	Binds to estrogen receptor

Figure 1 Example of "Estrogen Receptor Binding" TEST prediction for CEC mefenamic acid in the USEPA CompTox Chemicals Dashboard

We now have five classes for chronic toxicity hazard assessment:

- **CT1 – highest chronic toxicity:** estrogenicity value ≥ 0.5 AND mutagenicity value ≥ 0.5
- **CT2 – high chronic toxicity:** estrogenicity value ≥ 0.5 AND mutagenicity value < 0.5
- **CT3 – moderate chronic toxicity:** mutagenicity value ≥ 0.5 AND estrogenicity value < 0.5
- **CT4 – unknown chronic toxicity:** prediction of either both or one value (estrogenicity or mutagenicity) not possible, while the other (if available) is < 0.5
- **CT5 – no chronic toxicity:** both estrogenicity and mutagenicity value < 0.5

Occurrence, removal and toxicity data were collated for CEC in the high chronic hazard groups (groups CT1 and CT2 above), with occurrence, removal and toxicity data for CEC considered as moderate chronic risk (CT3) to be included in future updates.

This update does not affect the ECHIDNA Group 1 (33 CEC) and Group 2 (102 CEC) priority CEC but does change the CEC predicted to have high chronic toxicity potential. The current version of ECHIDNA included 112 high chronic toxicity potential CEC, but there are now 174 high chronic toxicity potential CEC in the Global CEC Risk Ranking Tool. There was some overlap between the previous high chronic toxicity potential CEC and the current high chronic potential CEC (CT1 and CT2), with occurrence, removal and toxicity data collated for the additional CEC. These data were collected using the same processes as outlined previously (Neale et al., 2023).

3 Addition of new matrices

The addition of new matrices (e.g., biosolids/WWTP sludge, groundwater and recycled water) was identified as the highest priority in Milestone 1. Therefore, the Global CEC Risk Ranking Tool was expanded to include seven different matrices: wastewater influent, wastewater effluent, surface water, drinking water, recycled water, groundwater and biosolids/WWTP sludge. While biosolids are a sub-class of treated wastewater sludge, both biosolids and wastewater sludge were combined here to maximise data availability. Occurrence data for the above matrices were searched for all priority chemicals (Group 1, Group 2, CT1 and CT2).

The previous version of ECHIDNA included the maximum reported concentration for each CEC detected in the different matrices but did not consider geographic location. We have included the country where the sample was collected in the Global CEC Risk Ranking Tool, allowing users to find data relevant to their location. In some cases, we provided region rather than country (e.g., to de-identify industry data). We have occurrence data from many countries for some frequently monitored CEC (e.g., wastewater effluent concentrations for over 30 countries for 17β-estradiol), while other less commonly monitored CEC may only have occurrence data for one country.

The collated occurrence data came from several sources including project partner data, publicly available databases and reports, and peer-reviewed literature. Project partner data were labelled as "Industry data", with only country or region information provided. Project partners also recommended several databases, including UKWIR Chemical Investigations Programme (CIP) (https://ukwir.org/water-chemicals-investigation-programme), RIWA-Rijn Waterdata Dashboard (https://www.riwa-rijn.org/data-dashboard/), UBA "Pharmaceuticals in the Environment" database v3 (https://www.umweltbundesamt.de/en/database-pharmaceuticals-in-the-environment-0#undefined) and USEPA Unregulated Contaminants in Drinking Water (https://www.epa.gov/dwucmr). Relevant reports included Arp et al. (2023) and Saaristo et al. (2023). These resources were searched for both chemical name and Chemical Abstracts Service (CAS) registry number to find occurrence data for priority CEC, with data gaps filled, where possible, by searching the peer reviewed literature.

Overall, occurrence data in at least one of the matrices could be found for 264 of the priority CEC, with no data available for 45 of the priority CEC. We now have 4942 occurrence data points in the Global CEC Risk Ranking Tool from 87 countries. We have:

- wastewater influent data for 223 CEC
- wastewater effluent data for 244 CEC
- surface water data for 254 CEC
- drinking water data for 128 CEC
- recycled water data for 96 CEC
- groundwater data for 121 CEC
- biosolids/WWTP sludge data for 165 CEC

For the project partner provided data, we have also included CEC that were analysed but below the analytical detection limit. These have been flagged with a "<" symbol. Of the recycled water data, only 31 CEC were found above the limit of detection, with the remaining 65 CEC below the limit of detection.

4

Risk quotient for biosolids/WWTP sludge

With occurrence data for biosolids/WWTP sludge now included in the Global CEC Risk Ranking Tool, it was necessary to estimate the risk of CEC in biosolids/sludge. This is not as straightforward as calculating a risk quotient (RQ) for water matrices as it is necessary to estimate the predicted concentration in soil or the predicted daily intake from food. The risk of CEC in biosolids/sludge was assessed based on the Step 1 screening approach outlined in the European Commission Joint Research Centre report "Screening risk assessment of organic pollutants and environmental impacts from sewage sludge management" (Huygens et al., 2022). The equations used in this report were partly based on the Technical Guidance Document on Risk Assessment (European Commission, 2003) and REACH R.16 guidance (ECHA, 2016). RQ for both soil organisms and humans were estimated based on a 10-year period of continuous sludge application on agricultural soil, which was based on the approach in Huygens et al. (2022).

The risk quotient for the soil compartment after 10 years of continuous sludge application on agricultural land ($RQ_{soil\ 10\ years}$) was estimated using Equation 1:

$$RQ_{soil\ 10\ years} = \frac{PECsoil_{soil\ 10\ years}}{PNEC_{soil}} \quad (1)$$

Where:

$PEC_{soil\ 10\ year}$ is the predicted environmental concentration for a CEC in units of mg/kg in soil after 10 years of continuous sludge application on agricultural land (calculated based on Appendix 1)

$PNEC_{soil}$ is the predicted no-effect concentration for a CEC in units of mg/kg in soil

$PEC_{soil\ 10\ year}$ is calculated based on the detected CEC concentration in sludge and a series of assumptions regarding sludge application rate, soil depth, rainfall rate and soil properties. Standard default values from European Commission (2003) and ECHA (2016) were used, with more information in Appendix 1.

$PNEC_{soil}$ is not readily available, so $PNEC_{soil}$ in units of mg/kg was estimated using Equation 2:

$$PNEC_{soil} = \frac{K_{soil\text{-}water}}{RHO_{soil} \cdot PNEC_{water} \cdot 1000} \quad (2)$$

Where:

RHO_{soil} is the bulk density of wet soil, with a default value of 1700 kg/m^3

$K_{soil\text{-}water}$ is the soil-water partition coefficient in units of m^3/m^3 (calculated using Equation S3 in Appendix 1)

$PNEC_{water}$ is the predicted no-effect concentration for a CEC in units of mg/L in water

Note: 1000 is a conversion factor to convert mg/L to mg/m^3

$PNEC_{water}$ includes both experimental and predicted values and were collected from the NORMAN Ecotoxicity Database, with the values included in the Global CEC Risk Ranking Tool.

The risk quotient for humans after 10 years of continuous sludge application on agricultural land ($RQ_{human\ 10\ years}$) was calculated using Equation 3:

$$RQ_{human\ 10\ years} = \frac{(\text{Total Daily Intake}_{10\ years}/BW)}{\text{ADI or TDI or RfD}} \quad (3)$$

Where:

$\text{Total Daily Intake}_{10\ years}$ is the daily contaminant intake from food in units of mg/day estimated after 10 years of continuous sludge application on agricultural land (calculated based on Appendix 2)

BW is body weight, with a default value of 70 kg

ADI or TDI or RfD is the acceptable daily intake, tolerable daily intake or reference dose in units of mg/kg bw/day

$\text{Total Daily Intake}_{10\ years}$ includes intake from fish, root vegetables, leaf vegetables, drinking water, meat and milk, with default intake values from European Commission (2003) used. The approach assumes that intake is exclusively from within the contaminated system, so represents a worst-case scenario.

ADI, TDI or RfD were already included in ECHIDNA for many CEC. If ADI, TDI or RfD values were not available, TDI was calculated by dividing the no observable adverse effects level (NOAEL) by a standard safety factor of 1,000 (composed of 10× for intraspecies, 10× for interspecies, and 10× for database uncertainty). If a NOAEL was not available, NOAEL was estimated using the rat LD_{50} values from the USEPA CompTox Chemicals Dashboard and an assessment factor of 17,000 based on Kramer et al. (1996). This was similar to the approach used for deriving interim water quality values (IWQV) in ECHIDNA. All ADI, TDI or RfD values used to derive RQ_{human} are disclosed in the tool.

All equations used for the calculations are provided in Appendices 1 and 2.

5 Regional regulatory information

Expansion of regional regulatory information was identified as a secondary priority in Milestone 1, with the addition of guidelines from China, India and Japan suggested to provide broader applicability. As a result, we have added the following drinking water guidelines:

- Japan Drinking Water Quality Standard
- Indian Standard Drinking Water
- Chinese Standards for Drinking Water Quality
- South African National Standard 241-1:2015 Drinking Water Specification

We have also added the following additional ecosystem protection guidelines:

- Canadian Water Quality Guidelines
- Japanese Environmental Quality Standards for Water Pollution
- Chinese Environmental Quality Standards for Surface Water
- South African Water Quality Guidelines - Aquatic ecosystems

All existing guidelines in ECHIDNA were checked for any updates since 2020. This resulted in some compounds moving to Priority Group 6 if a guideline was available. For example, the Australian Drinking Water Guidelines now have values for perfluorohexanesulfonic acid (CAS 355-46-4) and perfluorobutanesulphonic acid (CAS 375-73-5), so these chemicals are no longer technically considered CEC.

We have focused on human and ecological health thus far, but there is scope to expand to guidelines for other water uses (e.g., irrigation) in future iterations of the Global CEC Risk Ranking Tool.

References

Arp, H.P.H., Hale, S. and Neumann, M. 2023 PMT/vPvM assessment of REACH registered Substances Detected in Wastewater Treatment Plant Effluent, Freshwater Resources and Drinking Water, German Environment Agency, https://www.umweltbundesamt.de/en/publikationen/pmtvpvm-assessment-of-reach-registered-substances.

ECHA 2016 Guidance on information requirements and Chemical Safety Assessment, Chapter R.16: Environmental exposure assessment, Version 3.0, ECHA-16-G-03-EN.

European Commission 2003 Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances, Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market, Part I.

Huygens, D., Garcia-Gutierrez, P., Orveillon, G., Schillaci, C., Delre, A., Orgiazzi, A., Wojda, P., Tonini, D., Egle, L. and Jones, A. 2022 Screening risk assessment of organic pollutants and environmental impacts from sewage sludge management, Joint Research Centre.

Judson, R.S., Magpantay, F.M., Chickarmane, V., Haskell, C., Tania, N., Taylor, J., Xia, M., Huang, R., Rotroff, D.M., Filer, D.L., Houck, K.A., Martin, M.T., Sipes, N., Richard, A.M., Mansouri, K., Setzer, R.W., Knudsen, T.B., Crofton, K.M. and Thomas, R.S. 2015. Integrated Model of Chemical Perturbations of a Biological Pathway Using 18 In Vitro High-Throughput Screening Assays for the Estrogen Receptor. Toxicological Sciences 148(1), 137-154.

Kramer, H., Van den Ham, W., Slob, W. and Pieters, M. 1996. Conversion factors estimating indicative chronic no-observed-adverse-effect levels from short-term toxicity data. Regulatory Toxicology and Pharmacology 23(3), 249-255.

Neale, P.A., Melvin, S.D., Hancock, M. and Leusch, F.D.L. 2023. ECHIDNA (Emerging CHemIcals Database for National Awareness): a framework to prioritise contaminants of emerging concern in water. Journal of Water and Health 21(9), 1357-1368.

Saaristo, M., Sharp, S., Zhang, S. and Taylor, M.P. 2023 Emerging contaminants in recycled water, Publication 2054, Environment Protection Authority Victoria, https://www.epa.vic.gov.au/sites/default/files/epa/publications/2054-recycled-water-emerging-contaminants_report_may2023.pdf.

Appendix 1: Equations used to estimate predicted environmental concentrations in soil

Equation S1

$$Kp_{soil} = K_{oc} \cdot \text{fraction organic carbon in standard soil}$$

Where:

Kp_{soil} is solids-water partition coefficient in soil (L/kg)

K_{OC} is organic carbon-water partition coefficient (L/kg)

Fraction of organic carbon in standard soil is 0.02 (default)

Equation S2

$$K_{air\text{-}water} = \frac{HENRY}{R \cdot TEMP}$$

Where:

$K_{air\text{-}water}$ is air-water partitioning coefficient

HENRY is Henry's law constant (Pa m^3/mol) converted to atm m^3/mol based on conversion factor of 101325 (1 atm = 101325 Pa)

R is gas constant (8.314 Pa m^3/mol K)

TEMP is temperature at air-water interface (285 K)

Equation S3

$$K_{soil\text{-}water} = Fair_{soil} \cdot K_{air\text{-}water} + Fwater_{soil} \cdot Fsolid_{soil} \cdot \frac{Kp_{soil}}{1000} \cdot RHO_{solid}$$

Where:

$K_{soil\text{-}water}$ is soil-water partitioning coefficient (m^3/m^3)

$Fair_{soil}$ is fraction air in soil, with a default value of 0.2 (m_{air}^3/m_{soil}^3)

$K_{air\text{-}water}$ is air-water partitioning coefficient (Equation S2)

$Fwater_{soil}$ is fraction water in soil, with a default value of 0.2 (m_{water}^3/m_{soil}^3)

$Fsolid_{soil}$ is fraction solid in soil, with a default value of 0.6 (m_{solid}^3/m_{soil}^3)

Kp_{soil} is solids-water partition coefficient in soil (L/kg) (Equation S1)

RHO_{solid} is density of the solid phase, with a default value of 2500 kg/m^3

Equation S4

$$Csoil_{initial} = \frac{C_{sludge} \cdot APPL_{sludge}}{DEPTH_{soil} \cdot RHO_{soil}}$$

Where:

$Csoil_{initial}$ is CEC concentration in soil due to sludge in first year at t=0 (mg/kg)

C_{sludge} is CEC concentration in dry biosolids/WWTP sludge (mg/kg)

$APPL_{sludge}$ is dry biosolids/WWTP sludge application rate, with a default value of 0.5 kg/m^2/year

$DEPTH_{soil}$ is mixing depth of soil, with a default value of 0.2 m

RHO_{soil} is bulk density of wet soil, with a default value of 1700 kg/m^3

Equation S5

$$K_{leach} = \frac{Finf_{soil} \cdot RAIN_{rate}}{K_{soil\text{-}water} \cdot DEPTH_{soil}}$$

Where:

K_{leach} is pseudo first-order rate constant for leaching from soil layer (d)

$Finf_{soil}$ is fraction of rainwater that infiltrates into soil, with a default value of 0.25

$RAIN_{rate}$ is rate of precipitation, with a default of 1.925×10^{-3} m/d (700 mm/year)

$K_{soil\text{-}water}$ is soil-water partitioning coefficient (m^3/m^3) (Equation S3)

$DEPTH_{soil}$ is mixing depth of soil, with a default value of 0.2 m

Equation S6

$$Kbio_{soil} = \frac{\ln 2}{DT50bio_{soil}}$$

Where:

$Kbio_{soil}$ is first order rate constant for biodegradation in bulk soil (d)

$DT50bio_{soil}$ is half-life for biodegradation of the CEC in soil (d)

Equation S7

$$DIFFwater = 2.0 \cdot 10^{-9} \sqrt{\frac{32}{MOLW}}$$

Where:

DIFFwater is molecular diffusivity of the substance in the water phase (m^2/d)

MOLW is molecular weight of the substance (kg/mol)

Equation S8

$$DIFFgas = 2.57 \cdot 10^{-5} \sqrt{\frac{18}{MOLW}}$$

Where:

DIFFgas is molecular diffusivity of the substance in the gas phase (m^2/d)

MOLW is molecular weight of the substance (kg/mol)

Equation S9

$$FRs.soil = \frac{Fsolid_{soil}}{Fair_{soil} \cdot K_{air\text{-}water}/(Kp_{soil} \cdot RHO_{solid}/1000) + Fwater_{soil}/(Kp_{soil} \cdot RHO_{solid}/1000) + Fsolid_{soil}}$$

Where:

FRs.soil is mass fraction of the substance in the solid phase of soil

$Fsolid_{soil}$ is fraction solid in soil, with a default value of 0.6 (m_{solid}^3/m_{soil}^3)

$Fair_{soil}$ is fraction air in soil, with a default value of 0.2 (m_{air}^3/m_{soil}^3)

$K_{air\text{-}water}$ is air-water partitioning coefficient (Equation S2)

Kp_{soil} is solids-water partition coefficient in soil (L/kg) (Equation S1)

RHO_{solid} is the density of the solid phase, with a default value of 2500 kg/m^3

$Fwater_{soil}$ is fraction water in soil, with a default value of 0.2 (m_{water}^3/m_{soil}^3)

Equation S10

$$FRw.soil = \frac{Fwater_{soil}}{Fair_{soil} \cdot K_{air\text{-}water} + Fwater_{soil} + Fsolid_{soil} \cdot Kp_{soil} \cdot RHO_{solid}/1000}$$

Where:

FRw.soil is mass fraction of the substance in the water phase of soil

$Fwater_{soil}$ is fraction water in soil, with a default value of 0.2 (m_{water}^3/m_{soil}^3)

$Fair_{soil}$ is fraction air in soil, with a default value of 0.2 (m_{air}^3/m_{soil}^3)

$K_{air\text{-}water}$ is air-water partitioning coefficient (Equation S2)

$Fsolid_{soil}$ is fraction solid in soil, with a default value of 0.6 (m_{solid}^3/m_{soil}^3)

Kp_{soil} is solids-water partition coefficient in soil (L/kg) (Equation S1)

RHO_{solid} is density of the solid phase, with a default value of 2500 kg/m^3

Equation S11

$$FRa.soil = 1 - FRw.soil - FRs.soil$$

Where:

FRa.soil is mass fraction of the substance in the air phase of soil

FRw.soil is mass fraction of the substance in the water phase of soil (Equation S10)

FRs.soil is mass fraction of the substance in the solid phase of soil (Equation S9)

Equation S12

$$Deff_{soil} = FRa.soil \frac{DIFFgas.Fair_{soil}^{1.5}}{Fair_{soil}} + FRw.soil. \frac{DIFFwater.Fwater_{soil}^{1.5}}{Fwater_{soil}} + FRs.soil \cdot \frac{SOLIDdiff.soil}{Fsolid_{soil}}$$

Where:

$Deff_{soil}$ is effective diffusion coefficient (m^2/d)

FRa.soil is mass fraction of the substance in the air phase of soil (Equation S11)

DIFFgas is molecular diffusivity of the substance in the gas phase (m^2/d) (Equation S8)

$Fair_{soil}$ is fraction air in soil, with a default value of 0.2 (m_{air}^3/m_{soil}^3)

FRw.soil is mass fraction of the substance in the water phase of soil (Equation S10)

DIFFwater is molecular diffusivity of the substance in the water phase (m^2/d) (Equation S7)

$Fwater_{soil}$ is fraction water in soil, with a default value of 0.2 (m_{water}^3/m_{soil}^3)

FRs.soil is mass fraction of the substance in the solid phase of soil (Equation S9)

SOLIDdiff.soil is solid phase diffusion coefficient in the soil compartment, with a default value of 6.37×10^{-12} m^2/d

$Fsolid_{soil}$ is fraction solid in soil, with a default value of 0.6 (m_{solid}^3/m_{soil}^3)

Equation S13

$$Veff_{soil} = FRw.soil \frac{RAIN_{rate}.Finf_{soil}}{Fwater_{soil}} + FRs.soil. \frac{SOLIDadv.soil}{Fsolid_{soil}}$$

Where:

$Veff_{soil}$ is effective advection (with penetrating porewater) (m)

FRw.soil is mass fraction of the substance in the water phase of soil (Equation S10)

$RAIN_{rate}$ is rate of precipitation, with a default of 1.925×10^{-3} m/d (700 mm/year)

$Finf_{soil}$ is fraction of rainwater that infiltrates into soil, with a default value of 0.25

$Fwater_{soil}$ is fraction water in soil, with a default value of 0.2 (m_{water}^3/m_{soil}^3)

FRs.soil is mass fraction of the substance in the solid phase of soil (Equation S9)

SOLIDadv.soil is rate of advective downward transport of soil particles, with a default value of 6.34×10^{-12} m^2/d

$Fsolid_{soil}$ is fraction solid in soil, with a default value of 0.6 (m_{solid}^3/m_{soil}^3)

Equation S14

$$d_p = \frac{Veff_{soil} + \sqrt{Veff_{soil}^{\ 2} + Deff_{soil} \cdot 4 \cdot kdeg_{soil}}}{2 \cdot kdeg_{soil}}$$

Where:

d_p is substance-dependent penetration depth (m)

$Veff_{soil}$ is effective advection (with penetrating porewater) (m) (Equation S13)

$Deff_{soil}$ is effective diffusion coefficient (m^2/d) (Equation S12)

$kdeg_{soil}$ is rate constant for degradation in bulk soil (d) (*note: no other information provided about $kdeg_{soil}$, so we have used $Kbio_{soil}$, first order rate constant for biodegradation in bulk soil (d) (Equation S6)*)

Equation S15

$$kasl_{soil} = \left(Veff_{soil} + \frac{Deff_{soil}}{d_p} \right)$$

Where:

$kasl_{soil}$ is partial mass-transfer coefficient at soil side at the air-soil interface (m/d)

$Veff_{soil}$ is effective advection (with penetrating porewater) (m) (Equation S13)

$Deff_{soil}$ is effective diffusion coefficient (m^2/d) (Equation S12)

d_p is substance-dependent penetration depth (m) (Equation S14)

Equation S16

$$\frac{1}{k_{volat}} = \left(\frac{1}{kasl_{air} \cdot \frac{k_{air\text{-}water}}{k_{soil\text{-}water}}} + \frac{1}{kasl_{soil}} \right) \cdot DEPTH_{soil}$$

Where:

k_{volat} is pseudo-first order rate constant for volatilisation from soil

$kasl_{air}$ is partial mass transfer coefficient at air-side of the air-soil interface, with a default value of 1.05×10^{-3} m/s

$K_{air\text{-}water}$ is air-water partitioning coefficient (Equation S2)

$K_{soil\text{-}water}$ is soil-water partitioning coefficient (m^3/m^3) (Equation S3)

$kasl_{soil}$ is partial mass-transfer coefficient at soil side at the air-soil interface (m/d) (Equation S15)

$DEPTH_{soil}$ is mixing depth of soil, with a default value of 0.2 m

Equation S17

$$k = K_{volat} + K_{leach} + Kbio_{soil}$$

Where:

k is first order rate constant for removal from top soil (d)

k_{volat} is pseudo-first order rate constant for volatilisation from soil (Equation S16)

K_{leach} is pseudo first-order rate constant for leaching from soil layer (d) (Equation S5)

$Kbio_{soil}$ is first order rate constant for biodegradation in bulk soil (d) (Equation S6)

Equation S18

$$Csoil_{max} = Csoil_{initial} \cdot \left(\frac{1-\exp^{(-k \cdot 365)^{Napp}}}{1-\exp^{(-k \cdot 365)}} \right)$$

Where:

$Csoil_{max}$ is maximum CEC concentration in soil ($mg/kg_{wet\ weight}$)

$Csoil_{initial}$ is CEC concentration in soil due to sludge in first year at t=0 (mg/kg) (Equation S4)

k is first order rate constant for removal from top soil (d) (Equation S17)

Napp is number of application events, which is set to 10

Equation S19

$$TWAC_{soil}\ (t) = Csoil_{max} \cdot \left(\frac{1-\exp^{(-k \cdot t)}}{(k \cdot t)} \right)$$

Where:

$TWAC_{soil}$ (t) is time weighted average CEC concentration in soil, over a period t ($mg/kg_{wet\ weight}$)

$Csoil_{max}$ is maximum CEC concentration in soil ($mg/kg_{wet\ weight}$) (Equation S18)

k is first order rate constant for removal from top soil (d) (Equation S17)

t is time period, with t = 30 used for soil organisms and t = 180 used for modelling transfer from soil to crops for human intake

Equation S20

$$PEC_{soil\ 10\ year} = TWAC_{soil}\ (30\ d)$$

Where:

$PEC_{soil\ 10\ year}$ is predicted environmental concentration for a CEC in soil after 10 years of continuous sludge application on agricultural land ($mg/kg_{wet\ weight}$)

$TWAC_{soil}$ (30 d) is time weighted average CEC concentration in soil, over a period of 30 d ($mg/kg_{wet\ weight}$) (Equation 19)



Appendix 2: Equations used to estimate human intake

Equation H1

$$C_{liq} = \frac{Clocal_{crop\ transfer} \cdot RHO_{soil}}{K_{soil\text{-}water} \cdot 1000}$$

Where:

C_{liq} is CEC concentration in soil porewater (mg/L)

$Clocal_{crop\ transfer}$ is time weighted average CEC concentration in soil after 180 d (e.g., $TWAC_{soil}$ (180 d)) ($mg/kg_{wet\ weight}$) (Equation S19)

RHO_{soil} is bulk density of wet soil, with a default value of 1700 kg/m^3

$K_{soil\text{-}water}$ is soil-water partitioning coefficient (m^3/m^3) (Equation S3)

Equation H2

$$\text{Eq Rate Runoff Event} = C_{sludge} \cdot APPL_{sludge} \cdot 10 \cdot \exp^{\left(-4 \cdot \frac{\ln(2)}{DT50soil}\right)}$$

Where:

Eq Rate Runoff Event is equivalent rate for runoff at the time of the runoff event (g/ha)

C_{sludge} is CEC concentration in dry biosolids/WWTP sludge (mg/kg)

$APPL_{sludge}$ is dry biosolids/WWTP sludge application rate, with a default value of 0.5 $kg/m^2/year$

10 is to convert units of mg/m2 (Csludge × $APPL_{sludge}$) to g/ha

$DT50_{soil}$ is half-life of the CEC in soil (d) (*note: we have used $DT50bio_{soil}$, half-life for biodegradation of the CEC in soil (d), here*)

Equation H3

$$\text{Input runoff} = \frac{\text{Eq Rate Runoff Event} \cdot \text{Runoff\%} \cdot \text{FW ratio}}{1000}$$

Where:

Input runoff is input via runoff (mg/m^2)

Eq Rate Runoff Event is equivalent rate for runoff at the time of the runoff event (g/ha) (Equation H2)

Runoff % is runoff percentage, with a default value of 5%

FW ratio is ratio of field to waterbody, with a default value of 10

Equation H4

$$Fwaterphase_{runoff} = \frac{Water\ depth}{Water\ depth + \left(Eff\ sed\ depth \cdot RHO_{sed} \cdot OC \cdot \frac{K_{OC}}{100}\right)}$$

Where:

$Fwaterphase_{runoff}$ is fraction of CEC entering in water phase via runoff

Water depth is depth of surface water, with a default value of 30 cm

Eff sed depth is effective sediment depth of the surface water, with a default value of 1 cm

RHO_{sed} is sediment bulk density, with a default value of 0.8 kg/L

OC is sediment organic carbon content, with a default value of 5%

K_{OC} is organic carbon-water partition coefficient (L/kg)

Equation H5

$$Input\ runoff_{sw} = Input\ Runoff \cdot Fwaterphase_{runoff}$$

Where:

$Input\ runoff_{sw}$ is runoff input via the water phase (mg/m^2)

Input runoff is input via runoff (mg/m^2) (Equation H3)

$Fwaterphase_{runoff}$ is fraction of CEC entering in water phase via runoff (Equation H4)

Equation H6

$$Cwater_{initial} = \frac{Input\ runoff_{sw} \cdot 100}{Water\ depth}$$

Where:

$Cwater_{initial}$ is local CEC concentration in surface water after initial application (µg/L)

$Input\ runoff_{sw}$ is runoff input via the water phase (mg/m^2) (Equation H5)

Water depth is depth of surface water, with a default value of 30 cm

Equation H7

$$k_{total} = \frac{\ln(2)}{DT50_{biowater}} + kres$$

Where:

K_{total} is first order rate constant for removal from water phase (d)

$DT50_{biowater}$ is half-life for degradation in water (d)

kres is first order rate constant for residence time in a water body, with a default value of 0.025 d (based on residence time of 40 days)

Equation H8

$$Cwater_{max}=Cwater_{initial}\cdot\left(\frac{1-exp^{(-k_{total}\cdot 365)^{Napp}}}{1-exp^{(-k_{total}\cdot 365)}}\right)$$

Where:

$Cwater_{max}$ is maximum CEC concentration in water (µg/L)

$Cwater_{initial}$ is local CEC concentration in surface water after initial application (µg/L) (Equation H6)

K_{total} is first order rate constant for removal from water phase (d) (Equation H7)

Napp is number of application events, which is set to 10

Equation H9

$$TWAC_{water}=Cwater_{max}\cdot\left(\frac{1-exp^{(-k_{total}\cdot t)}}{(k_{total}\cdot t)}\right)$$

Where:

$TWAC_{water}$ is time weighted average CEC concentration in surface water over a period of 180 days (µg/L)

$Cwater_{max}$ is maximum CEC concentration in water (µg/L) (Equation H8)

K_{total} is first order rate constant for removal from water phase (d) (Equation H7)

t is time period, with t = 180 d used for modelling transfer from soil to crops for human intake

Equation H10

$$\log BCF_{fish}=0.85\cdot\log K_{ow}-0.7$$

Where:

BCF_{fish} is bioconcentration for fish on wet weight basis ($L/kg_{wet\ weight}$)

K_{OW} is octanol-water partition coefficient

NB: This is for CEC with log K_{ow} less than or equal to 6

Equation H11

$$\log BCF_{fish}=-0.20\cdot\log K_{ow}^{2}+2.74\cdot\log K_{ow}-4.72$$

Where:

BCF_{fish} is bioconcentration for fish on wet weight basis ($L/kg_{wet\ weight}$)

K_{OW} is octanol-water partition coefficient

NB: This is for CEC with log K_{OW} greater than 6

Equation H12

$$C_{fish}=0.5\cdot(TWAC_{water}+PEC_{regional})\cdot BCF_{fish}\cdot BMF$$

Where:

C_{fish} is CEC concentration in fish (mg/kg$_{wet\ weight}$)

$TWAC_{water}$ is time weighted average CEC concentration in surface water over a period of 180 days (µg/L) (Equation H9) *note: converted from µg/L to mg/L*

$PEC_{regional}$ is background concentration in mg/L, which we have assumed is 0

BCF_{fish} is bioconcentration for fish on wet weight basis (L/kg$_{wet\ weight}$) (Equation H10 and H11)

BMF is biomagnification factor in fish based on log K_{OW} (see below)

Log K_{OW}	BMF
<4.5	1
4.5-5	2
5-8	10
8-9	3
>9	1

Equation H13

$$K_{plant\text{-}water}=Fwater_{plant}+Flipid_{plant}\cdot K_{ow}{}^{b}$$

Where:

$K_{plant\text{-}water}$ is partition coefficient between plant tissue and water (mg.m plant^3/mg.m water^3)

$Fwater_{plant}$ is volume fraction of water in plant tissue, with a default value of 0.65

$Flipid_{plant}$ is volume fraction of lipid in plant tissue, with a default value of 0.01

K_{OW} is octanol-water partition coefficient

b is correction for differences between plant lipid and octanol, with a default value of 0.95

Equation H14

$$C_{root}=\frac{K_{plant\text{-}water}}{RHO_{plant}}\cdot C_{liq}\cdot 1000$$

Where:

C_{root} is C EC concentration in the root tissue of plant (mg/kg$_{wet\ weight}$)

$K_{plant\text{-}water}$ is partition coefficient between plant tissue and water (mg.m plant^3/mg.m water^3) (Equation H13)

RHO_{plant} is bulk density of plant tissue, with a default value of 700 kg/m^3

C_{liq} is CEC concentration in soil porewater (mg/L) (Equation H1)

NB: 1000 is needed to give the final units of mg/kg (m^3 is equivalent to 1000 L)



Equation H15

$$C_{leaf}=\frac{0.0392\exp^{\frac{(\log K_{ow}-1.78)^2}{2.44}}}{\frac{432}{0.0006+\frac{0.0013+0.00002K_{ow}^{0.95}}{K_{air\text{-}water}}+0.035}}\cdot C_{liq}\cdot 1000$$

Where:

C_{leaf} is CEC concentration in the leaf tissue of plant (mg/kg$_{wet\ weight}$)

K_{OW} is octanol-water partition coefficient

$K_{air\text{-}water}$ is air-water partitioning coefficient (Equation S2)

C_{liq} is CEC concentration in soil porewater (mg/L) (Equation H1)

Equation H16

$$C_{drw}=\frac{TWAC_{water}}{1000}\cdot F_{pur}$$

Where:

C_{drw} is concentration in drinking water (mg/L)

$TWAC_{water}$ is time weighted average CEC concentration in surface water over a period of 180 days (µg/L)

F_{pur} is purification factor for surface water

F_{pur} was estimated by the multiplying purification factors based on log K_{OW} and Henry's law constant for each CEC. The factors were provided in European Commission (2003). Only storage in open reservoirs was considered.

	log K_{OW}			**Henry's law constant (Pa m^3/mol)**	
	<4	4-5	>5	<100	>100
Storage in open reservoir	1	1/4	1/16	1	1/2

Equation H17

$$BTF_{meat}=10^{-7.6+\log K_{OW}}$$

Where:

BTF_{meat} is biotransfer factor for meat (beef) ((mg/kg)/(m/d))

K_{OW} is octanol-water partition coefficient

Note: The estimation can be used for CEC with log K_{OW} ranging from 1.5 to 6.5. Outside this range, the minimum or maximum log K_{OW} is used

Equation H18

$$BTF_{milk}=10^{-8.1+\log k_{OW}}$$

Where:

BTF_{milk} is biotransfer factor for milk ((mg/kg)/(m/d))

K_{OW} is octanol-water partition coefficient

Note: The estimation can be used for CEC with log K_{OW} ranging from 3 to 6.5. Outside this range, the minimum or maximum log K_{OW} is used

Equation H19

$$C_{meat}=BTF_{meat}(C_{grass}\cdot IC_{grass}+TWAC_{soil}(180\ d)\cdot IC_{soil}+C_{drw}\cdot IC_{drw})$$

Where:

C_{meat} is CEC concentration in meat ($mg/kg_{wet\ weight}$)

BTF_{meat} is biotransfer factor for meat ((mg/kg)/(m/d)) (Equation H17)

C_{grass} is concentration in grass (i.e., C_{leaf}) ($mg/kg_{wet\ weight}$) (Equation 15)

IC_{grass} is daily intake of grass, with a default value of 67.6 kg/d

$TWAC_{soil}$ (180 d) is time weighted average CEC concentration in soil over 180 d ($mg/kg_{wet\ weight}$) (Equation S19)

IC_{soil} is daily intake of soil, with a default value of 0.46 kg/d

C_{drw} is concentration in drinking water (mg/L) (Equation H16)

IC_{drw} is daily intake of water, with a default value of 55 L/d

Equation H20

$$C_{milk}=BTF_{milk}(C_{grass}\cdot IC_{grass}+TWAC_{soil}(180\ d)\cdot IC_{soil}+C_{drw}\cdot IC_{drw})$$

Where:

C_{milk} is CEC concentration in milk ($mg/kg_{wet\ weight}$)

BTF_{milk} is biotransfer factor for milk ((mg/kg)/(m/d)) (Equation H18)

C_{grass} is concentration in grass (i.e., C_{leaf}) ($mg/kg_{wet\ weight}$) (Equation 15)

IC_{grass} is daily intake of grass, with a default value of 67.6 kg/d

$TWAC_{soil}$ (180 d) is time weighted average CEC concentration in soil over 180 d ($mg/kg_{wet\ weight}$) (Equation S19)

IC_{soil} is daily intake of soil, with a default value of 0.46 kg/d

C_{drw} is concentration in drinking water (mg/L) (Equation H16)

IC_{drw} is daily intake of water, with a default value of 55 L/d

Equation H21

$$\text{Human intake} = C_{fish} \cdot I_{fish} + C_{root} \cdot I_{root} + C_{leaf} \cdot I_{leaf} + C_{meat} \cdot I_{meat} + C_{milk} \cdot I_{milk} + C_{drw} \cdot I_{drw}$$

Where:

Human intake is total daily human intake (mg/kg)

C_{fish} is CEC concentration in fish ($mg/kg_{wet\ weight}$) (Equation H12)

I_{fish} is daily human intake of fish, with a default value of 0.115 $kg_{wet\ weight}/d$

C_{root} is CEC concentration in the root tissue of plant ($mg/kg_{wet\ weight}$) (Equation H14)

I_{root} is daily human intake of root vegetables, with a default value of 0.384 $kg_{wet\ weight}/d$

C_{leaf} is CEC concentration in the leaf tissue of plant ($mg/kg_{wet\ weight}$) (Equation H15)

I_{leaf} is daily human intake of leaf vegetables, with a default value of 1.2 $kg_{wet\ weight}/d$

C_{meat} is CEC concentration in meat ($mg/kg_{wet\ weight}$) (Equation H19)

I_{meat} is daily human intake of meat, with a default value of 0.301 $kg_{wet\ weight}/d$

C_{milk} is CEC concentration in milk ($mg/kg_{wet\ weight}$) (Equation H20)

I_{milk} is daily human intake of milk, with a default value of 0.561 $kg_{wet\ weight}/d$

C_{drw} is CEC concentration in drinking (mg/L) (Equation H16)

I_{drw} is daily human intake of drinking water, with a default value of 2 L/d