

Minnesota's Aquatic Toxicity Profiles

Methods and application



Minnesota Pollution Control Agency

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Abbreviations

ATP	Aquatic toxicity profile
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service
CTD	Comparative Toxicogenomics Database
ECOSAR	Ecological structure activity relationships
EDSP	Endocrine Disruptor Screening Program
EPA	U. S. Environmental Protection Agency
HBV	Health based value
HC5	5% hazard concentration – concentration that affects 5% of species
HD5	5% hazard dose – dose that affects 5% of species
HQ	Hazard quotient
HRL	Health Risk Limit
ICE	Interspecies correlation estimation
K_{ow}	Octanol-water partition coefficient
K_{oc}	Organic carbon-water partition coefficient
LC50	Concentration that is lethal to 50% of individuals tested
LOEC	Lowest observed effect concentration
LRAT	Long-range atmospheric transport
LTV	Lowest toxicity value
MDH	Minnesota Department of Health
MPCA	Minnesota Pollution Control Agency
NOAEL	No observed adverse effect level
NOEC	No observed effect concentration
OECD	Organization for Economic Co-operation and Development
P2	Pollution prevention
PBT	Persistent, bioaccumulative, toxic
PNEC	Predicted no-effect concentration
RAA	Risk Assessment Advice
SSD	Species sensitivity distribution
SW	Saltwater
t_{1/2}	Half-life

Introduction

For several years, the Minnesota Pollution Control Agency (MPCA) has been collecting occurrence data for a highly diverse set of contaminants that includes pharmaceuticals and personal care products, flame retardants, and industrial chemicals. Many of these contaminants have been detected at low concentrations in the aquatic environment across all of Minnesota.

These contaminants may have a variety of adverse impacts on aquatic life including the ability to disrupt the endocrine system or other biological systems. However, toxicity data and associated regulatory or screening values for many, if not most, of these contaminants is lacking, which makes it difficult to put the occurrence data into context. This has made it challenging to characterize the potential impact of these contaminants to aquatic life.

The MPCA wanted a way to characterize the available contaminant monitoring data in order to make informed decisions about its water quality, pollution prevention, and monitoring programs. To that end, it was necessary to develop a process to evaluate the Minnesota occurrence data the MPCA and others have been collecting for years. The aquatic toxicity profile (ATP) developed by the MPCA will be used to characterize the potential for contaminants detected in Minnesota's environment to cause adverse effects to aquatic life.

ATPs use a weight-of-evidence approach to gain a broad understanding of the potential impacts associated with the presence of specific contaminants in the aquatic environment. ATPs differ from the standard approach used to set regulations in many ways. The ATP is a non-regulatory screening tool that uses the precautionary principle. In other words, this is a conservative approach that is more likely to overestimate potential effects, rather than possibly overlooking effects.

For MPCA's purposes, the ATPs focus on chemicals that have been monitored and detected in Minnesota waters. The goal is to determine the contaminants of highest concern, when compared to other contaminants. The MPCA does not have the funding or resources to monitor or pursue the ever-growing number of contaminants that may be found in the environment. ATPs are a useful tool to screen and prioritize contaminants based on their likely environmental impacts. While MPCA is focused on evaluating contaminants that have been detected in Minnesota's waters, the ATP methodology may also be applied to contaminants that have not been monitored.

What is aquatic life?

The term 'aquatic life' includes all organisms that reside in water for all or most of their life such as fish, aquatic invertebrates, and plants. It also includes generally terrestrial organisms such as amphibians, aquatic reptiles, birds, and mammals that rely on aquatic systems in some way - either as a source of food, habitat, or for the completion of some portion of their life cycle. This holistic definition of aquatic life provides a basis for considering the potential range of species affected by contaminants in Minnesota.

What are aquatic toxicity profiles?

ATPs provide a broad overview of chemical-specific information including physicochemical properties, occurrence, toxicity, and production/importation volume. The information compiled in the ATP will be used to prioritize chemicals for monitoring and for making chemical-specific recommendations for follow-up. The results of the ATP are not regulatory in any fashion. While MPCA will focus on compounds that have been detected in Minnesota, these methods could be adapted to accommodate other uses.

Methods

The ATP process is a rapid assessment of the available information relevant to each contaminant. Information sources may include publicly available databases, modeling tools, and limited (i.e., non-exhaustive) literature and internet searches. While guidelines are in place for completing the ATP, there may be situations where the instructions do not apply and best professional judgment is required. In these situations, the author of the ATP will clearly explain their use of professional judgment in the worksheet and/or the summary profile.

Each ATP consists of two parts: a worksheet (Attachment A) and a summary profile (Attachment B). The worksheet is used to capture relevant information available primarily from publicly available models and databases. It is intended to facilitate a rapid screening-level assessment for each subject chemical. It is not an exhaustive literature search. Links are included for ease of use, as are guidelines for interpretation of findings. The summary profile provides a brief description of the information captured in the worksheet, including the subject chemical's ranking in terms of priority for follow-up.

Both parts of the ATP are publicly available and will be posted to MPCA's external website. However, the summary profile will likely be most useful as a communication and decision-making tool.

Worksheet instructions

Prior to completing a new worksheet, save the template under a new name. Templates are best saved according to: subject contaminant, author's last name, and date. For example: Chemical_Author_MMDDYY. Basic instructions and links are also in the worksheet for ease of use.

Contaminant properties

The U. S. Environmental Protection Agency (EPA's) EPI (Estimation Programs Interface) Suite™ (EPA 2012b) is a collection of physicochemical property and environmental fate models that is available as a free download (<https://www.epa.gov/tsca-screening-tools/epi-suite™-estimation-program-interface#download>). It is a screening-level tool that is well-suited for use in the ATP process. It is very easy to use, requiring only a single input (e.g. Chemical Abstracts Service (CAS) number, chemical name, or SMILES notation). Please note that metals and inorganics in general are typically not suitable for modeling in EPI Suite™. The intended application of EPI Suite is organic chemicals.

The CAS number is the preferred way to search for contaminant information. This will ensure that information is gathered for the right chemical (although, diligence should be used to verify the CAS number used, as there are instances where multiple CAS numbers exist for a chemical, or the CAS number has changed over time). CAS numbers can be readily obtained on the internet. Relevant properties are entered into Table 1 and interpreted using the guidelines described below. The guidelines described below are commonly used, primarily coming from an internationally harmonized classification system (OECD 2001).

Table 1. Physical-chemical properties (EPI Suite™)

Property	Value	Units	Interpretation
Molar mass		g/mol	-
Solubility		mg/L	
log K _{ow}		--	
log BAF		--	
log BCF		--	
log K _{oc}		--	
Henry's Law Constant		atm·m ³ /mol	
Half-life in water			
Half-life in sediment			
Half-life in air			
Half-life in soil			
Predicted to readily biodegrade?		--	
PBT?		--	

Guidelines for interpretation of Table 1:

A chemical will be considered to have the potential to accumulate in biota and/or sediment if it has measured or predicted partitioning properties that exceed the following guidelines:

Bioaccumulation potential

- Log K_{ow}, log BAF, or log BCF ≥ 4

Sediment accumulation potential:

- Log K_{oc} ≥ 3

Interpretation of half-lives in water, sediment and soil (Degradation)

A chemical will be considered persistent if it has measured or predicted half-lives (t_{1/2}) that exceed the following guidelines:

Abiotic degradation half-life thresholds

- t_{1/2} in water > 2 months
- t_{1/2} in sediment > 6 months
- t_{1/2} in soil > 6 months

Additionally, if the chemical is not predicted to be readily biodegradable, as determined in EPI Suite, the chemical will be determined to be persistent.

Biotic degradation threshold

- EPI Suite determination that chemical is not predicted to readily biodegrade

A finding of moderate or high volatility coupled with an atmospheric half-life greater than two days is an indication that long-range atmospheric transport (LRAT) is possible and may be considered in the overall evaluation of the contaminant in the environment. Contaminants that may be susceptible to LRAT may be candidates for air deposition modeling, which can be used when selecting monitoring sites.

Atmospheric half-life threshold

- t_{1/2} in air > 2 days

Volatility (Henry's Law constant)

- Non-volatile: ($< 3 \times 10^{-7}$ atm m³/mol)
- Low volatility: (3×10^{-7} to 1×10^{-5} atm m³/mol)
- Moderate volatility: (1×10^{-5} to 1×10^{-3} atm m³/mol)
- High volatility: ($> 1 \times 10^{-3}$ atm m³/mol)

LRAT potential

- $t_{1/2} > 2$ days + moderate to high volatility

If the contaminant meets the criteria above for persistence and bioaccumulation and also falls into Category 1 or 2 for toxicity (Table 7) then it is designated persistent, bioaccumulative, and toxic (PBT). A chemical may also be designated as being any combination of these attributes (e.g., not P or B, but T).

Enter the interpretation for each value in the Interpretation column of Table 1. This information will be used to answer questions later in the worksheet.

Environmental occurrence

Search available databases, reports, and peer-reviewed literature to determine if the contaminant has been detected in Minnesota surface waters, sediment, or biota. Links to monitoring data or reports can be found on our ATP [webpage](#).

If the contaminant has been detected, complete Table 2 by filling in the highest concentration detected for that media. Some useful links are included for convenience. Using these links does not indicate that a complete and exhaustive search was conducted. A brief internet search for available literature should also be conducted.

The original focus of the ATPs is on contaminants that have been detected in Minnesota. As such, it was not anticipated that there would be contaminants that had no environmental occurrence data for Minnesota. However, these methods can be adapted to accommodate situations where the contaminant has not been detected. When the contaminant has been analyzed but not detected, the detection limit could be used as a basis for comparison to toxicity. That is, the detection limit could be treated as the detected concentration. If the toxicity of a contaminant is greater than the detection limit, and the contaminant has been analyzed but not detected, then adverse effects are not expected based on the available data for environmental concentrations.

Another adaptation could be made when a contaminant has not been monitored in Minnesota. Table 2 could be left blank, and the priority level question of "Do detected concentrations in MN exceed toxicity?" could simply be removed from the evaluation.

Table 2. Occurrence of contaminant in Minnesota's environment

Media	Water (µg/L)	Sediment (mg/kg)	Biota (ng/g ww) (species)
Maximum concentration (Source)			

Toxicity

The first step in the process to assess the toxicity of the subject contaminant is to conduct a brief internet search for benchmarks or PNECs (predicted no effect concentrations). These risk-based toxicity values can typically be found in both peer-reviewed literature and government documents, including international governments. Record any existing freshwater benchmarks or PNECs in Table 3. Add as

many rows as necessary to accommodate the number of values found. Include sources for all values. If values are available, the toxicity data used to derive the value should be entered into Table 4. Cite all data sources and include full citation in the References section.

Table 3. Benchmarks or PNECs

Type	Water (µg/L)	Sediment (mg/kg dw)	Tissue (ng/g ww)	Secondary poisoning (mg/kg -bw)	Source

In addition to searching for benchmarks and PNECs, conduct a search in EPA’s ECOTOX (https://cfpub.epa.gov/ecotox/quick_query.htm) for aquatic toxicity data. Toxicity information found in ECOTOX (and from other literature sources) are referred to as “measured” toxicity values for the purpose of this document, in that they were calculated from toxicity testing, and not estimated from a computer program.

If the contaminant is bioaccumulative (as determined in Table 1), also search for terrestrial toxicity data. Chemicals that are not bioaccumulative are less likely to appreciably accumulate in biota, and therefore less likely to elicit effects in organisms that consume biota. Therefore, when the contaminant is not bioaccumulative, toxicity to terrestrial organisms are not included in the ATP.

The European Chemicals Agency also has a compilation of registration dossiers which include an array of information about the chemical of interest, including ecological toxicity data (<https://echa.europa.eu/information-on-chemicals/registered-substances>). The toxicological studies in the database have been evaluated, and many of them indicate that the studies are acceptable for use in regulatory decision-making. Record these endpoints in Table 4, and cite the source.

Record the lowest acute and chronic toxicity values for as many species (including aquatic plants and algae) as possible. For example, if there are ten *Daphnia magna* studies, five fathead minnow studies, and one rainbow trout study, record the lowest acute and chronic values for *D. magna* and fathead minnow, as well as the single value for rainbow trout. Be sure to use values from studies with valid endpoints (e.g. LC50, EC10, NOEC, etc.) Do not use endpoints such as bioconcentration factor (BCF). Record this information in Table 4, adding as many rows as necessary to accommodate the toxicity data found. Cite all data sources and include full citation in the References section.

After looking in ECOTOX, do a brief internet search for any additional aquatic and terrestrial toxicity data and enter those values in Table 4. Again, if multiple values are available for the same species, choose the lowest acute and chronic toxicity values.

Table 4. Measured toxicity values – ECOTOX or literature

Species	Endpoint	Outcome	Concentration (units)	Source	Used in ICE?

Ideally, measured toxicity data will be used to evaluate the potential of each contaminant to cause adverse effects in the environment. If acute toxicity data are available, EPA’s web program, the Interspecies Correlation Estimation (ICE), can be used to estimate the acute toxicity of untested species (Raimondo et al. 2015). This tool can be used for both aquatic species and terrestrial wildlife

(mammalian and avian) species. The web version of ICE is available for use online (<https://www3.epa.gov/webice/>). Modeled data (such as those values that are modeled in ecological structure activity relationships (ECOSAR) are *not* appropriate for use in ICE (Barron et al. 2012).

ICE can be used with only one acute value, for a species that is modeled in ICE. Not all test species are modeled in ICE, so it may happen that acute toxicity data are available, but the species are not modeled in ICE, and therefore, an ICE estimate cannot be calculated. In this case, indicate in Table 4 that the acute value was not used in ICE, and use the lowest toxicity value (LTV) in Table 7.

Use ICE to complete Table 5, if measured *acute* toxicity data are available to do so (Table 4). Using the available measured acute toxicity value(s), the toxicity of multiple species can be estimated in one batch to create a species sensitivity distribution (SSD). From this distribution, a 5% hazard concentration/dose (HC/HD5) value can be calculated. The HC or HD5 is the concentration or dose from the SSD that is not expected to affect 95% of the species in the SSD. The SSD will likely include saltwater species in the extrapolation. Be sure to uncheck these species before accepting the HC5. Record the HC5 for aquatic species and HD5 for terrestrial wildlife species (if applicable), and record the 95% confidence interval for each. The acute HC5 or HD5 value generated by ICE should be used to determine a chemical's overall acute toxicity category whenever possible (Table 7).

If the chemical of concern is an herbicide or if measured or estimated toxicity values indicate that algae or plants are the most sensitive species, an SSD using algae (if measured toxicity values are available) should be completed within the aquatic life SSD module.

Table 5. Predicted HC/HD5 values, with 95% confidence intervals (ICE)

Species	HC5 (µg/L) or HD5 (mg/kg-bw)	95% Confidence Interval (µg/L or mg/kg-bw)
Aquatic		
Terrestrial wildlife		
Algae (if applicable)		

It is likely that measured toxicity data will be unavailable for many contaminants. When measured acute and/or chronic data are not available for aquatic organisms, modeled toxicity data should be used, if available. EPA's ECOSAR aquatic toxicity model is used to predict a chemical's acute and chronic toxicity to fish, aquatic invertebrates, and aquatic plants (EPA 2012a). ECOSAR software is available as a free download (<https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model>).

Certain types of chemicals are not suitable for modeling in ECOSAR. These include inorganic and organometallic chemicals and polymers, and chemicals with a molecular weight greater than 1,000 g/mol (EPA 2012a). In addition, ECOSAR is not able to account for unique properties of nanomaterials. ECOSAR is useful for modeling neutral organics, organic chemicals with excess toxicity, and surfactants.

For neutral organics, the mode of toxic action is narcosis - a reversible, drug-induced loss of consciousness. Narcosis is also referred to as baseline toxicity. Chemicals with excess toxicity and surfactants have a more specific mode of toxic action and are modeled differently than neutral organics. For more detailed information on the inner workings of ECOSAR, please see: <https://www.epa.gov/sites/production/files/2015-09/documents/ecosartechfinal.pdf>

ECOSAR is used primarily to predict toxicity to freshwater organisms. Sometimes toxicity estimates for terrestrial or saltwater species are available. Estimates for saltwater species are not typically used by the MPCA as they are not relevant to Minnesota. ECOSAR cannot be used to predict toxicity to terrestrial organisms.

If no measured aquatic toxicity data are available, use ECOSAR to complete Table 6. Searching by CAS number is the most efficient and accurate way to search in ECOSAR. Enter the lowest acute value and lowest chronic value and record the taxa associated with each value. Do not use values denoted as saltwater (SW), or any values for mysids (some mysid values are not listed as SW, but any mysid values in ECOSAR are saltwater or modeled on saltwater). Indicate whether the LTV was measured or modeled in parentheses in the taxa column. For example: Fish, 96-h LC50 (modeled). Also, indicate chemical class chosen if more than one class is modeled.

Table 6. Predicted lowest toxicity values (ECOSAR – freshwater species)

Duration	Taxa	Concentration (µg/L)
Acute		
Chronic		

When all data have been collected and modeled appropriately, summarize the findings by entering the acute and chronic values into the toxicity summary table (Table 7). Aquatic acute values can be:

- The HC5 modeled in ICE
- The measured LTV if it is lower than the HC5 calculated in ICE or the HC5 cannot be calculated in ICE
- The LTV predicted in ECOSAR

Aquatic chronic values can be either

- The measured LTV
- The LTV predicted in ECOSAR

Use Figure 1 to determine which aquatic life value to utilize in the summary table, Table 7.

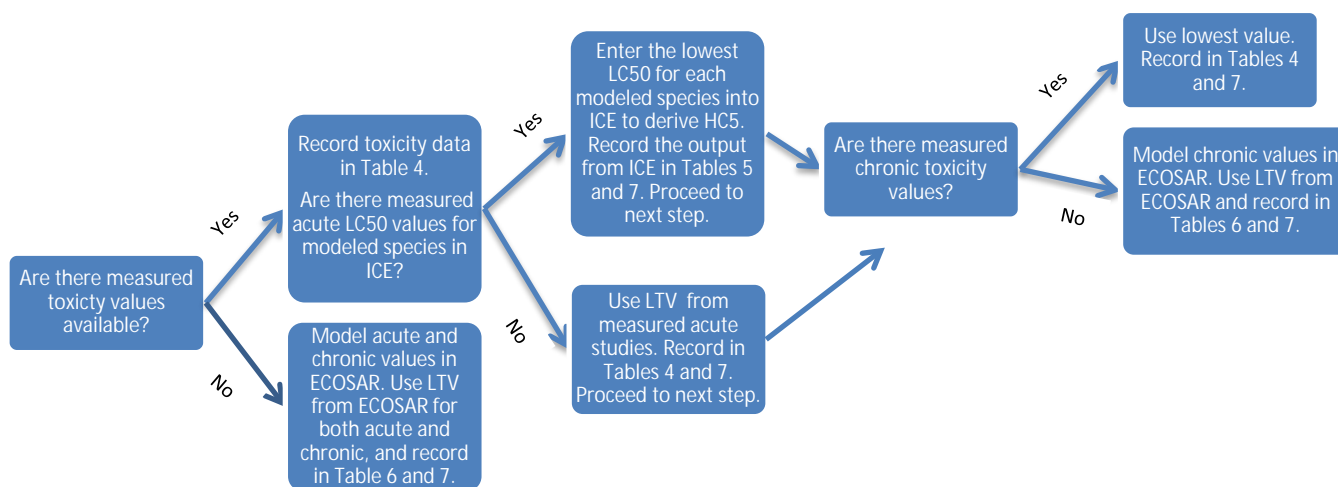


Figure 1. Decision tree for choosing aquatic life toxicity values based on available data of the subject chemical.

Terrestrial acute values can be

- The HD5 modeled in ICE
- The LTV, if it is lower than the HD5 or the HD5 cannot be calculated

Use Figure 2 to determine which value to utilize. Terrestrial chronic values require a measured LTV. If no measured toxicity data are available for terrestrial organisms, indicate "N/A" in Table 7 for the terrestrial toxicity values.

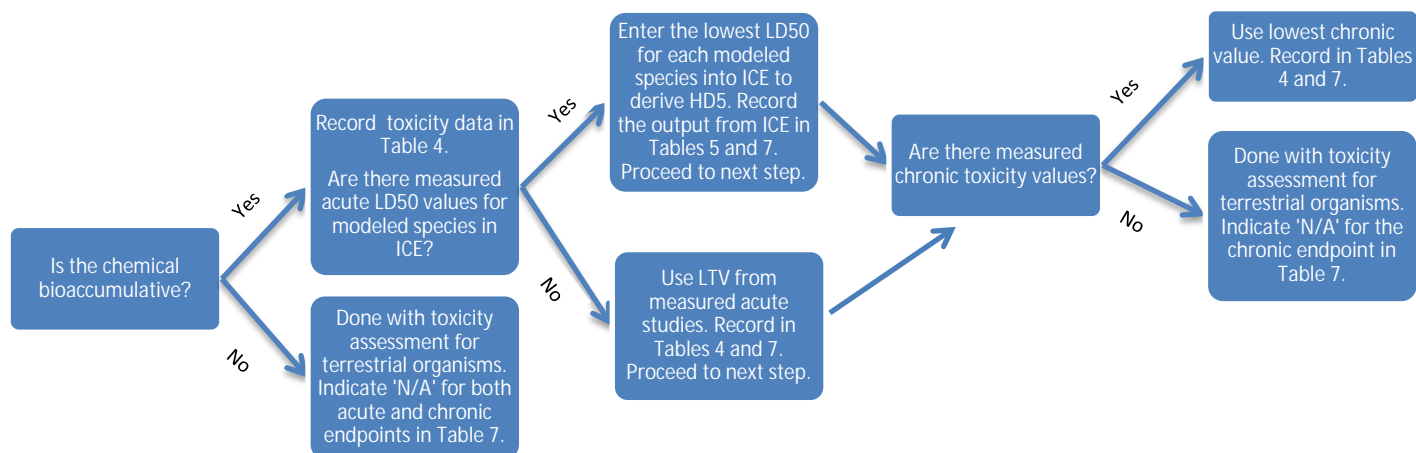


Figure 2. Decision tree for choosing terrestrial life toxicity values based on available data and properties of the subject chemical.

The toxicity values in Table 7 are used to determine whether a contaminant is toxic as defined in the guidelines given below. A contaminant will be considered toxic if either the acute HC/HD5, and/or the acute or chronic LTV falls into either category 1 or 2 of the corresponding guidelines.

Table 7. Toxicity summary

	Toxicity Value (units)	ICE, measured LTV, or ECOSAR?	Toxicity Category
Aquatic acute			
Aquatic chronic			
Terrestrial acute			
Terrestrial chronic			

N/A = Not available

Guidelines for interpretation of toxicity data in Table 7:

Interpretation of acute values for aquatic life (ICE, measured LTV or ECOSAR):

- $\leq 1,000 \mu\text{g/L}$ = Very toxic, Acute category 1
- $> 1,000$ to $\leq 10,000 \mu\text{g/L}$ = Toxic, Acute category 2
- $> 10,000$ to $\leq 100,000 \mu\text{g/L}$ = Harmful, Acute category 3
- $> 100,000 \mu\text{g/L}$ = Not classified, Acute category 4

Interpretation of chronic values for aquatic life (measured LTV or ECOSAR):

- $\leq 10 \mu\text{g/L}$ = Very toxic, Chronic category 1
- > 10 to $\leq 1,000 \mu\text{g/L}$ = Toxic, Chronic category 2
- $> 1,000$ to $\leq 10,000 \mu\text{g/L}$ = Harmful, Chronic category 3
- $> 10,000 \mu\text{g/L}$ = Not classified, Chronic category 4

Interpretation of acute values for terrestrial wildlife (measured LTV or ICE):

- $\leq 5 \text{ mg/kg-bw}$ = Very highly toxic, Acute category 1
- > 5 to $\leq 50 \text{ mg/kg-bw}$ = Highly toxic, Acute category 2
- > 50 to $\leq 300 \text{ mg/kg-bw}$ = Moderately toxic, Acute category 3

- > 300 to ≤ 2,000 mg/kg-bw μg/L = *Slightly toxic, Acute category 4*
- > 2,000 mg/kg-bw = *Practically nontoxic, Acute category 5*

Interpretation of chronic values for terrestrial wildlife (measured LTV):

- ≤ 0.05 mg/kg-bw = *Very highly toxic, Acute category 1*
- > 0.05 to ≤ 0.5 mg/kg-bw = *Highly toxic, Acute category 2*
- > 0.5 to ≤ 3 mg/kg-bw = *Moderately toxic, Acute category 3*
- > 3 to ≤ 20 mg/kg-bw μg/L = *Slightly toxic, Acute category 4*
- > 20 mg/kg-bw = *Practically nontoxic, Acute category 5*

The classifications of acute toxicity described above are commonly used, coming from an internationally harmonized classification system (United Nations 2003; OECD 2001). Harmonized classification systems for chronic effects are not available for use, so the categories used for chronic values were derived from the acute categories. Chronic effects typically occur at concentrations lower than acute effects, and many studies have evaluated the ratio between acute and chronic effects. The acute-to-chronic ratio varies depending upon the species and chemical tested, and can encompass a wide range of values. An acute-to-chronic extrapolation of 100 has been demonstrated to be protective for greater than 90% of evaluated chemicals, while an acute-to-chronic extrapolation of 10 may only be protective for approximately 50% of chemicals (May et al. 2016). Similar results have been reported, with a 90th percentile of ACRs close to 100 (73-80) (Lange et al. 1998, Raimondo et al. 2007). Therefore, to err on the side of caution, an acute-to-chronic conversion of 100 was used in this preliminary screening.

Endocrine disruption

Some contaminants may disrupt the endocrine system of organisms at concentrations lower than what may cause overt toxic effects like death or decreased growth. Therefore, the screening review process includes a review of any potential endocrine effects. The Endocrine Disruptor Screening Program (EDSP) was developed by the EPA to assess chemicals for the potential to affect endocrine pathways, and uses a tiered approach for evaluating chemicals. Currently, a limited number of chemicals have been assessed under the Tier I analysis, but some high-throughput assays have been completed on a much larger number of chemicals.

Search the EDSP database (<http://actor.epa.gov/edsp21/>) using the CAS number. Select the “Bioactivity Summary” tab. Count the number of active assays in each category (i.e., estrogen, androgen, or thyroid) and record in Table 8. Any activity in any of these assays will be considered evidence of potential for endocrine disruption.

Search the list of chemicals that have undergone Tier I EDSP testing to determine if complete Tier I results are available (<https://www.epa.gov/endocrine-disruption/endocrine-disruptor-screening-program-tier-1-screening-determinations-and>). If Tier I results are available for the compound, add a brief overview of the results of the appropriate tests in Table 8. To do this, scan the executive summary and indicate if there was information available that the compound interacts with the estrogen, androgen or thyroid pathways, and whether EPA recommended Tier II testing. Any activity in any of these assays is considered evidence of potential for endocrine disruption.

Table 8. EPA Endocrine Disruptor Screening Program (EDSP)

Screened in EDSP?	
Number of active estrogen assays	
Number of active androgen assays	
Number of active thyroid assays	
Tier I assessment completed?	

A literature search should also be conducted to determine whether any *in vivo* testing has been conducted that would provide evidence of potential for endocrine activity. Any literature should be recorded in Table 9.

Table 9. Evidence of endocrine activity in peer-reviewed literature

Species	Endpoint	Outcome	Concentration (units)	Source

Hazard quotients

A hazard quotient (HQ) can be used as a quick reference to determine whether the contaminant is present in the environment at levels that are higher or lower than the level that is expected to cause toxicity. To calculate a HQ, simply divide the maximum detected concentration (Table 2) by the toxicity value (Table 7) from the same media. If there are documented *in vivo* studies that indicate clear endocrine disruption results (Table 9), a HQ for endocrine effects may also be calculated. Record any calculated HQs in Table 10. Add as many rows as necessary to accommodate HQs for various media and effects.

If data for measured concentrations of the contaminant in fish tissue are available (Table 2), an HQ can be calculated to assess whether the tissue concentration may be at a level that poses a risk to fish. Ideally, the fish tissue concentration that is toxic to fish would be obtained from a peer-reviewed study. However, these studies are sparse and measured data are unlikely to be readily available for most contaminants. If no data are available, the aquatic toxicity values in Table 7 can be converted to a toxic tissue value using the bioaccumulation factor (BAF) (not the log BAF). Table 1 contains the log BAF, which can be converted to the BAF by raising the base to the power of 10. Multiplying the aquatic toxicity value by the BAF will give you a tissue concentration in units of ng/g. This value can be compared to measured fish tissue data to determine the HQ.

Terrestrial chronic doses cannot be compared directly to measured tissue concentrations. However, the toxic dose can be converted to a concentration using a conversion factor that accounts for body weight and daily food intake of relevant species (Attachment C). To convert the toxic dose to a concentration, simply multiply the dose by the appropriate conversion factor, which will change the units from a dose format (mg/kg – bw) to a concentration format (mg/kg). Upon conversion, an HQ can then be calculated using the measured concentration in fish tissue and the converted concentration. This HQ can be used to assess whether measured chemical concentrations in tissue are likely to harm terrestrial wildlife that consume biota.

If the HQ is > 1, the likelihood of adverse effects is increased. If the HQ is < 1, the likelihood of adverse effects is lower. A significant exceedance of an HQ over 1 may elevate the priority of the contaminant, particularly if the contaminant was determined to be of low or intermediate priority. Likewise, if the HQ is <1 but approaching 1, specific mention of this should be made in environmental implications section. Given other findings in the profile, an HQ close to 1 may elevate the priority of the contaminant. The magnitude of the HQ should be explicitly described in the environmental implications section of the summary profile. Specific recommendations in the summary profile may be determined by the magnitude of the HQ.

Table 10. Hazard quotients

Type of Toxicity Value	Toxicity Value (units)	Maximum Detected Concentration (units)	Resulting Hazard Quotient	Media

Production volume

A high production volume chemical is defined by the EPA as any chemical that is produced in or imported to the U.S. at a rate of at least 1 million pounds per year. It is assumed that chemicals with higher production volumes are more likely to be detected in the environment. Both the EPA and OECD have list of high production volume chemicals. If the subject chemical is on one of these lists, then answer “yes” to the high production volume question in Table 11. If the chemical is not on these lists, do a brief internet search of sales and production data. If production or importation is less than 1 million pounds per year, then answer “no”. The production volume, if less than 1 million pounds per year, may be recorded in the supplemental information section of the worksheet.

EPA high production volume chemicals list:

https://iaspub.epa.gov/sor_internet/registry/substreg/list/details.do?listId=74

[EPA HPV Challenge Program](#) (reviews of high production volume chemicals)

OECD high production volume chemicals list:

[http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono\(2009\)40&doclanguage=en](http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2009)40&doclanguage=en)

Priority level

The priority level is set for each chemical by completing Table 11 using information collected in the worksheet. The findings in this table can also be summarized in bullet points in the environmental implications section of the summary profile. Priority in the context of an ATP simply refers to the level of concern associated with one contaminant as compared to another, based on physicochemical properties, effects (e.g., toxicity and endocrine activity), and occurrence information. Assigning any priority level to a contaminant does not imply any specific action will be taken, only that a screening-level assessment of the contaminant has been completed and that a certain level of priority has been given based on the information available about the contaminant.

Each “yes” answer is given a score of 1, while each “no” answer receives a score of 0. The total score is used to determine the priority level for each chemical, as follows:

0 to 2 = low priority



3 to 4 = intermediate



5 to 6 = high priority



The colored symbol specific to each priority level (as indicated above) is placed at the top of each summary profile to provide the reader with an instant sense of where the chemical falls in terms of priority.

Table 11. Priority level

Question	Table or section	Answer (yes or no)	Score
Is the contaminant persistent in the environment?	1		
Does the contaminant have the potential to accumulate?	1		
Is the chemical toxic?	7		
Do detected concentrations in MN exceed toxicity?	10		
Is there evidence of endocrine disruption?	8 and 9		
Is this a high production volume chemical?	Production volume		
Total			
Priority level			

Supporting information

When reviewing a contaminant, record any unique properties or information that may be useful for further evaluation of the contaminant in Table 12. You may add as many rows as needed to capture the information. While this information will not be used to directly assign a priority level to the contaminant, the information may be useful in determining appropriate follow-up.

Table 12. Supporting information relevant to subject contaminant

Notes	Source

Information on the potential of a contaminant to alter gene expression (Table 13) and results from high-throughput screening assays (Table 14) should be examined and included in this section.

The Comparative Toxicogenomics Database (CTD) is a publically-available resource that compiles and centralizes scientific data and makes connections between genes/proteins and contaminants (Davis et al. 2015). While this database is geared towards human health, many genes act in similar ways in human and aquatic organisms. By understanding which genes or proteins may be affected by exposure to a contaminant, information about potential modes of toxic action may be able to be inferred. This information is used as supporting information only, as gene interactions may indicate where effects may be elicited or indicate possible modes of action, but actual effects to an organism’s growth, reproduction or survival may not be realized.

Complete a chemical search in the CTD (<http://ctdbase.org/>) using the CAS number. Record the top interacting genes in Table 13. For each of the top interacting genes, in the CTD, search by gene and scan the list of associated organisms to determine if the gene is relevant to aquatic life. For each gene, complete a Google search and/or utilize <http://www.genecards.org> to find the function of the gene. Briefly summarize this information in the Table 13.

Table 13. Top gene interactions (Comparative Toxicogenomics Database)

Gene	Function	Relevant to aquatic life?

The Toxicity Forecaster (ToxCast) is an EPA effort developed to screen large numbers of contaminants while reducing animal-based laboratory testing. Over 2,500 chemicals have been evaluated using high-throughput screening assays that expose proteins or living cells to the contaminant of concern in an automated fashion. The results of the screening assays demonstrate changes in biological activity, which can indicate potential for toxic effects. This information is used as supporting information only, as activity in a given *in vitro* assay may indicate where effects may be elicited or indicate possible modes of action, but actual effects to an organism’s growth, reproduction or survival may not be realized.

Use the CAS number to do a chemical search in the ToxCast database (<https://comptox.epa.gov/dashboard>). Assays will be sorted, first by whether or not the subject contaminant was active in that assay, and then by sensitivity. Record the top 10 active assays in Table 14. The intended target of the assay can be used to gain insight into possible adverse effects of chemical exposure. Record any relevant findings in the toxic mode of action section in the summary profile. The AC50 (the concentration at 50% of maximum activity) can be compared to environmental concentrations to provide additional context to the concentration that causes gene activation.

Table 14. Top 10 active assays from ToxCast.

Assay Name	Intended Target Family	AC50 (µg/L)

Human-health based values

While the aquatic toxicity profiles are meant to address concerns related to aquatic life, it can be useful to record the human-health based guidance values that may exist in Minnesota. The Minnesota Department of Health (MDH) has Health Risk Limits (HRLs), Health Based Values (HBVs) and Risk Assessment Advice (RAA) for contaminants found in drinking water. HRLs have been promulgated into rule, while HBVs are derived using the same methodology as HRLs, but have not been promulgated into rule yet. When the needed data are not available for development of an HBV or HRL, RAA may be developed to provide guidance. RAA may also be developed using a method that is different from published methodology.

Obtain any existing drinking water values (including HRLs, HBVs and RAA) by searching the MDH's guidance value page (<http://www.health.state.mn.us/divs/eh/risk/guidance/gw/table.html>). If more than one type of value is available for the contaminant, record the most recent value, as indicated by the subscript. For example, if HRL₉₃ and HBV₁₅ are available for the contaminant, use the HBV₁₅ value, as this indicates that the HBV was derived in 2015, and the HRL₉₃ was derived in 1993. The newest value more accurately reflects the most up-to-date science available. Record the lowest value (e.g., for chronic or cancer) for the most recent value type in Table 15.

For pharmaceuticals and pesticides, MDH has also developed water screening values, which were developed using a rapid assessment method that is more conservative (has a greater margin of safety) than values that are derived by a more in-depth assessment. The results of the assessment are not intended to be definitive estimates of risk, but to determine a lower-bound conservative water guidance value, which if exceeded in sampling results, could trigger additional evaluation of the contaminant.

Obtain any existing water screening values for pharmaceuticals (<http://www.health.state.mn.us/divs/eh/risk/guidance/dwec/pharmproj.html>) or pesticides (<http://www.health.state.mn.us/divs/eh/risk/guidance/dwec/rapidpest.html>). The values are provided in the worksheet strictly for informational purposes and will not be used in decision making within the context of the ATP.

Table 15. Minnesota's human-health based values

Type of value	µg/L

Summary profile instructions

The summary profile synthesizes the detailed information captured in the worksheet to provide the user with a broad understanding of the subject contaminant in a very rapid way. Prior to completing a new profile, save the template under a new name, preferably the same name as the corresponding worksheet. Templates should be saved according to subject contaminant.

Contaminant overview

The contaminant overview at the top of the profile provides a very brief summary of chemical-specific information including what the chemical is used for, potential environmental sources, and why there is concern or interest in that chemical.

Environmental implications

This section provides an overview of the potential adverse effects of each contaminant at environmentally-relevant concentrations. Information from the worksheet, particularly Tables 7 and 10, is provided in a bullet-point summary. Additional information from the "Supporting information" section can also be described here.

Toxic mode of action

Whenever possible, the toxic mode of action should be recorded. This information may be useful when considering potential additive effects of contaminants in a mixture. A brief internet search can be conducted to determine whether this information is available. Toxicity studies used in the worksheet will likely provide some insight. Additional clues about toxic mode of action may also be available in the following databases:

www.ctdbase.org
https://aopwiki.org/wiki/index.php/Main_Page
<http://www.genome.jp/kegg/pathway.html?sess=2764b8338258d6286de91bbebe6faf46>

Record information in bullet points in this section of the summary profile.

Relevant media for monitoring

Physicochemical properties captured in Table 1 of the worksheet are used to make recommendations regarding the most appropriate environmental media for monitoring. Some chemicals are best monitored in water. Others are more relevant to sediment and/or biota. Summarize those findings by simply stating “water”, “biota”, “sediment” or any combination of the three. The information provided in this section can be used to enhance study planning.

Are there seasonal considerations for monitoring?

Some chemicals may be present at higher concentrations in a given season. For example, chemicals used to de-ice airplanes are likely to be present at higher concentrations during winter months when ice is an issue. Knowledge of seasonality can be used to plan more focused monitoring efforts and thus, better characterize actual impacts to the environment.

Important degradates

Some chemicals may degrade to compounds that are of equal, or even greater, concern than the parent compound. Known degradates and any information about monitoring, environmental occurrence, and toxicity should be included in this section.

Recommendations for follow-up

Each ATP summary will have a recommendation for follow-up, based upon the following considerations:

- Overall priority of contaminant – a contaminant that is low priority will have different follow-up actions than a contaminant that is high priority.
- Availability of monitoring data in the state
 - Source of monitoring data – which agencies or groups are collecting monitoring data for the contaminant? Are the methods used for detection appropriate?
 - Current monitoring – is there ongoing monitoring for the contaminant by either MPCA or other agencies or groups? If other groups are routinely monitoring for the contaminant in the appropriate matrices and seasons, there is less of a need for follow-up monitoring by MPCA.
 - Amount of available monitoring data – has the contaminant been evaluated extensively, or are the studies that evaluated the contaminant limited? Recommendations may be made for additional sampling for limited datasets of contaminants with high toxicity or concern.
 - Considerations of seasonal or source impacts – do available monitoring data adequately describe potential seasonal or source impacts? If the contaminant is expected to be detected at higher levels during certain seasons, monitoring may be recommended during those times. For contaminants that are likely released at specific areas/sources, those locations may be recommended for monitoring.
 - Appropriate media monitoring – Based on physicochemical properties, have the appropriate media been monitored? For a hydrophobic or accumulative contaminant, water may not be the best media to sample, but water is the most commonly sampled media. Follow-up

- sampling could be focused on other media if it is likely that the contaminant is partitioning to another medium.
- Applicability to agency work/programs – a contaminant that is more closely tied to agency work or programs would be considered differently for follow-up than those contaminants that would have less impact on agency work or programs. Information about high priority contaminants may be shared with programs within the agency to ensure those contaminants are addressed appropriately. The contaminant may also be recommended to MDH's Contaminants of Emerging Concern program for evaluation.
 - Supporting information – information that was discovered when developing the ATP that influence the implications of the contaminant in the environment. Does the contaminant have a similar mode of action to another contaminant that it is often detected with? If many contaminants have the same mode of action, the additive effect of the mixture of compounds could affect aquatic life differently than exposure to contaminants with different modes of action.
 - Degradates – if a contaminant was demonstrated to have important degradates, those contaminants could be targeted for evaluation as well. The relative toxicity of those compounds could be considered with any other information collected about the degradates to potentially consider for additional monitoring.

How will the MPCA use the worksheet and profile?

ATPs can be used in a number of ways. Contaminants that show the greatest potential for causing harm in Minnesota's environment may be prioritized for monitoring. Recommendations will be made as to the most appropriate media for monitoring, as well as seasonal considerations, and thus will be useful in study planning.

Some contaminants may be good candidates for pollution prevention (P2) activities. Those contaminants will be referred directly to our P2 staff.

ATPs will likely be a useful internal and external communication tool. Managers can use the information in the summary profile to rapidly gain understanding of the environmental implications of specific contaminants found in Minnesota waters. That information can be readily shared with other managers, legislators, and the public.

Internally, several MPCA programs can use the ATPs to inform their work. ATPs may be useful to staff who work in P2, Stressor ID, Effluent Limits, Water Quality Standards, Closed Landfill, Emergency Response, Stormwater, and Feedlots, among others.

Requests for ATP

Anyone can request an ATP for a specific contaminant at any time by contacting the authors of this guidance. Alternatively, the worksheet is a step-by-step description of the ATP process, and could therefore be used by any interested party to develop their own ATP.

References

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- US EPA. 2012b. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. United States Environmental Protection Agency, Washington, DC, USA.

Attachment A

ATP Worksheet

Aquatic toxicity profile worksheet

Chemical information

Chemical name:

CAS number:

Date:

Author:

Table 1. Physical-chemical properties (EPISUITE)

Property	Value	Units	Interpretation
Molar mass		g/mol	-
Water solubility		mg/L	
log K _{ow}		--	
log BAF		--	
log BCF		--	
log K _{oc}		--	
Henry's Law Constant		atm·m ³ /mol	
Half-life in water			
Half-life in sediment			
Half-life in air			
Half-life in soil			
Predicted to readily biodegrade?		--	
PBT?		--	

In EPISUITE, search for the chemical by CAS number. Record the physical-chemical properties of the contaminant in Table 1 and the interpretation of the properties, using the following guidelines.

Guidelines for interpretation of Table 1:

Log K_{ow}, BAF, BCF and log K_{oc}

- Log K_{ow} is found under the KOWWIN tab. The experimentally derived value should be recorded if available, and the estimated value is recorded if it is the only available value.
- Log BAF and log BCF are found under the BCFBAF tab. Only one BAF value is available, but for the BCF, a regression-based method and Arnot-Gobas method are present. Preference is typically given to the Arnot-Gobas method, if both are available.
- Log K_{oc} is found under the KOCWIN tab. MCI and Kow methods are available, and preference is typically given to the MCI method, if both are available.

Interpretation of log K_{ow}, BAF, BCF and log K_{oc}

A chemical will be considered to have the potential to accumulate in biota and/or sediment if it has measured or predicted partitioning properties that exceed the following guidelines:

Bioaccumulation potential

- Log K_{ow}, log BAF, or log BCF ≥ 4

Sediment accumulation potential

- Log K_{oc} ≥ 3

Half-lives in water, sediment, and soil

- Water, sediment and soil abiotic degradation half-lives are found under the Fugacity tab. If necessary, convert to an easily assessed unit of time (e.g., a half-life of 8,000 hours can be converted to approximately 11 months or 333 days).
- For biotic degradation, open the BLOWIN tab. The “Ready Biodegradability Prediction” provides a yes or no answer as to whether the chemical is predicted to readily biodegrade.

Interpretation of half-lives in water, sediment and soil (Degradation)

A chemical will be considered persistent if it has measured or predicted half-lives ($t_{1/2}$) that exceeds the following guidelines:

Abiotic degradation half-life thresholds

- $t_{1/2}$ in water > 2 months
- $t_{1/2}$ in sediment > 6 months
- $t_{1/2}$ in soil > 6 months

Additionally, if the chemical is not predicted to be readily biodegradable, as determined in EPISuite, the chemical will be determined to be persistent.

Biotic degradation threshold

- EPISuite determination that chemical is not predicted to readily biodegrade

If the chemical exceeds any of the abiotic or biotic degradation thresholds, the chemical is determined to be persistent.

Half-life in air and volatility

- Atmospheric half-life is found under the Fugacity tab, as the half-life in air. If necessary, convert to an easily assessed unit of time.
- Henry's Law Constant is found under the HENRYWIN tab. Bond, Group and Experimental methods are available, and preference is typically given to the experimental data, then the Group method, and lastly the Bond method, depending on which data are available.

A finding of moderate or high volatility coupled with an atmospheric half-life greater than 2 days is an indication that long-range atmospheric transport (LRAT) is possible and should be considered in the overall evaluation of the contaminant in the environment.

Atmospheric half-life threshold

- $t_{1/2}$ in air > 2 days

Volatility (Henry's Law constant)

- Non-volatile: ($< 3 \times 10^{-7}$ atm m³/mol)
- Low volatility: (3×10^{-7} to 1×10^{-5} atm m³/mol)
- Moderate volatility: (1×10^{-5} to 1×10^{-3} atm m³/mol)
- High volatility: ($> 1 \times 10^{-3}$ atm m³/mol)

LRAT potential

- $t_{1/2} > 2$ days + moderate to high volatility

If the contaminant meets the criteria above for persistence and bioaccumulation and also falls into Category 1 or 2 for toxicity (Tables 7) then it is designated PBT. A chemical may also be designated as being any combination of these attributes (e.g., not P or B, but T).

Enter the interpretation for each value in the Interpretation column of Table 1. This information will be used to answer questions later in the worksheet.

Environmental occurrence

Table 2. Occurrence of contaminant in Minnesota’s environment

Media	Water (µg/L)	Sediment (mg/kg)	Biota (ng/g ww) (species)
Maximum concentration (Source)			

Toxicity

Table 3. Benchmarks or PNECs

Type	Water (µg/L)	Sediment (mg/kg dw)	Tissue (ng/g ww)	Secondary poisoning (mg/kg –bw)	Source

1. Perform a brief internet search to obtain any PNECs or benchmarks that have been previously derived for the contaminant. Record the values and their sources in Table 3, and provide full citations in the References section.
2. If the contaminant is a pesticide, in addition to the internet search, ensure that you search for the contaminant on the EPA’s aquatic life benchmark list for pesticides: <https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/aquatic-life-benchmarks-pesticide-registration#benchmarks>

Table 4. Measured toxicity values – ECOTOX or literature

Species	Endpoint	Outcome	Concentration (units)	Source	Used in ICE?

1. Visit https://cfpub.epa.gov/ecotox/quick_query.htm
2. Enter the CAS number in the “Chemical Entry” box
3. Under “Report Format,” select “Excel Format.”
4. Return to the top of the page and click on the “Perform Query for Aquatic Data” button.
5. Download the Excel spreadsheet and save it in the folder of the subject chemical, using the chemical name and date accessed in the file name (e.g., Chemical_ECOTOX_MMDDYY).
6. Filter the column “Media Type” to remove anything designated as “SW.”
7. Convert any endpoints that are in molar concentrations (mM, µM, M) to µg/L using the molar mass of the compound).
8. Select the entire dataset, then select “Sort & Filter” and do a custom sort. Sort first by endpoint (A to Z), then species specific name (A to Z), then mean concentrations, including those converted from molar concentrations (from smallest to largest).
9. The mean concentration may not be labeled the same way for each downloaded dataset. Sort through the available options and choose the most appropriate. Do not use endpoints such as “BCF” – only use valid toxicological endpoints such as LC50, EC10, NOEC, LOEC etc. Then hide any unneeded columns to make the data easier to view.

10. If the contaminant is bioaccumulative (as determined from the log K_{ow} , BAF or BCF in Table 1), repeat the process, but instead of clicking on the button for aquatic data, select "Perform Query for Terrestrial Data".
11. Also search by CAS number within the European Chemicals Agency's registration information: <https://echa.europa.eu/information-on-chemicals/registered-substances>. Click on the test substance below the search box, and scroll down to the section called "Regulations and regulatory activities." Click on the link to the "Registration dossier." Use the control panel on the left to obtain relevant information about the contaminant, including "Ecotoxicological information" for use in Table 4. Include all relevant toxicological studies, including acute, chronic and sediment studies.
12. Perform a brief literature search to obtain any toxicity studies, including aquatic plant/algae studies, that may be available but are not in ECOTOX.
13. Enter into Table 4 the lowest acute and chronic toxicity value for each species (for each species, there could be two values – one for acute and one for chronic). Include the endpoint (e.g., chronic EC50), the outcome (e.g., reproduction) and the units of measure. If endpoints related to endocrine disruption are included in the database, record those data in Table 9. When developing Table 5, the information about ICE will be added to Table 4. Also include aquatic plant and algae data in Table 4, if available.
14. Cite all relevant data sources and include full citation in the References section.

Table 5. Predicted HC/HD5 values, with 95% confidence intervals (ICE)

Species	HC5 (µg/L) or HD5 (mg/kg-bw)	95% Confidence Interval (µg/L or mg/kg-bw)
Aquatic		
Terrestrial wildlife		
Algae (if applicable)		

1. Visit <https://www3.epa.gov/webice/>
2. Under the "Species Sensitivity Distribution" Section, choose "ICE Aquatic."
3. For every aquatic species for which measured acute LC50 toxicity values are available (use Table 4), choose the species from the drop down menu (if the species is available), and click "Add." Indicate in Table 4 that the species used was used in ICE. If no measured toxicity data for species modeled in ICE are available, use the acute LTV from Table 4 as the aquatic acute value in Table 7.
4. In the table that is generated, enter the LC50 value for each species (in µg/L). When all toxicity data are entered, click the "Calculate SSD" button.
5. Determine if any saltwater species are included in the resulting SSD. If saltwater species are included, de-select these values by unchecking the box next to the species. The HC5 will automatically update. The following species are saltwater species used in ICE and should be removed from the estimation:

Atlantic silverside	<i>Menidia menidia</i>
Banana prawn	<i>Fenneropenaeus merguensis</i>
Bigscale mullet	<i>Chelon macrolepis</i>
Blue shrimp	<i>Litopenaeus stylirostris</i>
Calanoid copepod	<i>Acartia tonsa</i>
Eastern oyster	<i>Crassostrea virginica</i>
Harpacticoid copepod	<i>Tigriopus japonicus</i>
Harpacticoid copepod	<i>Tisbe battagliai</i>
Inland silverside	<i>Menidia berrylina</i>
Mysid	<i>Americamysis bahia</i>
Mysid	<i>Metamysidopsis insularis</i>

Pinfish
 Pink shrimp
 Polychaete
 Polychaete
 Sheepshead minnow
 Starfish
 Striped mullet
 Tidewater silverside

Lagodon rhomboides
Farfantepenaeus duorarum
Hydroides elegans
Neanthes virens
Cyprinodon variegatus
Asterias forbesi
Mugil cephalus
Menidia peninsulae

6. Record the HC5 and 95% confidence interval.
7. If the contaminant is bioaccumulative (as determined by the $\log K_{ow}$, BCF or BAF in Table 1), repeat the process from Step 1 using the "ICE wildlife" SSD module, where data are available. Input terrestrial wildlife acute LD50 values. Rat data can be used.
8. HD5 values can be thought of as secondary poisoning values, or the concentration that may be toxic to wildlife eating contaminated food (such as fish). Compare MN fish tissue data (if available) to determine whether detected concentrations may pose a risk to terrestrial wildlife.

Use Figure 1 to determine which aquatic life values to utilize in the summary table, Table 7.

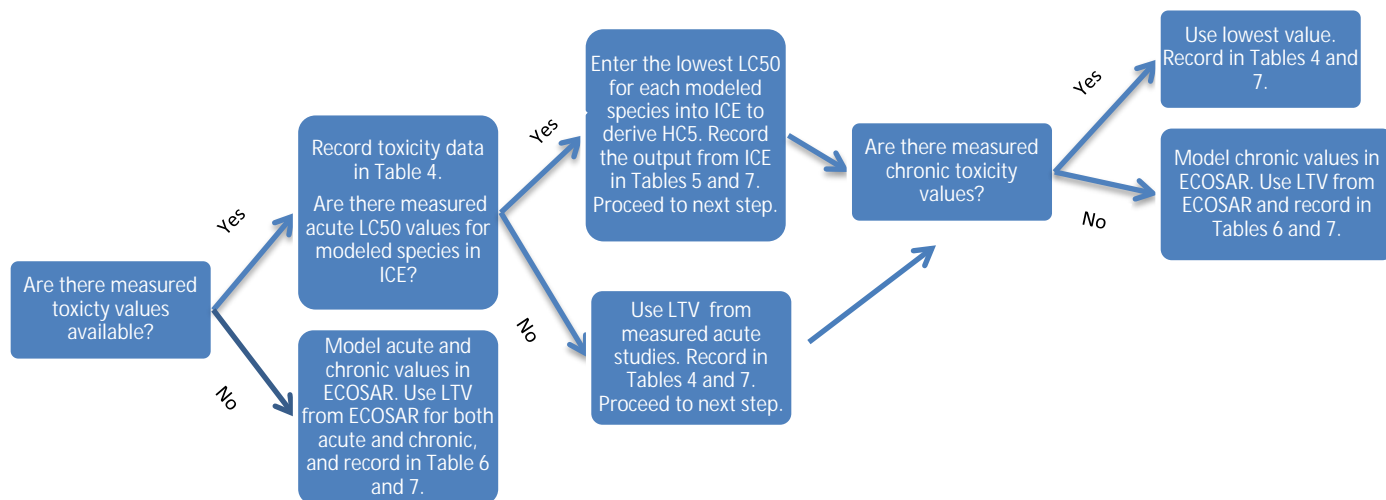


Figure 1. Decision tree for choosing aquatic life toxicity values based on available data of the subject chemical.

Use Figure 2 to determine which terrestrial toxicity value to utilize. Terrestrial chronic values require a measured LTV. If no measured toxicity data are available for terrestrial organisms, indicate "N/A" in Table 7 for the terrestrial toxicity values.

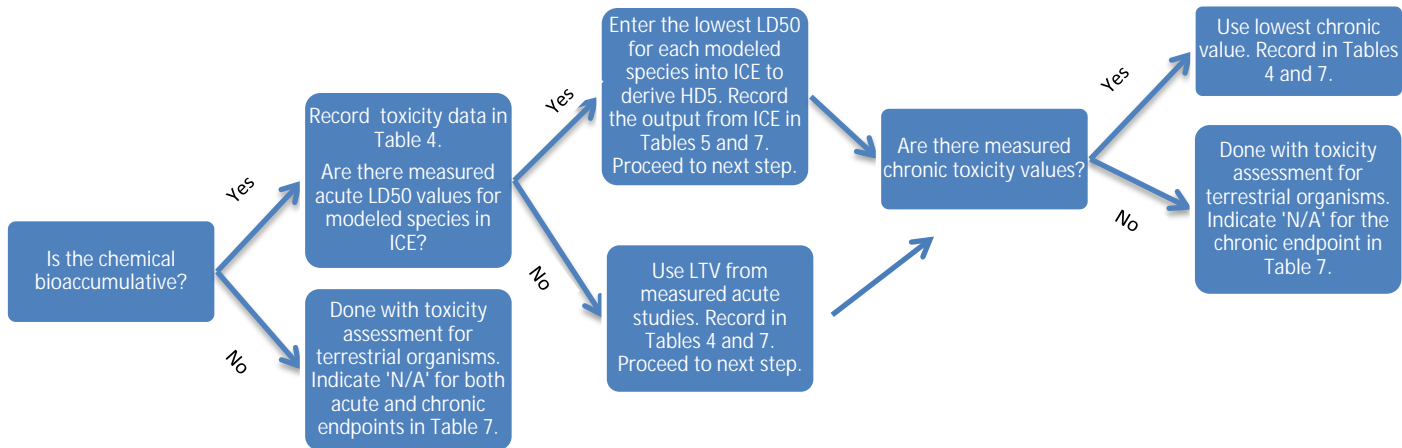


Figure 2. Decision tree for choosing terrestrial life toxicity values based on available data and properties of the subject chemical.

Table 6. Predicted lowest toxicity values (ECOSAR – freshwater species)

Duration	Taxa	Concentration (µg/L)
Acute		
Chronic		

1. Perform search in ECOSAR using CAS number.
2. Use lowest toxicity values (LTV) for both acute (LC50, EC50) and chronic (ChV) toxicity. Convert the concentration to µg/L prior to entering the values into Table 6.
3. Indicate whether LTV was measured or modeled in parentheses under "Taxa" For example: Fish, 96-h LC50 (modeled). Also indicate chemical class chosen if results for more than one chemical class are provided.
4. Use only data for freshwater species. All species in ECOSAR indicated by (SW) are saltwater species. Any data for mysids are also saltwater values (even if it is not designated with SW).

Table 7. Toxicity summary

	Toxicity Value (units)	ICE, measured LTV, or ECOSAR?	Toxicity Category
Aquatic acute			
Aquatic chronic			
Terrestrial acute			
Terrestrial chronic			

N/A = Not available

Guidelines for interpretation of Table 7:

Interpretation of acute values for aquatic life (ICE, measured LTV or ECOSAR):

- ≤ 1,000 µg/L = Very toxic, Acute category 1
- > 1,000 to ≤ 10,000 µg/L = Toxic, Acute category 2
- > 10,000 to ≤ 100,000 µg/L = Harmful, Acute category 3
- > 100,000 µg/L = Not classified, Acute category 4

Interpretation of chronic values for aquatic life (measured LTV or ECOSAR):

- ≤ 10 µg/L = Very toxic, Chronic category 1
- > 10 to ≤ 1,000 µg/L = Toxic, Chronic category 2

>1,000 to ≤10,000 µg/L = Harmful, Chronic category 3

>10,000 µg/L = Not classified, Chronic category 4

Interpretation of acute values for terrestrial wildlife (measured LTV or ICE):

≤ 5 mg/kg-bw = Very highly toxic, Acute category 1

> 5 to ≤ 50 mg/kg-bw = Highly toxic, Acute category 2

> 50 to ≤ 300 mg/kg-bw = Moderately toxic, Acute category 3

> 300 to ≤ 2,000 mg/kg-bw µg/L = Slightly toxic, Acute category 4

> 2,000 mg/kg-bw = Practically nontoxic, Acute category 5

Interpretation of chronic values for terrestrial wildlife (measured LTV):

≤ 0.05 mg/kg-bw = Very highly toxic, Acute category 1

> 0.05 to ≤ 0.5 mg/kg-bw = Highly toxic, Acute category 2

> 0.5 to ≤ 3 mg/kg-bw = Moderately toxic, Acute category 3

> 3 to ≤ 20 mg/kg-bw µg/L = Slightly toxic, Acute category 4

> 20 mg/kg-bw = Practically nontoxic, Acute category 5

Table 8. EPA Endocrine Disruptor Screening Program (EDSP)

Screened in EDSP?	
Number of active estrogen assays	
Number of active androgen assays	
Number of active thyroid assays	
Tier I assessment completed?	

1. Use the CAS number to do a chemical search in the EDSP <http://actor.epa.gov/edsp21/>.
2. Select the "Bioactivity Summary" tab.
3. Count the number of active assays in each category and enter in Table 8.
4. Search list of chemicals in Tier 1 EPA EDSP <https://www.epa.gov/endocrine-disruption/endocrine-disruptor-screening-program-tier-1-screening-determinations-and>
5. Add brief overview of Tier 1 results, if available.
6. Any activity in any of these assays will be considered evidence of endocrine activity.

Table 9. Evidence of endocrine activity in peer-reviewed literature

Species	Endpoint	Outcome	Concentration (units)	Source

Table 10. Hazard quotients

Type of Toxicity Value	Toxicity Value (units)	Maximum Detected Concentration (units)	Resulting Hazard Quotient	Media

1. Where data are available for both toxicity and detections in Minnesota from the same media (e.g., water), record in Table 10 the toxicity values and the type of value (e.g., aquatic chronic) from Table 7.
2. Record in Table 10 the maximum detected concentration from the same media (use Table 2).
3. For each type of toxicity value, calculate the HQ by dividing the maximum detected concentration by the toxicity value.

Production volume

If the subject chemical is on one of these lists, then answer “yes” to the question in Table 11.

If the chemical is not on these lists, do a brief internet search of sales and production data. If production or importation is less than 1 million pounds per year, then answer “no” to question 6.

EPA high production volume chemicals list:

https://iaspub.epa.gov/sor_internet/registry/substreg/list/details.do?listId=74

[EPA HPV Challenge Program](#) (reviews of high production volume chemicals)

OECD high production volume chemicals list:

[http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono\(2009\)40&docLanguage=en](http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2009)40&docLanguage=en)

Priority level

Each “yes” answer is given a score of 1, while each “no” answer receives a score of 0. The total score is used to determine the priority level for each chemical, as follows:

0 to 2 = low priority



3 to 4 = intermediate priority



5 to 6 = high priority



The colored symbol specific to each priority level (as indicated above) is placed at the top of each summary profile to provide the reader with an instant sense of where the chemical falls in terms of priority.

Table 11. Priority level

Question	Table or section	Answer (yes or no)	Score
Is the contaminant persistent in the environment?	1		
Does the contaminant have the potential to accumulate?	1		
Is the chemical toxic?	7		
Do detected concentrations in MN exceed toxicity?	10		
Is there evidence of endocrine disruption?	8 and 9		
Is this a high production volume chemical?	Production volume		
Total			
Priority level			

Supporting information

Table 12. Supporting information relevant to subject contaminant

Notes	Source

Table 13. Top gene interactions (Comparative Toxicogenomics Database)

Gene	Function	Relevant to aquatic life?

1. Perform a chemical search in the CTD using the CAS number <http://ctdbase.org/>.
2. On the "Basics" page, find "Top Gene Interactions" and enter the abbreviated gene name into table.
3. For each of the top 10 genes, search by gene in CTD. Click on each gene to obtain the full name of the gene, and record with the abbreviated gene name. Also, scan the list of associated organisms, under the "NCBI Gene IDs" section. If any aquatic organisms are present, answer "yes" under Relevant to aquatic life?
4. Do google search to find function of gene and disease implications (www.genecards.org often provides good summaries of gene functions). Briefly summarize in table.

Table 14. Top 10 active assays from ToxCast.

Assay Name	Intended Target Family	AC50 (µg/L)

1. Go to CompTox Dashboard at <https://comptox.epa.gov/dashboard>
2. Must use FireFox or Google Chrome. Internet Explorer will not work.
3. Enter CAS number into search bar on home page
4. Click on the "ToxCast in Vitro Data tab"
5. Scroll down the page to the "Download as:" options
6. Select Excel

7. Open the Excel table and save it in the folder of the subject chemical. Be sure to change the file extension to .xlsx. Include the chemical name and date of access in the file name. Example: *Chemical_ToxCast_MMDDYY.xlsx*
8. Click the "Sort & Filter" tab
9. Select custom sort
10. First, sort Column "Hit Call" by Order "A to Z". This will sort all Active assays to the top of the list
11. Second, sort Column "AC50" by Order "smallest to largest". This will sort assay results from most sensitive to least sensitive.
12. Click "OK"
13. Add a column to the spreadsheet called "Molar Mass". Enter the molar mass (g/mol) of the subject chemical.
14. The AC50 given in ToxCast is in units of $\mu\text{mol/L}$. Add a column called "AC50 $\mu\text{g/L}$ ". In this column multiply the AC50 ($\mu\text{mol/L}$) by the molar mass. This will convert the units of the AC50 to $\mu\text{g/L}$. Do this for the first 10 assays on the list.
15. Complete Table 14 using the data from the Excel file along with your calculated AC50.

Human-health based values

Table 15. Minnesota's human-health based values

Type of value	$\mu\text{g/L}$

1. Go to list of MDH's Health-based water guidance at <http://www.health.state.mn.us/divs/eh/risk/guidance/gw/table.html> and determine if the contaminant has a HRL, HBV or RAA. Record the lowest value of the most recently derived health-based guidance value and indicate what type (e.g., HRL) of value.
2. If there is no HRL, HBV or RAA, and the contaminant is a pharmaceutical, record the screening value from <http://www.health.state.mn.us/divs/eh/risk/guidance/dwec/pharmproj.html> and indicate the type of value is a screening value.

References

Attachment B

ATP summary profile

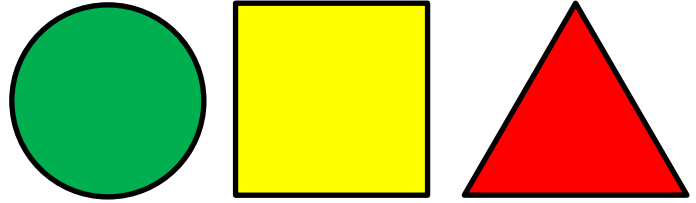
Summary profile

Chemical name:

Acronym:

CAS RN:

Use category:



Summary

Contaminant overview

Provide a very brief (3-4 sentence) overview describing: 1) what the chemical is used for, 2) potential environmental sources, and 3) why there is concern about this chemical.

Copy and paste appropriate shape in corner based on priority level determined in the worksheet: green circle = low, yellow square = medium; red triangle = high.

Environmental Implications

Summarize in bullet points the potential adverse effects of the chemical at concentrations found in the environment. At a minimum, use Table 10 and the supporting information section on the worksheet.

Toxic mode of action

Relevant media for monitoring

Water, sediment, and/or biota

Are there seasonal considerations for monitoring?

Important degradates

Known degradates and any information about monitoring, environmental occurrence, and toxicity should be included in this section.

Recommendations

Date:

Author:

Attachment C

No observed adverse effect level (NOAEL) conversion factors

Factors for converting NOAELs (dose) into NOECs (concentration)

Species	Age/study	Conversion factor (body weight/daily food intake)
Rat (<i>Rattus norvegicus</i>)	>6 weeks	20 ^a
Rat	<6 weeks	10 ^a
Rat	28 and 90 days	10 ^a
Rat	Two generation study first mating	12.5 ^a
Rat	Two generation study overall	8.3 ^a
Mouse (<i>Mus musculus</i>)	28 and 90 days	8.3 ^a
Vole (<i>Microtus spp</i>)	-	8.3 ^a
Rabbit (<i>Oryctolagus cuniculus</i>)	-	33.3 ^a
Dog (<i>Canis domesticus</i>)	Adult/all	40 ^a
Monkey (<i>Macaca spp</i>)	-	20 ^a
Chicken (<i>Gallus domesticus</i>)	-	8 ^a
Bufflehead (<i>Bucephala albeola</i>)	-	2.4 ^b
Common goldeneye (<i>Bucephala clangula</i>)	-	3.2 ^b
Mallard (<i>Anas platyrhynchos</i>)	-	4.3 ^b
Long-tailed duck (<i>Clangula hyemalis</i>)	-	3.2 ^b
Wood duck (<i>Aix sponsa</i>)	-	2.9 ^b
American wigeon (<i>Anas Americana</i>)	-	3.1 ^b
Lesser scaup (<i>Aythya affinis</i>)	-	3.1 ^b
Common merganser (<i>Mergus merganser</i>)	-	3.7 ^b
Red-breasted merganser (<i>Mergus serrator</i>)	-	4.8 ^b
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	-	9.1 ^b
Osprey (<i>Pandion haliaetus</i>)	-	5.0 ^b
Belted kingfisher (<i>Megaceryle alcyon</i>)	-	2.0 ^b
Common loon (<i>Gavia immer</i>)	-	5.6 ^b
Common tern (<i>Sterna hirundo</i>)	-	1.6 ^b
Herring gull (<i>Larus argentatus</i>)	-	3.4 ^b
Ring-billed gull (<i>Larus delawarensis</i>)	-	5.9 ^b
Great blue heron (<i>Ardea herodias</i>)	-	4.5 ^b
American mink (<i>Neovison vison</i>)	-	4.2 ^b
River Otter (<i>Lontra canadensis</i>)	-	10.0 ^b
Snapping turtle (<i>Chelydra serpentina</i>)	-	76.9 ^b
American bullfrog (<i>Rana catesbeiana</i>)	-	62.5 ^b

^aEuropean Commission (2011). Guidance Document Number 27, Technical Guidance for Deriving Environmental Quality Standards. Technical Report-2011-055 ed. Europe. European Commission.

^bCCME (1999). Protocol for the derivation of Canadian tissue residue guidelines for the protection of wildlife that consume aquatic biota. Winnipeg, Canada. Canadian Council of Ministers of the Environment. Environment Canada.