ITRC (Interstate Technology & Regulatory Council). 2023. *Contaminants of Emerging Concern Framework* CEC-1. Washington, D.C.: Interstate Technology & Regulatory Council, CEC Team. https://cec-1.itrcweb.org/.

This Fact Sheet has been organized into the following subsections:


- Section 1: Introduction
- Section 2: Process for Prioritizing CEC
  - Section 2.1: Occurrence
  - Section 2.2: Toxicity
  - Section 2.3: Physical-chemical Properties That Inform Fate and Transport and Chemical Behavior
- Section 3: Sources of Key Variables to Consider When Evaluating Potential Toxicity and Exposure
  - Section 3.1: Human Health Risk
  - Section 3.2: Ecological Risks
  - Section 3.3: Properties That Inform Fate and Transport
- Section 4. Schemes for Interpreting Information on Variables


## 1. INTRODUCTION

This Identification of Key CEC Variables Fact Sheet presents the key variables that may be used as criteria to prioritize actions to address a contaminant of emerging concern (CEC). In addition, this Fact Sheet contains suggested resources that can be used to determine the best available scientific information for these variables. The lack of scientific information on any one variable or multiple variables (e.g., exposure, toxicity, fate, and transport) poses a need for further research or data gathering to reduce the uncertainty and increase the accuracy when evaluating the risk posed by a CEC.

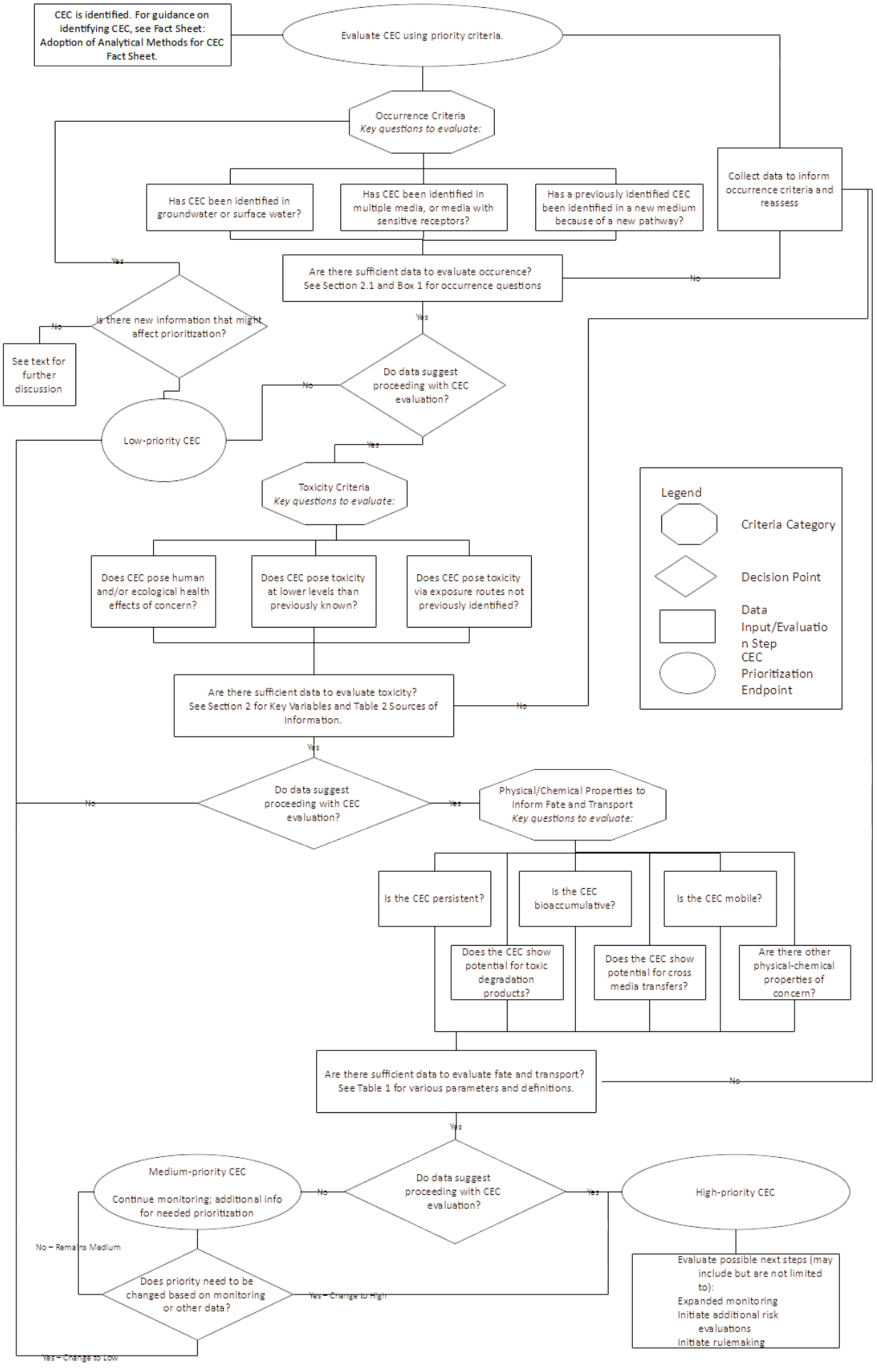
Section 2 provides a process flowchart on how to approach the evaluation of CEC, the specific types of information about the CEC that need to be considered as part of prioritization, and the order in which the information should be considered. Section 3 summarizes key variables that are important for newly identified risks stemming from the exposure and toxicity domains and includes sources where both empirical and estimated (calculated) variable information can be found. Section 4 summarizes available schemes and tools for prioritizing and/or interpreting CEC data.

Concerns about contaminants emerge because human activities relating to substances (e.g., the built environment, production, use, and disposal) release contaminants into the environment and/or lead to exposures that then may become public and environmental health concerns. These contaminants become recognized through detection and identification in environmental media locally, regionally, or globally. The term "**CEC**" **refers to substances and microorganisms, including physical, chemical, biological, or radiological materials known or anticipated to be present in the environment, that may pose newly identified risks to human health or the environment.** Thousands of chemicals are released into and identified in the environment, and communities, regulators, and policy makers need to know how to determine which of these CEC should be prioritized.

The flowchart presented in Figure 1 was newly developed by the Interstate Technology and Regulatory Council (ITRC) CEC Team to identify a logical process for evaluating CEC other than pathogens and radiologicals. The process uses prioritization criteria and assumes the CEC (which has presumably been identified as the result of an event, a concern from the media or public, or a discovery of new information) can be measured in the environment (see the Adoption of Analytical Methods for CEC Fact Sheet). The process flowchart is intended primarily for chemical contaminants. Due to the unique characteristics of biological (microbials) and radiological materials and the lack of expert resources within the ITRC CEC Team, process flowcharts for those CEC are not currently available but may be considered in future efforts. Additionally, this Fact Sheet addresses CEC with direct effects to human and ecological endpoints and does not consider those that may have indirect effects, such as chemicals, for example, that may impact climate change or deplete ozone in the upper atmosphere.

## 2. PROCESS FOR PRIORITIZING CEC

**Figure 1. Process Flowchart for prioritizing CEC (download)**


CEC is identified. For guidance on identifying CEC, see Fact Sheet: Adoption of Analytical Methods for CEC Fact Sheet.
Evaluate CEC using priority criteria.
Occurrence Criteria
Key questions to evaluate:
Has CEC been identified in groundwater or surface water?
Has CEC been identified in multiple media, or media with sensitive receptors?
Has a previously identified CEC been identified in a new medium because of a new pathway?
Collect data to inform occurrence criteria and reassess
Are there sufficient data to evaluate occurence? See Section 2.1 and Box 1 for occurrence questions
No
Yes
Is there new information that might affect prioritization?
No
See text for further discussion
Yes
Do data suggest proceeding with CEC evaluation?
No
Low-priority CEC
Yes
Toxicity Criteria
Key questions to evaluate:
Does CEC pose human and/or ecological health effects of concern?
Does CEC pose toxicity at lower levels than previously known?
Does CEC pose toxicity via exposure routes not previously identified?
Are there sufficient data to evaluate toxicity? See Section 2 for Key Variables and Table 2 Sources of Information.
No
Yes
Do data suggest proceeding with CEC evaluation?
No
Yes
Physical/Chemical Properties to Inform Fate and Transport
Key questions to evaluate:
Is the CEC persistent?
Is the CEC bioaccumulative?
Is the CEC mobile?
Does the CEC show potential for toxic degradation products?
Does the CEC show potential for cross media transfers?
Are there other physical-chemical properties of concern?
Are there sufficient data to evaluate fate and transport? See Table 1 for various parameters and definitions.
No
Yes
Medium-priority CEC
Continue monitoring; additional info for needed prioritization
No
Do data suggest proceeding with CEC evaluation?
Yes
High-priority CEC
No – Remains Medium
Does priority need to be changed based on monitoring or other data?
Yes – Change to High
Yes – Change to Low
Evaluate possible next steps (may include but are not limited to):
Expanded monitoring
Initiate additional risk evaluations
Initiate rulemaking
Legend
Criteria Category
Decision Point
Data Input/Evaluation Step
CEC Prioritization Endpoint

Ultimately, the intent of this process is to designate a CEC as low, medium, or high priority to inform the next evaluation steps and decision-making options (Table 1). The designations are based on occurrence, risk/toxicity, potential for exposure to receptors, and physical-chemical characteristics that inform mobility, bioaccumulation potential, and/or environmental degradation. These designations involve a certain degree of professional judgment that must be applied when weighing different factors and evidence.

**Table 1. CEC prioritization**

| | **LOW-PRIORITY CEC** | **MEDIUM-PRIORITY CEC** | **HIGH-PRIORITY CEC** |
|---|---|---|---|
| Summary of Current Data | No significant concern | Additional information needed for further prioritization | Widespread or significant concern |
| Monitoring Follow-Up | No monitoring at this time | Continued monitoring | Expanded monitoring |
| Additional Steps | Watch for new information | Seek out new information that may inform a need for risk characterization | Additional risk characterization and potential rulemaking |

Table 1 summarizes the CEC prioritization scheme in terms of level of concern, monitoring follow-up, and potential additional steps. Each category is expanded on below:

- Low-priority CEC: A CEC that is present in the environment, but current data suggest it does not pose a significant threat and does not require further monitoring at this time, either due to infrequent occurrence, low risk/toxicity, minimal potential for exposure to receptors or absence of receptors, or physical-chemical characteristics that may suggest poor mobility, low bioaccumulation potential, or high environmental degradation rate. Watching for new information is important for potential reprioritization. Additionally, the possibility of toxic breakdown products should be considered.

- Medium priority CEC: A CEC that is present in the environment for which additional information is needed and should be sought out. Continued monitoring is recommended. New information (e.g., lower toxicity endpoint, sensitive health effect, new impacted medium (vapor/air), or new fate and transport characteristic) may require additional risk characterization to determine whether the medium-priority CEC is downgraded to a low priority, remains a medium priority, or is elevated to a high-priority CEC.

- High-priority CEC: A CEC that, based on its physical-chemical characteristics and occurrence, risk/toxicity, potential exposure pathways, and/or presence of receptors, is recommended for expanded monitoring, additional risk characterization, and potential rulemaking.

The science and information on CEC are evolving. Per- and polyfluoroalkyl substances (PFAS) are a notable example. Compound classes and mixtures may also emerge as CEC. *CEC can be shifted between priority levels at any time.* For example, a low-priority CEC can be reintroduced into the evaluation process at any time based on new data (e.g., new information on toxicity, exposure pathways or impacted media) and can result in reconsideration of its CEC status. As such, reevaluation, or reassessment of any given CEC should periodically occur depending on the latest information. As shown in the flowchart, additional data could result in the reclassification of a CEC's priority.

To differentiate among the low, medium, and high priorities, the CEC flowchart considers three categories of criteria for prioritizing CEC. These are, in sequence: occurrence, toxicity, and physical-chemical properties that inform fate and transport and chemical behavior. Following the risk assessment paradigm, occurrence and toxicity are considered first—the consideration of occurrence before toxicity was selected for practical purposes. These are discussed in the following sections.

## 2.1 Occurrence

**Box 1 – Example Data Sufficiency Questions**

- Is the analytical method adequate for the need (i.e., is the detection and/or reporting level sufficiently sensitive)?
- Are there data of sufficient quantity/quality to evaluate?
- Are results reproducible?
- What media are data available for?
- Are there sufficient quality assurance/quality control (QA/QC) samples to validate the data?
- Were data collected using/following proper standards and guidelines?
- Were enough samples collected to indicate the presence of the substance in the environment?

The identification of a CEC in groundwater or surface water used for drinking water purposes is often a priority compared to other environmental media because of direct exposures to humans through drinking water and other household uses of water. For this reason, groundwater or surface water is often the first exposure source assessed and is highlighted in the flowchart. Depending on the situation, concerns over other exposure sources may predominate. For example, the occurrence of a CEC in soil may lead to a higher priority assignment depending on several factors, including land use (e.g., residential, day care, or school) or presence of sensitive subpopulations (e.g., children). Another example could be consumption of recreationally caught fish where a bioaccumulative CEC may be present at levels of concern even when it is nondetectable in surface water. CEC may also be identified in consumer products, which could lead to various exposure sources and pathways (e.g., dermal exposure, ingestion of contaminated food, inhalation of contaminated house dust, etc.). Overall, detection in multiple media adds to the concern due to the combined exposures to these multiple media (e.g., water, wastewater, air, soil, and biota) and likely multiple exposure routes (e.g., ingestion, dermal contact, inhalation) and higher potential for cross-media transfer. Importantly, an already regulated, well-established contaminant may be identified as a potential CEC. This could be due to new information that indicates potential for toxicity at lower exposure levels, its identification in a new media (e.g., air), or awareness of migration along a new exposure pathway (e.g., vapor intrusion).

Proximity of the CEC to sensitive receptors, and the exposure sources (e.g., drinking water, bathing, ingestion, recreation) and exposure routes (e.g., ingestion, inhalation, and dermal absorption) for those receptors, are also critical inputs to the occurrence evaluation. For drinking water, the source type (private well, public water system, groundwater- vs. surface water–based system, etc.) would also need to be evaluated. Agencies may also consider analyzing wastewater samples from treatment plants to detect and quantify the presence of the CEC, which can provide valuable information on its occurrence and distribution, as CEC often enter the environment through wastewater effluent.

An analogous process can be applied to ecological exposures. For example, occurrence in aquatic ecosystems (surface water and sediment) is often the first exposure question to evaluate if there is enhanced mobility and biological transfer potential within complex food webs. Occurrence in soil can lead to higher prioritization based on the presence of sensitive receptors (such as endangered species or valued keystone species), or the CEC may be susceptible to uptake by herbivorous or carnivorous animals via vegetation or soil biota. The priority assignment may also consider whether occurrence can affect the diversity and abundance of ecological communities.

When evaluating the occurrence criteria, agencies will want to consider analytical data sufficiency factors such as those identified in Box 1. Adequate characterization can be taken into account when making a decision about whether a CEC needs further evaluation or should be prioritized as a CEC. When data are not sufficient to make a judgment, the flowchart recommends additional data collection and reassessment. If sufficient data are found to be available, the reviewer determines whether (1) the CEC is a low priority (in which case, it would not be evaluated further in the flowchart) or (2) evaluation should proceed to a risk/toxicity assessment to determine next steps (e.g., monitoring/surveillance).

## 2.2 Toxicity

A toxicity value provides a concentration or dose above which exposure per unit of time may result in unacceptable health risks (for expmle, milligrams per kilogram body weight pre day [mg/kg bw/day])

The toxicities posed by a CEC are evaluated in relation to human health–based and/or ecological health effects. Many CEC may have information available on chemical characteristics but no available information on toxicity. For other CEC, toxicity information may be available but information about new exposure routes or exposure media may be lacking. In many cases, toxicity data may be limited and may not include the types of studies typically used to evaluate health effects in federal and/or state risk assessments. Toxicity data should be vetted to determine whether it can provide an adequate assessment of human health or ecological risks. Other potential considerations for evaluating CEC include the identification of toxicities at lower levels than previously known or identification of toxicities for one or more additional exposure routes. Toxicity evaluations (whether for human health or ecological receptors) will inform the degree to which a CEC poses a risk. This evaluation should also potentially include sensitive subpopulations that would be specific to a given site and CEC. Details

regarding specific toxicity information are discussed in Section 3: Sources of Key Variables to Consider When Evaluating Potential Toxicity and Exposure.

For a toxicity assessment to be meaningful, the extent and quality of information is a consideration. When incomplete toxicity data impede the development of numerical toxicity values, other tools may be used to develop or estimate toxicity values (see Section 3.3, Table 2: Sources of key variables information). For all estimates, an explanation of uncertainties, data sources, and assumptions should be provided to allow for clarity and transparency (see the Risk Perception and Communication Fact Sheet).

After reviewing toxicity information, three questions are considered:

- Does the CEC pose human and/or ecological health effects of concern?
- Does the CEC pose toxicity at lower levels than previously known?
- Does the CEC pose toxicity via exposure routes not previously identified?

Pathways to consider should include the potential for toxicity by uptake via the food chain (e.g., via feed, animal products, or edible plants). If data are insufficient to assess these factors, additional data should be collected for reassessment (see Section 3: Sources of Key Variables to Consider When Evaluating Potential Toxicity and Exposure). If data are available, an assessment can be made as to whether a specific CEC should be prioritized. For ecological toxicity, it is important to note that a variety of endpoints may need to be considered in addition to acute mortality, such as behavioral changes, reproductive damage, sex changes, etc. If the assessment indicates sufficient toxicity data, the next step is to consider the physical-chemical property criterion.

**Box 2 – Potential Additional Questions Regarding Physical-Chemical Mobi8lity and Transport**

- Was free product encountered in groundwater or siil?
- Were degaradation products identified in the analyzed media?
- Does the CEC have uniue characteristics (e.g., foam, amphiphilic) which affect transport?
- Can the CEC migrate along preferential pathways such as utility corridors or backfill?
- Is the CEC moving or behaving defferently than other substances detected in the area

### 2.3 Physical-chemical Properties That Inform Fate and Transport and Chemical Behavior

Physical-chemical properties influence how long a CEC remains in the environment and the environmental media in which it is present. They inform how the CEC's potential for exposure could increase, through its persistence in the environment, bioaccumulation, mobility, toxic degradation products, cross-media transfer, or other factors. This is the final step for determining whether a CEC should be considered a high-priority CEC. See Table 3 in Section 3.3 for a brief description of various properties used to determine persistence, bioaccumulation, and mobility.

These attributes reflect the potential for CEC to remain in the environment and cause exposure to human and ecological receptors. Physical-chemical properties may be empirical or estimated. Consideration may be given to the circumstances that dictate collection of site-specific data. Published data may be used when available. Data used to establish these properties also need to be of sufficient quality. Box 2 identifies additional considerations relative to physical-chemical mobility and transport.

## 3. SOURCES OF KEY VARIABLES TO CONSIDER WHEN EVALUATING POTENTIAL TOXICITY AND EXPOSURE

Assessments of CEC require some information on the CEC's toxicity as well as information on potential exposures. When considering toxicity, regulatory agencies usually consider chronic (cancer or noncancer), subchronic (noncancer, reproductive, or developmental), and acute (noncancer) health effects. Federal and state environmental and health agencies establish toxicity values, but the values generated can vary due to several factors. These can include the scientific information available at the time the value was developed, the consideration of a sensitive health effect or endpoint, and the choice of uncertainty factors (for noncancer endpoints). When no federal or state-developed toxicity value is available, or when toxicologists need to consider new information, the state may need to conduct its own toxicological assessment to develop a value that is defensible based on best available information. Many states prefer to use existing toxicity values developed by authoritative agencies or do not have the resources to develop their own values, while other states develop

their own toxicity values when necessary. Some states may choose to develop their own values if they do not agree with the scientific basis of available values; some states may be required to make different assumptions (e.g., regarding risk); and some states may also decide the available values are not applicable to or representative of conditions and situations present in their respective state (e.g., exposure of specific populations, water quality differences for aquatic life values, etc.). To facilitate a valid process for deciding which toxicity values should be applied in any given risk evaluation, the United States Environmental Protection Agency (USEPA) and many states use a hierarchy of sources (ECOS 2007; ITRC 2005; 2008; OSWER USEPA 2013, 3; 2009; ORD USEPA 2023d; 2015a). Table 2 presents a summary of sources relevant to the toxicity of a CEC.

There is less consensus on standard toxicity values and source hierarchies for ecological risk than for human health values. This is due to the wide variety of potential plant and animal receptors and differences in responses from exposure to environmental CEC. Defensible values require careful attention to study validity, endpoints, and uncertainty factors. Information on CEC of interest may be available in various databases curated by state agencies, federal sources (e.g., National Oceanic and Atmospheric Administration (NOAA), USEPA, the Department of Defense, and the Department of Energy), or national and international organizations.

When considering exposure pathways, physical-chemical criteria influence how long a chemical remains in the environment and the environmental media in which it is present and could increase the CEC's potential for exposure (persistence, degradation products), influence how it is taken up and processed in biota, and affect how it behaves in the food chain (e.g., bioaccumulation, cross-media transfer). Table 3 presents a brief description of key variables used to help prioritize CEC in relation to persistence, bioaccumulation, and mobility.

When standard approaches are not immediately applicable for use in evaluating CEC, the resources presented here can help states with decision-making regarding CEC. Table 2 summarizes sources of key variables and is explained in Sections 3.1 and 3.2.

Table 3 summarizes properties that inform fate and transport and is explained in Section 3.3.

## 3.1 Human Health Risk

Suitable criteria for considering risk to human health (i.e., toxicity values) may be available in multiple sources of widely varying quality and applicability. The sources are discussed below in three groupings without ranking relative importance. Table 2 provides a summary of each.

### 3.1.1 Group 1: U.S. Federal Values—IRIS, OW, ATSDR, PPRTV, and OPP

This group includes U.S. federal sources of human health toxicity values. For chemical exposures, the Integrated Risk Information System (IRIS) (ORD USEPA 2023d) is typically the preferred source for toxicity values because they are based on high-quality assessments that include internal and external reviews. IRIS includes cancer slope factors and inhalation risk values. The IRIS database may not include a value for the contaminant of interest, or the IRIS assessment may not have considered newly available information. Values may be available from other USEPA offices such as the Office of Water (OW) Health Advisories (OW USEPA 2023h) or the Office of Ground Water and Drinking Water (OW USEPA 2023i). These OW values are toxicity values developed by USEPA OW for use in drinking water health advisories or ambient water quality criteria. Another widely accepted source is the Agency for Toxic Substances and Disease Registry's (ATSDR) (ATSDR 2023) toxicity assessments for acute, intermediate, and chronic noncancer effects. ATSDR uses these to calculate peer-reviewed minimal risk levels for contaminants. The Provisional Peer Reviewed Toxicity Values (PPRTVs) (ORD USEPA 2023e) are developed to support the USEPA Superfund program for chemicals that do not have IRIS values or those with identified subchronic or acute health effects (which are not evaluated in IRIS). PPRTVs undergo both internal and external peer review but are considered a second-tier source by USEPA. The USEPA Office of Pesticide Programs (OPP) (OCSPP USEPA 2023c) generates health effects assessment for pesticides.

### 3.1.2 Group 2: State Values, ECHA, OECD, Other International Values, PubChem

Most states have their own processes for determining human health toxicity values. Generally, states use the Group 1 sources to initially identify their toxicity values; however, many states conduct their own toxicological assessments even when an IRIS value is available. Examples of these states are California (OEHHA 2016), New Jersey (NJDEP 2020), and Minnesota (MDH 2022). Toxicity values from the European Chemicals Agency's (ECHA) Guidance on Information Requirements and Chemical Safety Assessment (ECHA 2023d) and REACH (ECHA 2023h) and other countries (e.g., Canada and its provinces (Health Canada 2007) and Australia (Australian Government 2022)) may be considered when selecting

values. Selection of values from these sources when available will need to consider the toxicity assessment process, including evaluating principal studies (preferably peer reviewed and published/publicly available) and evaluating whether the risk assessment guidance used by other countries differs from USEPA's guidance. The value should be appropriate and sufficiently protective for the exposure scenario of interest. The Organisation for Economic Cooperation and Development (OECD) Echem Portal (OECD 2023a) and the National Library of Medicine's PubChem (PubChem 2023a) are excellent toxicity data resources but do not offer human health toxicity values that are used in human health risk assessment.

### 3.1.3 Group 3: Other Sources of Toxicity Data That Provide Supporting Evidence to Health Effects

If the level of concern for the CEC is potentially high based on other factors, and limited toxicity data are available, it may be advisable for the state to conduct a toxicological assessment. One resource that may provide additional weight of evidence to the assessment is the USEPA Toxicity Forecaster (ToxCast), which provides experimental and predictive data (ORD USEPA 2023g). ToxCast predictive capabilities are also available through the USEPA CompTox Dashboard (USEPA 2023a). A suite of models and tools are available for considering chemicals regulated under the Toxic Substances Control Act (OCSPP USEPA 2022b). Other estimation and modeling resources include the Toxicity Estimation Software Tool (TEST) (ORD USEPA 2023f), OPERA (NTP 2023), EpiSuite (OCSPP USEPA 2023a), Derex Nexus (Labcorp 2023), OncoLogic (OCSPP USEPA 2023b), and ToxTree (Jeliazkova et al. 2018).

## 3.2 Ecological Risks

Identification of suitable criteria for considering risk to the environment, wildlife, and water quality may be available from multiple sources of widely varying quality and applicability.

### 3.2.1 Group 1: Established CEC Frameworks

Many potential CEC may have already been evaluated as part of permitting requirements or other chemical management purposes using established CEC frameworks. A good starting point is the ECHA dossiers for new chemicals (ECHA 2023h), which assemble available information, including ecological and environmental toxicological data, as part of the European chemical classification process. As an example, for aquatic and terrestrial (soil) organisms, hazards may be represented under ECHA by the predicted no effect concentration values. The Chemicals Management Plan in Canada is a similar compilation of data (Government of Canada 2006).

### 3.1.2 Group 2: Established Media Concentrations or Screening Values Deemed Protective of Various Ecological Endpoints

Established media concentrations or screening values deemed protective of different ecological endpoints may have been established by various agencies. Unfortunately, they are typically established for well-known contaminants and may not be available for CEC. One source is the USEPA National Recommended Water Quality Criteria (OW USEPA 2022a) for surface water. Many states (e.g., Texas (TCEQ 2023), New Jersey (NJDEP 2010), and Oregon (Oregon DEQ 2023)) maintain surface water, sediment, and soil screening values for extensive lists of chemicals. Other sources include the USEPA regional office compilations for media concentrations (e.g., Region 3 (ORD USEPA 2015c), Region 4, (ORD USEPA 2015b), and Region 5 (USEPA 2023b)); the NOAA SquiRTs (NOAA 2023) screening value compilations for sediment, soil, and surface water; the Department of Energy (DOE) Oak Ridge National Laboratory Ecological Benchmark Tool for Chemicals (RAIS 2022a) as part of the Risk Assessment Information System (RAIS 2022b); and Los Alamos National Laboratory ECORISK Database (Kieling 2017). Many other countries also maintain similar databases. These values are generally, but not always, compilations developed from primary or secondary sources, can be based on widely different methodologies, and can be of varying quality and applicability. They are also generally limited to more common contaminants. Nevertheless, they are some of the primary sources to consider when evaluating a CEC.

### 3.2.3 Group 3: Compilations of Measured Toxicity Criteria and Bioaccumulation Potential from Exposures to CEC

These sources typically present a review of toxicity or bioaccumulation testing results available in the research literature and may or may not include the prioritization and selection of a preferred toxicity reference value (TRV). In the first group are databases of research results such as USEPA ECOTOX (Olker et al. 2022), which presents details of toxicity evaluations for a great many chemicals and species of aquatic and terrestrial biota. ECOTOX also now has several data summary tools that allow the user to summarize and manage data outcomes. A similar database for bioaccumulation and tissue residue studies in aquatic environments is the United States Army Corps of Engineers Environmental Residue Effects Database (USACE ERED) (USACE 2023). These sources present a wealth of information but require the user to have toxicological knowledge to determine the quality and applicability to the specific site and concern at hand. The scientific literature can be referenced for

additional information.

### 3.2.4 Group 4: Surrogates and Models

Potential CEC may be lacking in published empirical evaluations of potential toxicity and hazard to the environment. It may therefore be useful to consider modeling approaches for such chemicals. Among these are the USEPA Ecological Structure Activity Relationships (ECOSAR) (OCSPP USEPA 2022a) Predictive Model, a quantitative structure activity relationships (QSAR) model to estimate aquatic toxicity for organic chemicals. QSAR models can be accessed through the OECD QSAR Toolbox (OECD 2023b) and VEGA (VEGA HUB 2023). In the absence of useful data on the chemical of interest, it may also be possible to consider similar chemicals as surrogates for the chemical of interest. This is a common approach for chemicals that exist as very similar congeners or isomers that can be extrapolated across the chemical class. Resources identified in the prior human health toxicity section “Group 3: State Toxicological Assessment Using Available Information” may also provide values that can be considered for evaluation of potential impacts on ecological receptors (see ,for example, James and colleagues (2023), where high-throughput laboratory in vitro cell-line bioassay exposure-response data are being used as a surrogate for ecological risk thresholds).

### 3.2.5 Other Sources

In the absence of useful information in complied data sources for either human health or ecological toxicity, it may also be necessary to search and evaluate the primary research literature for information not already reflected in many of these sources. Some manufactured chemicals are proprietary, and existing human health and/or ecological toxicological information may not be publicly available. Values based on published scientific research are generally preferred to modeled data.

It is important to consider not only the exposure medium of concern, but also the biological organism level (individual, population, community, ecosystem) these data sources apply to. Toxicity data may be expressed in terms of toxicity (e.g., reference doses or effect concentrations) to an individual or populations of receptors or as values describing an effect at the community level (i.e., measures of diversity and abundance).

## 3.3 Properties That Inform Fate and Transport

Table 3 presents some indicators of persistence, bioaccumulation, and environmental partitioning. Persistence or bioaccumulation potential may be the result of direct empirical measurement or may be estimated from chemical-specific properties.

Some common sources for primary data (measured and/or estimated) used in the evaluation of environmental presence and exposure include the following:

- US EPA CompTox Dashboard (USEPA 2023a): The source presents chemistry, toxicity, and exposure information for more than 900,000 chemicals. Data and models presented in the dashboard can help with efforts to identify chemicals most in need of further testing.
- ATSDR Toxicological Profiles (ATSDR 2023): Peer-reviewed information reflecting a comprehensive and extensive evaluation, summary, and interpretation based on available toxicological, epidemiological, and fate and transport information.
- PubChem (PubChem 2023a): Comprehensive listing of chemicals and their physical-chemical, biological effect, and other attributes, including citations to original empirical data.
- EPISuite (OCSPP USEPA 2023a): A compendium of empirical and estimated physical, chemical, degradation, and bioaccumulation parameters, searchable by CAS number, SMILES structure, or name. This database focuses on attributes useful for estimating whether a chemical should be identified as a CEC.
- CRC Handbook of Chemistry and Physics (Rumble 2022): A classical source of comprehensive physical and chemical data for many chemicals.
- National Institutes of Standards and Technology (NIST) Chemistry WebBook (NIST 2023) Includes collected information on chemical and physical property data curated by the NIST Standard Reference Data Program and others.
- COSMO*therm* (COLaN 2023): Computational chemistry software program to predict thermodynamic properties.

Other countries also maintain compendia containing physical-chemical properties for thousands of chemicals. Some states specifically call out preferred sources for values to be used in a CEC evaluation. In addition, international and domestic

specialized databases for bioaccumulation and bioconcentration data, biodegradability constants, and environmental degradation rates are available (e.g., USACE ERED, USEPA Envirofate) (USACE 2023; USEPA 2023c).

Careful review and assessment of the data quality and applicability of the information from a data source, including any cited primary data, are essential to a comprehensive evaluation of the fate and transport characteristics of a chemical undergoing a CEC evaluation. Large ranges of empirical and measured values between sources may be present and could be problematic for the evaluation.

**Table 2. Sources of key variables information**

| Source (hyperlinked) | Categories of Variables Available | Responsible Agency | Summary |
|---|---|---|---|
| **Human Health Toxicity Group 1: U.S. Federal Values** | | | |
| IRIS (ORD USEPA 2023d) | Human health toxicity values: reference dose (RfD), reference concentration (RfC) inhalation unit risk (IUR) oral slope factor (OSF) weight of evidence for carcinogenicity | USEPA | The program characterizes and identifies the health hazards of chemicals found in the environment. It provides toxicity values for health effects resulting from chronic exposure to chemicals through the assessment of Hazard Identification and Dose-Response Assessment. |
| Office of Water (OW) (OA USEPA 2013) and Office of Ground Water and Drinking Water (OW USEPA 2023i) | Provides RfDs, OSFs, weight of evidence for carcinogenicity, Health Advisories (OW USEPA 2018), maximum contaminant levels, maximum contaminant level goals, and recommended human health-based water quality criteria for many different contaminants | USEPA | Information on toxicity criteria for and management of contaminants in surface waters and drinking water sources, for implementation of the Clean Water Act and Safe Drinking Water Act. |
| ATSDR ToxGuides (ATSDR 2021a) ATSDR Tox Profiles (ATSDR 2023) | Human health toxicity values: minimal risk levels noncancer toxicity factors for acute, intermediate (subchronic), and/or chronic exposure durations | CDC/ATSDR | The ATSDR program provides information on chemical and physical properties, sources of exposure, routes of exposure, minimal risk levels based on varying length of exposure, children's health, and health effects (ToxGuides™) (ATSDR 2021a) and a compilation of toxicological information on a given hazardous substance (ToxProfile) (ATSDR 2023). Established minimal risk levels can be found here. The Toxicological Profiles reflect a comprehensive and extensive evaluation, summary, and interpretation of available toxicological and epidemiological information on a substance. The program also offers additional toxicological resources (e.g., chemical classifications, health effects of exposure to toxic substances, etc.) and a database on a wide range of substances (Toxic substances Portal) (ATSDR 2021b). |

| | | | |
|---|---|---|---|
| PPRTVs (ORD USEPA 2023e) | Human health toxicity values: RfD, RfC, IUR, OSF, and weight of evidence for carcinogenicity | USEPA | The PPRTV (ORD USEPA 2023e) program provides toxicity information and values for chemicals of concern to the Superfund Program, focusing on those not addressed by IRIS. |
| OPP (OCSPP USEPA 2023c) | Ecological and human health toxicity values | USEPA | OPP provides ecological and human health risk assessment information for existing and new pesticides. |
| **Human Health Toxicity Group 2: State Values, ECHA, OECD, Other International Values, PubChem (Selected Examples of State Resources)** | | | |
| CA OEHHA (OEHHA 2016) | Noncancer reference exposure levels and cancer potency factors for toxic air contaminants; health protective exposure levels for contaminants in air, water, and soil; listing of cancer and reproductive toxicants under Proposition 65; and fish advisories. Toxicity factors for noncancer and cancer effects by the oral exposure route are also provided. | California | Chemical toxicity levels provided by the state of California. |
| NJDEP (NJDEP 2020) NJDEP (NJDEP 2023) | URF, Reference Concentrations Toxicity factors (RfDs, RfCs, CSFs, IURs) used for New Jersey drinking water, groundwater, surface water, and soil remediation standards | New Jersey | Air toxic criteria provided by the state of New Jersey. NJDEP Standards Compendium |
| MDH (MDH 2022) | Health-based values, health risk limits | Minnesota | Risk information on drinking water contaminants from the state of Minnesota. |
| Texas Commission on Environmental Quality (TCEQ) | Texas Risk Reduction Program (TRRP), e.g., Tiered Protective Concentration Levels for soil and groundwater; TRRP human health surface water risk-based evaluation levels (RBELs) | Texas | The TRRP program presents extensive guidance on identifying and developing toxicity criteria and physical-chemical characteristics for contaminants in soil, groundwater, surface water, and sediment. |

| | | | |
|---|---|---|---|
| Health Canada and Environment Canada (Health Canada 2007) | Toxicological reference values (TRVs) and guidance on Federal Contaminated Site Risk Assessment in Canada: Toxicological Reference Values (TRVs), Version 3.0, is a companion to Federal Contaminated Site Risk Assessment in Canada: Guidance on Human Health Preliminary Quantitative Risk Assessment (PQRA), Version 3.0, and to Federal Contaminated Site Risk Assessment in Canada, Part V: Guidance on Human Health Detailed Quantitative Risk Assessment for Chemicals (DQRAchem). | Health Canada | Provides guidance and advice on human health risk assessment and public involvement to other federal departments by reviewing human health risk assessment and integration of health issues in environmental assessments conducted under the Canadian Environmental Assessment Act. Risk assessment guidelines and approaches used by Health Canada to develop toxicity values may differ in some ways from those used by USEPA and states. Most Canadian provinces have their own requirements for carrying out risk assessments for contaminated sites (e.g., Ontario has requirements established under the Ontario Environmental Protection Act. |
| Australia Department of Climate Change, Energy, the Environment and Water (A); Department of Health and Aged Care (B) (Australian Government 2022) | A. Management plans for selected contaminants (e.g., PFAS) but no information on toxicity assessment or human toxicity values. B. Health-based guidance values expressed as tolerable daily intakes used for assessing potential exposure to contaminants through food, drinking water, and recreational water during site investigations. | Australia | A. Provides risk assessments to determine how chemicals will impact the environment at various stages of the chemical life cycle and manages the environmental risks from industrial chemicals through Industrial Chemicals and Environmental Management Standard (IChEMS). B. Collaborate with other Australian government agencies on policies and programs that aim to improve and maintain health-supporting environments including environmental and human health risk assessments. |
| Guidance on Information Requirements and Chemical Safety Assessment and REACH (ECHA 2023d; 2023h) | Under the Public Activities Coordination tool (PACT) Data generation and assessment (dossier evaluation (ECHA 2023c), substance evaluation, informal hazard assessment (PBTs (persistent, bioaccumulative, and toxic), and very persistent and very bioaccumulative (ECHA 2023g) Assessment of regulatory needs (ARN) Regulatory risk management | ECHA | Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) (ECHA 2023h) is a regulation of the European Union adopted to improve the protection of human health and the environment from the risks that can be posed by chemicals. ECHA provides information on substances that were assessed under REACH. The information provided includes a brief profile, REACH registered substance fact sheet, C&L Inventory (ECHA 2023b), biocidal active substance fact sheet (ECHA 2023e), the PACT (ECHA 2023f), and regulatory obligations. |

| | | | |
|---|---|---|---|
| Echem Portal (OECD 2023a) | Toxicity, exposure, use information, risk assessment data | OECD | OECD eChemPortal provides links to chemical hazard and risk information prepared for government chemical programs. It also provides toxicity, exposure, and use information on chemicals and access to any risk assessment data. Databases participating in eChemPortal include USEPA databases, ECHA, Canada, Japan, and Nordic countries). |
| PubChem (PubChem 2023a) | Toxicity and pharmacology information including links to chemical toxicity assessments, carcinogenicity classification, target organs, and human and nonhuman effects if available. | National Library of Medicine, National Institute of Health | PubChem, an open chemistry database that includes ToxNet (PubChem 2023b) data from Chemical Carcinogenesis Research Information System (CCRIS), ChemIDplus, Genetic Toxicology Data Bank (Gene-Tox), and Hazardous Substances Data Bank (HSDB) (HSDB 2023). |
| **Human Health Toxicity Group 3: Other Sources of Toxicity Data That Provide Supporting Evidence to Health Effects** | | | |
| ToxCast (ORD USEPA 2023g) | High-throughput screening assays endpoints—identify the potential of chemicals for toxic effects including endocrine disruption and neuro-developmental effects; includes predictive capabilities access through the ComTox Dashboard (USEPA 2023a). | USEPA | USEPA's Toxicity Forecaster (ToxCast) generates data and predictive models on thousands of chemicals using high-throughput screening methods and computational toxicology approaches to rank and prioritize chemicals. |
| The Toxicity Estimation Software Tool (TEST) (ORD USEPA 2023f) | A calculation tool that may be used to predict acute and developmental toxicity in the absence of appropriate animal toxicity or epidemiological studies. The modeled toxicity estimates provide another weight of evidence to the toxicological assessment of a chemical. | USEPA | Estimates the toxicity values and physical properties of organic chemicals based on an entered molecular structure using QSAR methods. |
| EpiSuite (OCSPP USEPA 2023a) | Physical-chemical properties Environmental fate properties | USEPA | Estimates physical-chemical and environmental fate properties. |
| OECD QSAR Toolbox | A software application intended to be used by governments, the chemical industry, and other stakeholders in filling gaps in (eco)toxicity data needed for assessing the hazards of chemicals. | OECD/ECHA | Identifies relevant structural characteristics and potential mechanism or mode of action of a target chemical based on other chemicals that have the same structural characteristics and/or mechanism or mode of action and uses existing experimental data to fill data gap(s). |
| OncoLogic (OCSPP USEPA 2023b) | Estimated carcinogenicity | USEPA / OECD | The OncoLogic™ model estimates carcinogenicity from chemical and use information based on a set of knowledge rules. |

| | | | |
|---|---|---|---|
| Derek Nexus (Labcorp 2023) | Skin sensitization | Lhasa Limited | Derek Nexus can predict a number of toxicological endpoints. It is expert, knowledge-based toxicology software that gives predictions for a variety of endpoints. |
| ToxTree (Jeliazkova et al. 2018) | Hazard estimation | Ideaconsult Ltd | ToxTree uses a decision-tree approach to estimate hazards. |
| **Ecological Toxicity Group 1: Established Evaluation Frameworks** | | | |
| ECHA REACH Dossiers (ECHA 2023i) | Hazard classification; use | ECHA | (See REACH above) |
| Chemicals Management Plan (Government of Canada 2006) | Risk assessment and risk management information | Health Canada | Assessment and management of risks to human health and the environment posed by chemical substances that can be found in food and food products, consumer products, cosmetics, drugs, drinking water, and industrial releases. |
| OPP (OCSPP USEPA 2023c) | Ecological and human health toxicity | USEPA | OPP provides ecological and human health risk assessment information for existing and new pesticides. |
| **Ecological Toxicity Group 2: Established Media Concentrations or Screening Values Deemed Protective of Various Ecological Endpoints** | | | |
| US EPA National Recommended Water Quality Criteria (OW USEPA 2022a) | Water quality criteria | USEPA | Summary tables of recommended water quality criteria for the protection of aquatic life and human health in surface water for approximately 150 pollutants. |
| State-level compilations available in most states (e.g., Texas (TCEQ 2023), New Jersey (NJDEP 2010), Oregon (Oregon DEQ 2023)) | Ecological screening criteria | Various | States provide ecological screening and risk assessment criteria and information. |
| Regional Screening (Region 3 (ORD USEPA 2015c), Region 4 (ORD USEPA 2015b), and Region 5 (USEPA 2023b, 5)) | Biological Technical Assistance Group (BTAG) Screening Values, Regional Ecological Risk Assessment (ERA) Guidance | USEPA | USEPA regions provide specific guidance to states, tribes, and local governments. |
| SquiRTs (NOAA 2023) | Sediment, soil, and surface water screening values | NOAA | Screening Quick Reference Tables (SquiRTs) provide information to evaluate potential risks from contaminated water, sediment, or soil. |

| | | | |
|---|---|---|---|
| Ecological Benchmark Tool for Chemicals (RAIS 2022a) | Ecological screening levels | DOE Oak Ridge National Laboratory | Contains ecological screening benchmarks for surface water, sediment, surface soil, and biota applicable to a range of aquatic organisms, soil invertebrates, mammals, and terrestrial plants. |
| ECORISK Database (Kieling 2017) | Ecological screening levels | DOE Los Alamos National Laboratory | Compilation of ecological screening levels to inform ecological risk assessments. |
| **Ecological Toxicity Group 3: Compilations of Measured Toxicity Criteria and Bioaccumulation Potential from Exposures to CEC** | | | |
| ECOTOX (Olker et al. 2022) | Toxicological endpoints | USEPA | The ECOTOXicology Knowledgebase contains single chemical toxicity data for aquatic life, terrestrial plants, and wildlife. |
| ERED (USACE 2023) | Residue-effects data | U.S. Army Corp of Engineers | The ERED contains residue-effects data, useful for understanding potential bioaccumulation from exposure to dredged sediment. |
| **Ecological Toxicity Group 4: Surrogated and Models** | | | |
| ECOSAR (OCSPP USEPA 2022a) | Acute and chronic toxicity | USEPA | ECOSAR is used to estimate toxicity to aquatic organisms, such as fish, aquatic invertebrates, and aquatic plants, by using computerized Structure Activity Relationships. |
| OECD QSAR Toolbox (OECD 2023b) | Ecotoxicity endpoints | OECD | Developed in collaboration with ECHA, fills ecotoxicity data for assessing the chemical hazards. |
| VEGA (VEGA HUB 2023) | Ecotoxicity endpoints | Istituto di Ricerche Farmacologiche Mario Negri | Provides a platform to access QSAR models. |

**Table 3. Properties that inform potential fate and transport**

| | **Property** | **Symbol** | **Description** |
|---|---|---|---|

| | | | |
|---|---|---|---|
| **Some Indicators of Persistence** | | | **Measures estimating persistence of chemicals in environmental compartments. Environmental persistence is a fundamental component of the classification process related to persistence, bioaccumulation, and toxicity (PBT).** |
| | Half-life | t ½ | Measures of environmental persistence are defined as the time required for the concentration of a substance in an environmental medium to diminish by one-half. Persistence criteria under several PBT classification schemes (e.g., the REACH Annex XIII PBT or very persistent and very bioaccumulative (vPvB) criteria) are defined on the basis of persistence half-lives in water and sediment. Analogous half-lives can be derived for volatilization from water to air, biotransformation, and other processes and are a common tool in evaluating fate and transport of substances. |
| | Biodegradability | | The capacity for microbial degradation of organic chemicals to base substances. Degradability is a key measure of persistence of chemicals and is usually tested by standard degradation tests. “Ready” degradability are chemicals that quickly and extensively degrade. “Inherent” biodegradability is the ability of a chemical to degrade to base products over a longer period of time. Definitions of “persistence” in several PBT classification schemes are defined from measures of biodegradability. Multiple experimental methods exist. |
| | Photodegradation and atmospheric oxidation potential | | Measures of chemical propensity to transformation under influence of sunlight and atmospheric oxidation processes. Note that photodegradation products may be of concern in their own right. |

| | | | |
|---|---|---|---|
| **Some Indicators of Bioaccumulation** | | | **Measured or estimated properties that estimate uptake and bioaccumulation to biota from environmental media. Can be based on standard tests or biokinetic models. Bioaccumulation is a fundamental component of the PBT classification process.** |
| | Bioaccumulation and bioconcentration factors | BAF/BCF | Measures describing the degree to which substances are taken up or accumulated into tissues, typically but not exclusively aquatic organisms, from the surrounding medium. The BAF describes the total ratio (at equilibrium) of the concentration in the tissue to the concentration in the medium. Definitions on bioaccumulation in PBT schemes are often based on BAF or BCF ranges. BAF and BCFs are derived from standardized bioaccumulation tests. A related concept, trophic biomagnification factors, considers the ability of some substances to bioaccumulate across ecological trophic levels (i.e., from consumers to primary predators to secondary predators). |
| | Biota-sediment accumulation factors | BSAF | A special case of bioaccumulation factors often applied in sediment, where the units are based on organic carbon normalized values in sediment and lipid content values in tissue. |
| | Biota and trophic transfer factors | BTF/TTF | Measures describing the transfer of substances between different levels of biota or between different organ systems in biota. These factors help describe the ability of a substance to biomagnify (i.e., increase in concentration in higher trophic levels). Also describe a propensity to particularly concentrate in milk, meat, or particular food items. |
| | Bioavailability and bioaccessibility | BA | Measures of how much a substance in the environment may enter living organisms. Many factors such as chemical forms, adsorption to environmental media, exposure route to the organism, and physiological characteristics of the organism affect this measure. Understanding bioavailability is essential to predict the biological effects of environmental contaminants. Bioavailability is usually measured as relative (where bioavailability is compared relative to a standard bioavailability) or absolute (where bioavailability directly measures the relationship between the environmental concentration and the effective dose in the organism). Bioaccessibility describes the physical ability of a substance to come into direct contact with a living organism in a form that may be bioavailable. |

| | | | |
|---|---|---|---|
| **Some Indicators of Environmental Partitioning and Fate** | | | **Measured or estimated properties that estimate the partitioning of chemicals between environmental media and between biota and environmental media.** |
| | Octanol-water partitioning coefficient | $K_{ow}$ | A measure of the partitioning coefficient of a chemical in a two-phase system of n-octanol and water. The octanol is considered a surrogate for organism lipids. The $K_{ow}$ describes the propensity of nonpolar organic chemicals to accumulate in organism lipids and is therefore used as a surrogate for bioaccumulation. Most PBT classification schemes use $K_{ow}$ to classify chemicals as bioaccumulative. $K_{ow}$ may not be an appropriate indicator of bioaccumulative potential for polar or charged contaminants. |
| | Organic carbon-sediment partitioning coefficient | $K_{oc}$ | A measure of the partitioning coefficient of a chemical between organic carbon (in soil, sediment, or particulates) and surrounding water. The $K_{oc}$ describes the propensity of nonpolar organics to exist as a freely dissolved form enhancing migration potential and bioavailability. The $K_{oc}$ is an important measure to estimate bioavailability and migration potential and thereby the potential to bioaccumulate or exert toxic effects. (While databases often include $K_{oc}$ values for polar and charged chemicals, it may not be appropriate in certain contexts; e.g., other soil components can influence adsorption for polar/charged compounds). |
| | Soil/sediment to water partitioning coefficient | $K_{d}$ | A measured value describing the amount of chemical adsorbed onto soil (or sediment) per amount of water. It is related to $K_{ow}$ and $K_{oc}$ but is an empirical measure considering the totality of factors affecting the partitioning. |
| | Octanol air partitioning coefficient | $K_{oa}$ | Analogous measure to the $K_{ow}$ but estimates the partitioning between volatile chemicals in air and biological tissue lipids, represented by n-octanol. It is used to predict partitioning among air, soil, vegetation, and aerosols. |
| | Fugacity | F | Fugacity describes the propensity of a substance to move among multiple environmental compartments (air, soil, sediment, and water) under given conditions, based on fugacity model outputs. These models use default parameters such as temperature and substance $K_{ow}$ to distribute a substance among compartments and are useful in evaluating transport and persistence. |
| | Particulate sorption | phi (φ) | Measure of the fraction of a substance adsorbed to atmospheric particulates |

| | | | |
|---|---|---|---|
| **Other Physical-Chemical Factors Informing Evaluations** | | | **Basic empirical or estimated physical-chemical properties that can provide insight into fate, transport, persistence, and bioaccumulation of chemicals** |
| | Henry's Law constant | H' or $K_H$ | A chemical-specific property predicting the volatility of a chemical. This measure is frequently used to classify chemicals as volatile or nonvolatile and affects persistence. |
| | Vapor pressure | P | A chemical-specific property that estimates the partitioning of a substance between liquid and air phase. It is related to H'. This measure is frequently used to classify chemicals as volatile or nonvolatile and affects persistence. |
| | Solubility | Wsol | Key indicator property predicting availability and migration potential of chemicals in aqueous environments via dissolution in water. Very insoluble substances have limited partitioning to the aqueous phase and high retardation factors and thereby have limited transport potential in aqueous systems. |
| | Boiling and melting points | BP, MP | Boiling and melting points are useful to understand environmental occurrence and transport potential of a substance. |

## 4. SCHEMES FOR INTERPRETING INFORMATION ON VARIABLES

A number of published prioritization schemes/approaches for a range of environmental media and contaminant groups are available. Table 4 summarizes select schemes and frameworks used to prioritize emerging contaminants/chemicals and is intended to represent a broad spectrum of national, international, and state frameworks. Table 4 serves as a resource for the states to explore alternative prioritization approaches (in addition to the one presented in this Fact Sheet) to facilitate development of their own programs to monitor, identify, and evaluate CEC.

**Table 4. Schemes for interpreting information on variables**

| Prioritization Approach/ Reference | Year Developed/ Updated | Environmental Media | Contaminant Group | Brief Summary of Approach / Links for Additional Information |
|---|---|---|---|---|
| USEPA Screening Risk of Emerging Contaminants (SIREN) (Guiseppi-Elie, Pollard, and Zambrana 2022) | 2023 | All | All | USEPA is developing a technical framework that may eventually be adaptable to states to support the agency's response to potential CEC. SIREN will consider factors such as potential hazards, exposure, persistence, bioaccumulation, and cross-media impacts. |

| | | | | |
|---|---|---|---|---|
| USEPA Contaminant Candidate List (CCL) (OW USEPA 2022b) | 2022 | Drinking Water | All emerging contaminant groups | The CCL is prepared every five years based on nominations from the public and comments received from the public and Science Advisory Board. The following three criteria are used to determine (prioritize) whether the contaminant on the CCL may require regulation: (1) the contaminant may have an adverse effect on the health of persons; (2) the contaminant is known to occur or there is a substantial likelihood that the contaminant will occur in PWSs with a frequency and at levels of public health concern; and (3) in the sole judgment of the Administrator, regulation of such contaminant presents a meaningful opportunity for health risk reduction for persons served by public water systems. Contaminant Candidate List 5 – CCL 5 ("Drinking Water Contaminant Candidate List 5-Final" 2022) |
| USEPA Unregulated Contaminant Monitoring Rule (UCMR) | 2021 | Drinking Water | All emerging contaminant groups | The USEPA UCMR requires that every five years all large public water systems and a subset of small public water systems monitor for a list of 30 contaminants that are not currently regulated. The goal of the UCMR program is to help the agency determine whether it should regulate a specific contaminant. |
| Watch List for European Union–Wide Surface Water Monitoring (Gomez Cortes et al. 2022) | 2022 | Surface Water | All emerging contaminant groups | Three pillars of information are used to select candidate substances for the Watch List. The first pillar is the outcome of the last review of substances for the third Watch List, the second is information from Member States and stakeholders, and the third is literature search and/or other information (Gomez Cortes et al. 2022). The three criteria used to prioritize substances for inclusion in the Watch List are (1) the need for more monitoring data to perform a risk assessment, (2) the existence of reliable information on the toxicity of the substances that points to a possible risk, and (3) sufficiently sensitive analytical methods exist for the substances. Selection of substances for the 4th Watch List under the Water Framework Directive (Gomez Cortes et al. 2022) |
| Association of State Drinking Water Administrators (ASDWA) (ASDWA 2020) | 2020 | Drinking Water | All emerging contaminant groups | Supports agencies' programs addressing potential risks from CEC in drinking water, including management and treatment options. |

| | | | | |
|---|---|---|---|---|
| Voluntary Groundwater Watch List – European Union (Kozel and Wolter 2018) | 2018 | Groundwater | All emerging contaminant groups | Watch list of pollutants is developed based on (1) the occurrence of substances in groundwater (based on monitoring data) and (2) the theoretical leaching potential of substances (based on the substance properties). The combined outcome of these two assessments ("Combined groundwater leaching potential score") is linked with the hazard potential of these substances to form a ranked list, the "Integrated groundwater score." Voluntary Groundwater Watch List (Kozel and Wolter 2018), Voluntary Groundwater Watch List Concept & Methodology (Kozel and Wolter 2018) |
| NORMAN Prioritization Framework (Dulio and von der Ohe 2013) | 2013 | Aquatic environment (water, sediment, suspended particulate matter and biota) | All emerging contaminant groups | The overall prioritization procedure is carried out in two successive stages. In the first stage, the NORMAN prioritization methodology uses a decision tree that classifies chemicals into six categories, based on identified ("categories" of) knowledge gaps and actions to be taken by the research community and public authorities to fill them. The second stage entails the prioritization of the substances within each (action) category on the basis of the criteria / indicators identified for each category (Dulio and von der Ohe 2013). NORMAN Prioritization framework for emerging substances (Dulio and von der Ohe 2013) |
| U.S. Department of Defense (DOD) Instruction 4715.18 (DOD 2019) | 2019 | All | All emerging contaminant groups | This DOD Instruction (DOD 2019) establishes an enterprise-wide program to identify emerging chemicals (ECs); assess the likelihood and severity of impacts associated with ECs to people, the environment, and DOD mission; and take management actions to reduce these impacts. To be considered an EC, a chemical must (1) be relevant to the DOD, (2) have a perceived or real threat to human health or the environment, and (3) have new or changing toxicity values or regulatory standards as a result of new science, detection capabilities, or exposure pathways (DOD 2019). |

| | | | | |
|---|---|---|---|---|
| Michigan | 2019 | All | All new or emerging chemical contaminants | The Natural Resources and Environmental Protection Act, 1994 PA 451, as amended, Parts 201 (remediation) and 213 (LUSTs), regulates facilities of environmental contamination. “New” contaminants detected in soil and groundwater are substances that are not listed in the Part 201 Cleanup Criteria Rules and therefore do not have cleanup criteria that can be used to determine whether a property is a “facility.” The Part 201 regulations require “facility” determination for any property with detected contaminants to ensure due care is met. The owners and operators of property that is contaminated are required to take actions to ensure that the contamination does not cause unacceptable exposures and assure the safe use of the property. (Due Care Obligations (michigan.gov) (EGLE 2019). |
| Minnesota | | | | MDH collaborates with partners and the public to identify contaminants of interest; investigates the health and exposure potential of CEC in water; and informs partners and the public of appropriate actions for pollution prevention and reducing exposures to contaminants that might be unhealthy. |
| REACH | 2022 | All | All new or emerging chemical contaminants | REACH seeks to identify substances of very high concern based on carcinogenic, mutagenic, or toxic for reproduction categorization and PBT/vPVB properties. Substances of Very High Concern Identification (ECHA 2023a) |

| | | | | |
|---|---|---|---|---|
| Toxicity Forecaster (ToxCast™) | 2022 | All | All new or emerging chemical contaminants | The Toxicity Forecaster (ToxCast) database contains the results from automated screening assays for thousands of chemicals and can be accessed using the CompTox Chemicals Dashboard (CompTox Chemicals Dashboard) (USEPA 2023a). These assays, termed high-throughput screening assays, expose living cells or isolated proteins to contaminants one at a time; following exposure, the cells and proteins are screened for changes in biologic activity that suggest biologic and potentially toxic effects. This *in silico* data provides information to assess the toxicity of specific contaminants, but it is not equivalent to traditional toxicity tests. Scientists are using this tool and related techniques in field studies to assist in the identification of CEC that may be impacting aquatic life and the prioritization of CEC for further research and identification. (Ankley et al. 2021; Blackwell et al. 2019) (ORD USEPA 2017a) ToxCast Owner's Manual – Guidance for Exploring Data, ToxCast Data: Example Use Cases and Scenarios for Exploring Data (ORD USEPA 2017b) |
| Toxic Substances Control Act (TSCA) | 2019–2020 | All | Chemical contaminants | The TSCA, as amended by the Frank R. Lautenberg Chemical Safety for the 21st Century Act, requires USEPA to evaluate the safety of existing chemicals. The first step in USEPA's process for evaluating the safety of existing chemicals is prioritization (OCSPP USEPA 2017), which is a risk-based screening process for designating chemical substances as either High-Priority Substances for risk evaluation or Low-Priority Substances. Preferences are given to prioritizing chemicals on the 2014 TSCA Work Plan (OCSPP USEPA 2014) and to considering certain criteria, such as hazard/exposure, persistence, and bioaccumulation. |
| California State Water Resources Control Board Constituents of Emerging Concern | 2023 | Water | Emerging chemicals and substances | The California Water Resources Control Board's Constituents of Emerging Concern program supports source control issues for emerging contaminants that are "hardest to treat, not regulated and/or routinely monitored, and have not been adequately tested for human or ecological toxicity." The webpage contains information and recommendations for strategic prioritization and characterization as well as potential rulemaking for constituents that impact California waters. |

## References


Ankley, G.T., J.P. Berninger, B.R. Blackwell, J.E. Cavallin, T.W. Collette, D.R. Ekman, K.A. Fay, et al. 2021. “Pathway-Based Approaches for Assessing Biological Hazards of Complex Mixtures of Contaminants: A Case Study in the Maumee River.” *Environmental Toxicology and Chemistry* 40 (4): 1098–1122. https://doi.org/10.1002/etc.4949.

ASDWA. 2020. “State CEC Rule Development and Management Strategies Toolkit.” Association of State Drinking Water Administrators. February 2020. https://www.asdwa.org/wp-content/uploads/2020/03/State-CEC-Rule-Development-and-Management-Strategies-Toolkit.pdf.

ATSDR. 2021a. “ToxGuidesTM.” February 10, 2021. https://wwwn.cdc.gov/TSP/ToxGuides/ToxGuidesLanding.aspx.

ATSDR. 2021b. “Toxic Substances Portal.” February 10, 2021. https://wwwn.cdc.gov/TSP/index.aspx.

ATSDR. 2023. “Toxicological Profiles.” March 7, 2023. https://www.atsdr.cdc.gov/toxprofiledocs/index.html.

Australian Government. 2022. “Environmental Toxins and Contaminants.” Text. Australian Government Department of Health and Aged Care. Australian Government Department of Health and Aged Care. July 8, 2022. https://www.health.gov.au/topics/environmental-health/what-were-doing/environmental-toxins-and-contaminants.

Blackwell, Brett R., Gerald T. Ankley, Paul M. Bradley, Keith A. Houck, Sergei S. Makarov, Alexander V. Medvedev, Joe Swintek, and Daniel L. Villeneuve. 2019. “Potential Toxicity of Complex Mixtures in Surface Waters from a Nationwide Survey of United States Streams: Identifying in Vitro Bioactivities and Causative Chemicals.” *Environmental Science & Technology* 53 (2): 973–83. https://doi.org/10.1021/acs.est.8b05304.

COLaN. 2023. “Cosmotherm | the CAPE-OPEN Laboratories Network.” 2023. https://www.colan.org/process-modeling-component/cosmotherm/.

DOD. 2019. “DOD Instruction 4715.18: Emerging Chemicals (ECs) of Environmental Concern.” September 4, 2019. https://www.esd.whs.mil/Portals/54/Documents/DD/issuances/dodi/471518p.pdf.

Dulio, Valeria, and Peter C. von der Ohe. 2013. *NORMAN Prioritisation Framework for Emerging Substances*.

ECHA. 2023a. “Authorisation.” European Chemicals Agency. 2023. https://echa.europa.eu/substances-of-very-high-concern-identification-explained.

ECHA. 2023b. “C&L Inventory.” 2023. https://echa.europa.eu/information-on-chemicals/cl-inventory-database.

ECHA. 2023c. “Dossier Evaluation Status.” 2023. https://echa.europa.eu/information-on-chemicals/dossier-evaluation-status.

ECHA. 2023d. “Guidance on Information Requirements and Chemical Safety Assessment.” European Chemicals Agency. 2023. https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment.

ECHA. 2023e. “Information on Biocides.” 2023. https://echa.europa.eu/information-on-chemicals/biocidal-active-substances.

ECHA. 2023f. “PACT – Public Activities Coordination Tool.” 2023. https://echa.europa.eu/pact.

ECHA. 2023g. “PBT/vPvB Assessments under the Previous EU Chemicals Legislation.” 2023. https://echa.europa.eu/information-on-chemicals/pbt-vpvb-assessments-under-the-previous-eu-chemicals-legislation.

ECHA. 2023h. “REACH – Registration, Evaluation, Authorisation and Restriction of Chemicals Regulation.” 2023. https://echa.europa.eu/information-on-chemicals/registered-substances.

ECHA. 2023i. “Registered Substances.” 2023. https://echa.europa.eu/information-on-chemicals/registered-substances.

ECOS. 2007. “Identification and Selection of Toxicity Values/Criteria for CERCLA and Hazardous Waste Site Risk Assessments in the Absence of IRIS Values.” *The Environmental Council of the States (ECOS)* (blog). April 23, 2007. https://www.ecos.org/documents/risk-assessment-identification-and-selection-of-toxicity-valuescriteria-for-cercla-and-hazardous-waste-site-risk-assessments-in-the-absence-of-iris-values/.

EGLE. 2019. “Due Care Obligations.” Michigan Department of Environment, Great Lakes, and Energy. May 2019. https://www.michigan.gov/-/media/Project/Websites/egle/Documents/Programs/RRD/Due-Care/EGLE-RRD-Due-Care-Guide.pdf

?rev=79e593d455c74612a6af450b61777c9b.

Federal Register. 2016. “Drinking Water Contaminant Candidate List 4-Final.” Federal Register. November 17, 2016. https://www.federalregister.gov/documents/2016/11/17/2016-27667/drinking-water-contaminant-candidate-list-4-final.

Gomez Cortes, Livia, Dimitar Marinov, Isabella Sanseverino, Anna Navarro Cuenca, Magdalena Niegowska Conforti, Elena Porcel Rodriguez, Francesco Stefanelli, and Teresa Lettieri. 2022. “Selection of Substances for the 4th Watch List under the Water Framework Directive.” Publications Office of the European Union, EUR 31148 EN. https://doi.org/10.2760/01939.

Government of Canada. 2006. “Chemicals Management Plan.” Program descriptions. October 27, 2006. https://www.canada.ca/en/health-canada/services/chemical-substances/chemicals-management-plan.html.

Guiseppi-Elie, Annette, Amina Pollard, and José Zambrana. 2022. “When to Sound an Alarm: Contaminants of Emerging Concern.” In . Lisbon, Portugal. https://cfpub.epa.gov/si/si_public_record_Report.cfm?dirEntryId=356113&Lab=CEMM.

Health Canada. 2007. “Guidance Documents – Contaminated Sites – Environmental and Workplace Health.” Guidance. May 9, 2007. https://www.canada.ca/en/health-canada/services/environmental-workplace-health/contaminated-sites/guidance-documents.html.

HSDB. 2023. “Hazardous Substances Data Bank (HSDB).” January 5, 2023. https://healthdata.gov/dataset/Hazardous-Substances-Data-Bank-HSDB-/ehtz-u4ky.

ITRC. 2005. “Examination of Risk-Based Screening Values and Approaches of Selected States. RISK-1.” Interstate Technology & Regulatory Council, Risk Assessment Resources Team. http://www.itrcweb.org.

ITRC. 2008. “Use of Risk Assessment in Management of Contaminated Sites. RISK-2.” Interstate Technology & Regulatory Council, Risk Assessment Resources Team. www.itrcweb.org.

James, C.A., R. Sofield, M. Faber, D. Wark, A. Simmons, L. Harding, and S. O’Neil. 2023. “The Screening and Prioritization of Contaminants of Emerging Concern in the Marine Environment Based on Multiple Biological Response Measures.” *Science of The Total Environment* 886: 163712. https://doi.org/10.1016/j.scitotenv.2023.163712.

Jeliazkova, Nina, Martin Martinov, Olga Tcheremenskaia, Molecular Networks, Patrik Rydberg, Svetlana Avramova, Nikolay Kochev, Vedrin Jeliazkov, and Luchesar Iliev. 2018. “Toxtree – Toxic Hazard Estimation by Decision Tree Approach.” Toxtree – Toxtree – Toxic Hazard Estimation by Decision Tree Approach. 2018. https://toxtree.sourceforge.net/.

Kieling, John. 2017. “Submittal of the ECORISK Database, Release 4.1,” October 19, 2017. https://rais.ornl.gov/documents/ECO_BENCH_LANL.pdf.

Kozel, Ronald, and Rüdiger Wolter. 2018. “Voluntary Groundwater Watch List Concept & Methodology.” 2018. https://circabc.europa.eu/d/d/workspace/SpacesStore/63f48ec1-6da8-4b5b-aed7-71e018324d71/Groundwater%20watch%20list.pdf.

Labcorp. 2023. “DEREK Nexus® Toxicology Modeling.” Labcorp Drug Development. 2023. https://drugdevelopment.labcorp.com/catalog/derek-nexus-toxicology-modeling.html.

MDH. 2022. “How Health-Based Values and Health Risk Limits Are Calculated.” October 3, 2022. https://www.health.state.mn.us/communities/environment/risk/rules/water/methods.html.

NIST. 2023. “NIST Chemistry WebBook, NIST Standard Reference Database Number 69.” 2023. https://doi.org/10.18434/T4D303.

NJDEP. 2010. “NJDEP SRP – Guidance: Ecological Screening Criteria.” New Jersey Department of Environmental Protection. August 31, 2010. https://www.nj.gov/dep/srp/guidance/ecoscreening/.

NJDEP. 2020. “How We Estimate Risk from Air Toxics.” State of New Jersey Department of Environmental Protection. January 28, 2020. https://www.nj.gov/dep/airtoxics/atrisk.htm.

NJDEP. 2023. “Compendium of Environmental Standards.” *Environmental Standards* (blog). January 31, 2023. https://dep.nj.gov/standards/list/.

NOAA. 2023. “SQuiRT Cards.” NOAA Office of Response and Restoration. March 9, 2023. https://response.restoration.noaa.gov/environmental-restoration/environmental-assessment-tools/squirt-cards.html.

NTP. 2023. “Open (Quantitative) Structure-Activity/Property Relationship App: OPERA.” March 29, 2023. https://ntp.niehs.nih.gov/whatwestudy/niceatm/comptox/ct-opera/opera.

OECD. 2023a. “eChemPortal.” 2023. https://www.echemportal.org/echemportal/.

OECD. 2023b. “The OECD QSAR Toolbox.” 2023. https://www.oecd.org/chemicalsafety/risk-assessment/oecd-qsar-toolbox.htm.

OEHHA. 2016. “Chemicals.” Text. OEHHA. May 6, 2016. https://oehha.ca.gov/chemicals.

Olker, Jennifer H., Colleen M. Elonen, Anne Pilli, Arne Anderson, Brian Kinziger, Stephen Erickson, Michael Skopinski, et al. 2022. “The ECOTOXicology Knowledgebase: A Curated Database of Ecologically Relevant Toxicity Tests to Support Environmental Research and Risk Assessment.” *Environmental Toxicology and Chemistry* 41 (6): 1520–39. https://doi.org/10.1002/etc.5324.

Oregon DEQ. 2023. “Department of Environmental Quality: Ecological Risk Assessments : Environmental Cleanup : State of Oregon.” 2023. https://www.oregon.gov/deq/hazards-and-cleanup/env-cleanup/pages/era.aspx.

PubChem. 2023a. “PubChem.” National Library of Medicine. 2023. https://pubchem.ncbi.nlm.nih.gov/.

PubChem. 2023b. “ToxNet Data.” 2023. https://pubchem.ncbi.nlm.nih.gov/docs/toxnet.

RAIS. 2022a. “Ecological Benchmark Tool for Chemicals.” Risk Assessment Information System. 2022. https://rais.ornl.gov/tools/eco_search.php.

RAIS. 2022b. “Welcome to the Risk Assessment Information System.” Risk Assessment Information System. 2022. https://rais.ornl.gov/index.html.

Rumble, John. 2022. *CRC Handbook of Chemistry and Physics*. 103rd ed. CRC Press.

TCEQ. 2023. “Ecological Risk Assessments.” Texas Commission on Environmental Quality. 2023. https://www.tceq.texas.gov/remediation/eco.

USACE. 2023. “ERED Database.” US Army Corps of Engineers. 2023. https://ered.el.erdc.dren.mil/.

USEPA. 2023a. “CompTox Chemicals Dashboard Chemical Lists.” United States Environmental Protection Agency. 2023. https://comptox.epa.gov/dashboard/chemical-lists.

USEPA. 2023b. “Region 5 RCRA Corrective Action, Ecological Screening Levels.” USEPA, Region 5 Waste, Ecological Data. 2023. https://archive.epa.gov/region5/waste/cars/web/html/esl.html.

USEPA. 2023c. “The EPA National Library Catalog | EPA National Library Network.” 2023. https://cfpub.epa.gov/ols/catalog/advanced_full_record.cfm?&FIELD1=SUBJECT&INPUT1=Bases&TYPE1=EXACT&LOGIC1=AND&COLL=&SORT_TYPE=MTIC&item_count=197.

USEPA, OA. 2013. “About the Office of Water.” Overviews and Factsheets. January 29, 2013. https://www.epa.gov/aboutepa/about-office-water.

USEPA, OCSPP. 2014. “TSCA Work Plan Chemicals.” Reports and Assessments. March 14, 2014. https://www.epa.gov/assessing-and-managing-chemicals-under-tsca/tsca-work-plan-chemicals.

USEPA, OCSPP. 2017. “Prioritizing Existing Chemicals for Risk Evaluation.” Overviews and Factsheets. United States Environmental Protection Agency. June 21, 2017. https://www.epa.gov/assessing-and-managing-chemicals-under-tsca/prioritizing-existing-chemicals-risk-evaluation.

USEPA, OCSPP. 2022a. “Ecological Structure Activity Relationships (ECOSAR) Predictive Model.” Data and Tools. 2022. https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model.

USEPA, OCSPP. 2022b. “Predictive Models and Tools for Assessing Chemicals under the Toxic Substances Control Act

(TSCA).” 2022. https://www.epa.gov/tsca-screening-tools.

USEPA, OCSPP. 2023a. “EPI SuiteTM-Estimation Program Interface.” Data and Tools. United States Environmental Protection Agency. 2023. https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

USEPA, OCSPP. 2023b. “OncoLogicTM – An Expert System to Evaluate the Carcinogenic Potential of Chemicals.” Data and Tools. United States Environmental Protection Agency. 2023. https://www.epa.gov/tsca-screening-tools/oncologictm-expert-system-evaluate-carcinogenic-potential-chemicals.

USEPA, OCSPP. 2023c. “Overview of Risk Assessment in the Pesticide Program.” Overviews and Factsheets. 2023. https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/overview-risk-assessment-pesticide-program.

USEPA, ORD. 2015a. “Regional Screening Levels (RSLs).” Data and Tools. September 10, 2015. https://www.epa.gov/risk/regional-screening-levels-rsls.

USEPA, ORD. 2015b. “Regional Ecological Risk Assessment (ERA) Supplemental Guidance.” Reports and Assessments. September 28, 2015. https://www.epa.gov/risk/regional-ecological-risk-assessment-era-supplemental-guidance.

USEPA, ORD. 2015c. “Biological Technical Assistance Group (BTAG) Screening Values.” Collections and Lists. September 29, 2015. https://www.epa.gov/risk/biological-technical-assistance-group-btag-screening-values.

USEPA, ORD. 2017a. “ToxCast Owner’s Manual – Guidance for Exploring Data.” Data and Tools. United States Environmental Protection Agency. October 25, 2017. https://www.epa.gov/chemical-research/toxcast-owners-manual-guidance-exploring-data.

USEPA, ORD. 2017b. “ToxCast Data: Accessing ToxCast Data and Scenarios for Exploring Data.” Data and Tools. United States Environmental Protection Agency. November 1, 2017. https://www.epa.gov/chemical-research/toxcast-data-accessing-toxcast-data-and-scenarios-exploring-data.

USEPA, ORD. 2023d. “Integrated Risk Information System.” Reports and Assessments. 2023. https://www.epa.gov/iris.

USEPA, ORD. 2023e. “Provisional Peer-Reviewed Toxicity Values (PPRTVs).” Collections and Lists. 2023. https://www.epa.gov/pprtv.

USEPA, ORD. 2023f. “Toxicity Estimation Software Tool (TEST).” Data and Tools. United States Environmental Protection Agency. 2023. https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test.

USEPA, ORD. 2023g. “Toxicity Forecasting.” Overviews and Factsheets. United States Environmental Protection Agency. 2023. https://www.epa.gov/chemical-research/toxicity-forecasting.

USEPA, OSWER. 2009. “Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part F, Supplemental Guidance for Inhalation Risk Assessment).” January 2009. https://rais.ornl.gov/documents/RAGS_F_EPA540R070002.pdf.

USEPA, OSWER. 2013. “Tier 3 Toxicity Value White Paper.” May 16, 2013. https://www.epa.gov/sites/default/files/2015-11/documents/tier3-toxicityvalue-whitepaper.pdf.

USEPA, OW. 2018. “2018 Edition of the Drinking Water Standards and Health Advisories Tables.” March 2018. https://www.epa.gov/system/files/documents/2022-01/dwtable2018.pdf.

USEPA, OW. 2022a. “National Recommended Water Quality Criteria Tables.” Data and Tools. 2022. https://www.epa.gov/wqc/national-recommended-water-quality-criteria-tables.

USEPA, OW. 2022b. “Contaminant Candidate List 5 – CCL 5.” Other Policies and Guidance. October 21, 2022. https://www.epa.gov/ccl/contaminant-candidate-list-5-ccl-5.

USEPA, OW. 2023h. “Drinking Water Health Advisories (HAs).” Collections and Lists. 2023. https://www.epa.gov/sdwa/drinking-water-health-advisories-has.

USEPA, OW. 2023i. “Ground Water and Drinking Water.” Collections and Lists. 2023. https://www.epa.gov/ground-water-and-drinking-water.

VEGA HUB. 2023. “Virtual Models for Property Evaluation of Chemicals within a Global Architecture.” 2023. https://www.vegahub.eu/.