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GUIDELINES FOR
FRESH & MARINE
WATER QUALITY

Toxicant default guideline values for aquatic ecosystem protection

Atrazine in marine water

Technical brief

October 2025

DRAFT

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New Zealand Government



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Summary

The default guideline values (DGVs) and associated information in this technical brief should be used in accordance with the detailed guidance provided in the [Australian and New Zealand Guidelines for Fresh and Marine Water Quality](#) website.

Atrazine (6-chloro-N²-ethyl-N⁴-isopropyl-1,3,5-triazine-2,4-diamine, CAS No. 1912-24-9) is a selective, systemic triazine herbicide or, more specifically, a chlorotriazine herbicide. Other chlorotriazine herbicides include propazine, simazine and terbuthylazine. Atrazine is a common photosynthesis-inhibiting herbicide used to control annual broad-leaved weeds and annual grasses in a wide range of crops as well as in non-agricultural settings (e.g. forestry, utilities).

The previous Australian and New Zealand DGV for atrazine in marine environments (13 µg/L for 95% species protection) was considered to be of low reliability as it was adopted from the freshwater DGV of moderate reliability based on acute toxicity data for 23 freshwater species. There are now considerably more data available on the chronic toxicity of atrazine to marine species, including data for phototrophic species (species that photosynthesise, e.g. plants, algae), which has enabled the derivation of improved DGVs.

Atrazine has a specific mode of action (inhibition of the photosystem II pathway) and a non-specific mode of action (formation of reactive oxygen species). The available evidence indicates there is no difference in the sensitivities of phototrophs and heterotrophs. The lowest reported chronic toxicity value to marine species is 3.5 µg/L [see 'Glossary and acronyms' for definitions]). The lowest reported acute toxicity value to marine species is 94 µg/L.

Very high reliability DGVs for atrazine in marine water were derived from chronic negligible-effect values and chronic estimated-negligible-effect values for 18 marine species belonging to 8 phyla. There was a good fit of the species sensitivity distribution to the toxicity data. Note that the DGVs derived here are expressed in terms of the active ingredient (atrazine) rather than commercial formulations. The DGVs relate to atrazine only, not to any of its breakdown products. The DGVs for 99%, 95%, 90% and 80% species protection are 1.2 µg/L, 3.1 µg/L, 4.8 µg/L and 8.3 µg/L, respectively. The 95% species-protection level for atrazine, 3.1 µg/L, is recommended when assessing ecosystems that are slightly to moderately disturbed.

A multi-generational toxicity study indicated that exposure of a copepod to atrazine increases the sensitivities of at least 2 subsequent generations. This was the only multi-generational study in the literature and, while it was included in the calculation of the atrazine marine DGVs, the majority of the toxicity data exposed a single generation. Therefore, the above DGVs (at all levels of species protection) should be treated with caution as they may not provide adequate protection to organisms that are continuously exposed to atrazine for multiple generations – and one generation may be as short as 40 days for short-lived organisms.

1 Introduction

Atrazine ($C_8H_{14}ClN_5$; Figure 1) is a selective, systemic herbicide (BCPC 2012) that belongs to the chlorotriazine group within the triazine family of herbicides. This group also includes propazine, simazine and terbuthylazine. It is the active ingredient of a variety of commercial herbicide formulations. At room temperature, atrazine is a colourless powder. Physicochemical properties of atrazine that may affect its environmental fate and toxicity are presented in Table 1.

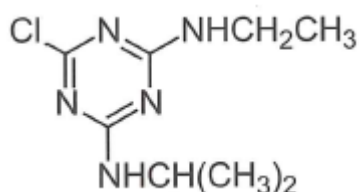


Figure 1 Structure of atrazine

Table 1 Summary of selected physicochemical properties of atrazine

Physicochemical property	Value
Molecular weight	215.7 atomic mass units ¹
Aqueous solubility	33 mg/L at pH 7 and 22 °C ¹ 35 mg/L at 20 °C ²
Logarithm of the octanol–water partition coefficient	2.5 at 25 °C ¹ 2.7 at pH 7 and 20 °C ²
Logarithm of the organic carbon–water partition coefficient	1.59–2.34 ^{1, 2}
Logarithm of the bioconcentration factor	0.63 ²
Half-life in water	14–20 days ¹ 105 to > 200 days in groundwater ¹
Half-life in soil	35–80 days in whole water–sediment system ¹ 80 days (water–sediment phase) ² 16–1,174 days, median 38.5 days in the field ¹ 29–66 days (in the field and lab at 20 °C, respectively) ² Longer under dry or cold conditions ^{1,3}

¹ BCPC (2012)

² Pesticide Properties Database (University of Hertfordshire 2013)

³ APVMA (2008).

Atrazine currently has approved label instructions for application to crops in Australia), including broom millet, lucerne, maize, rye, sorghum and sorghum (saccharine), sweet corn, potatoes, lupin, canola, cocksfoot, phalaris and sugar cane (APVMA 2008). Approved label instructions for non-agricultural uses include the application to pasture, fallow paddocks, utilities, infrastructure and timber plantations (APVMA 2022). In New Zealand, atrazine can be applied to linseed, established lucerne, maize, sweet corn and radiata pine forestry, and can be used in non-crop applications (ACVM 2022).

Atrazine exhibits moderate solubility in water and is moderately to highly mobile in soils, as indicated by its low logarithm of the organic carbon–water partition coefficient ($\log-K_{oc}$) value (Table 1). It does not adsorb strongly to soil particles. Therefore, atrazine has a high potential to be delivered to waterbodies, despite its moderate solubility in water. Atrazine is most effective when applied to wet soils and, therefore, has capacity to leach to groundwater and be transported in surface waters (Graymore et al. 2001). Surface runoff following large rain events may also deliver atrazine to aquatic ecosystems (Wallace et al. 2015). In the Great Barrier Reef lagoon, atrazine was detected each year from 2010 to 2016 at an average detection frequency of 70% (Grant et al. 2017; Grant et al. 2018; Gallen et al. 2019) and most recently at a detection frequency of 88% in the 2017–18 monitoring year (Gallen et al. 2019). Atrazine has a moderately short half-life ($t_{1/2}$) of 35–80 days in water–sediment systems (Table 1). The primary breakdown route of atrazine is via chemical hydrolysis, followed by degradation by soil microorganisms (APVMA 2008). The main degradation products of atrazine are desethyl-atrazine and desisopropyl atrazine, both of which have been widely detected in Australian marine waters. In the Great Barrier Reef lagoon, desethyl atrazine and desisopropyl atrazine were each detected in 50–80% of samples during the 2017–18 monitoring year (Gallen et al. 2019). These detection frequencies of atrazine and associated degradation products are very similar to those in rivers and creeks that discharge to the Great Barrier Reef (Turner et al. 2013a, 2013b; Wallace et al. 2014, 2015, 2016; Garzon-Garcia et al. 2015; Warne et al. 2020). However, the concentrations in the Great Barrier Reef lagoon are much lower and unlikely to constitute a risk to the marine biota in this system.

The previous Australian and New Zealand default guideline values (DGVs) for atrazine in marine environments was a low reliability value (using the ANZECC and ARMCANZ 2000 reliability scheme) based on the ANZECC and ARMCANZ (2000) moderate reliability freshwater DGVs for atrazine. At the time, data on the chronic toxicity of atrazine to marine species were only available for one species. More data on the chronic toxicity of atrazine to marine species are now available, which has enabled the derivation of improved DGVs, compared to the DGVs in ANZECC and ARMCANZ (2000). This technical brief provides revised DGVs for atrazine in marine water that supersede the ANZECC and ARMCANZ (2000) DGVs.

2 Aquatic toxicology

2.1 Mechanisms of toxicity

Atrazine is absorbed by plants principally through the plant roots. It is also absorbed through the foliage. It is then translocated acropetally (i.e. upwards from the base of plants to the apex) in the xylem and accumulates in the apical meristems and leaves (BCPC 2012). Atrazine is toxic to aquatic plants and algae because it inhibits electron transport in the photosystem II (PSII) complex (University of Hertfordshire 2013). Electron transport is a key process in photosynthesis that occurs in the thylakoid membranes of chloroplasts. Photosynthesis-inhibiting herbicides bind to the plastoquinone B (Q_B) protein binding site on the D1 protein in PSII. This prevents the transport of electrons to synthesise adenosine triphosphate (ATP, used for cellular metabolism) and nicotinamide adenine dinucleotide phosphate (NADPH, used in converting carbon dioxide [CO_2] to glucose) and, therefore, prevents CO_2 fixation (Wilson et al. 2000).

In addition to this main mode of action, exposure to PSII-inhibiting herbicides can lead to marked increases in the formation of reactive oxygen species (ROS), including the synthesis of singlet oxygen ($O=O$), superoxide (O_2^-) and hydrogen peroxide (H_2O_2) (Halliwell 1991). Reactive oxygen species are highly reactive forms of oxygen that readily react with, and bind to, biomolecules including DNA (deoxyribonucleic acid) and RNA (ribonucleic acid). Reactive oxygen species are created during normal cellular functioning, particularly in biochemical processes that involve the generation of energy (e.g. photosynthesis in chloroplasts and the Krebs cycle in the mitochondria of cells). In phototrophs (species that photosynthesise, e.g. macrophytes, diatoms, algae), ROS are formed when the absorbed light energy exceeds the ability to convert CO_2 to organic molecules, thus accumulating oxygen (Chen et al. 2012). Normal concentrations of ROS are involved in a number of cellular processes (Chen et al. 2012). However, prolonged exposure to elevated concentrations of ROS in plants, as a result of biotic stressors (e.g. disease) or abiotic stressors (e.g. PSII-inhibiting herbicides), can cause irreversible cell damage and ultimately lead to cell death (apoptosis). In heterotrophic organisms, atrazine increases expression of biomarkers for oxidative stress (e.g. Paulino et al. 2012; Lee et al. 2017).

Atrazine can also exert biochemical effects in non-target organisms. It is known to cause endocrine-disrupting effects (Mnif et al. 2011). For example, atrazine reportedly inhibits the production of testosterone and induces estrogen production in vertebrates (Deb 2005). Atrazine is classed as a Category 1 potential endocrine disruptor by the European Union, based on there being 'more or less comprehensive evidence' of endocrine-disrupting effects in exposed organisms (NIH 2023). Category 1 listed substances come under greater scrutiny with regards to regulation and, potentially, prohibition (ECHA 2023). However, the Warne et al. (2018) DGV derivation method does not explicitly consider endocrine disruption because it does not allow for the inclusion of endpoints that have not demonstrated ecological relevance (e.g. biochemical endpoints), which is often the case in studies of endocrine disruptors. Nevertheless, effects on ecologically relevant endpoints that can potentially be affected by endocrine disruption, such as reproduction, development and growth, are considered in DGV derivation. Endocrine-disrupting effects were not considered in the derivation of the DGVs for atrazine.

2.2 Toxicity

Although all available freshwater and marine toxicity data indicate that heterotrophic species as a group are less sensitive to atrazine than phototrophic species, there is substantial overlap in the sensitivities (Appendix A). Of the 11 marine heterotrophic species, 4 had toxicity values within the range of the 13 marine phototrophic species.

Toxicity values for diatoms ranged from 14 µg/L (5-day NOEL [see 'Glossary and acronyms' for definitions], biomass/growth rate/area under the curve) for *Skeletonema costatum* to 460 µg/L (3-day EC50, biomass/growth rate/area under the curve) for *Navicula incerta* (US EPA 2015). For green microalgae, toxicity values ranged from 11 µg/L (3-day EC50, abundance) for *Nephroselmis pyriformis* (Magnusson et al. 2008) to 431 µg/L (5-day EC50, biomass/growth rate/area under the curve) for *Dunaliella tertiolecta* (US EPA 2015). A 3-day EC50 of 77 µg/L (biomass/growth rate/area under the curve) has been reported for the brown macroalga *Monochrysis lutheri* (US EPA 2015), while 3-day and 5-day EC50s of 79 µg/L and 308 µg/L (biomass/growth rate/area under the curve), respectively, have been reported for the red microalga *Porphyridium cruentum* (US EPA 2015). Toxicity values for the macrophyte eel grass (*Zostera marina*) ranged from 10 µg/L (21-day NOEL, leaf count) to 1,000 µg/L (21-day LOEC, shoot length) (Hershner et al. 1982). There did not appear to be any differences in the sensitivities of the 6 marine phototrophic taxonomic groups to atrazine.

Atrazine toxicity values for heterotrophic species ranged from 3.5 µg/L to 197,850 µg/L. Toxicity values for fish ranged from 20 µg/L (15-day LOEC, length) for red drum (*Sciaenops ocellatus*) (Applebaum 2008) to 16,200 µg/L (96-hour LC50, mortality) for sheepshead minnow (*Cyprinodon variegatus*) (Hall et al. 1994). For crustaceans, toxicity values ranged from 3.5 µg/L (41-day NOEC, nonviable offspring) for a copepod (*Amphiascus tenuiremis*) (Bejarano and Chandler 2003) to 197,850 µg/L (96-hour LC50, mortality) for the sand fiddler crab (*Uca pugilator*) (US EPA 2015).

3 Factors affecting toxicity

As with many organic chemicals, dissolved and particulate organic matter and suspended solids affect atrazine bioavailability and toxicity. However, any such effect would be relatively minor given the low log- K_{oc} value of atrazine (Table 1). A major review by Knauer et al. (2016) concluded that suspended solids did not significantly affect the toxicity and bioavailability of a range of pesticides, including atrazine, to aquatic species. The presence of dissolved organic matter also did not decrease the toxicity of atrazine to periphyton communities (Nikkilä et al. 2001). Thus, the available evidence indicates that there is insufficient binding of atrazine to suspended solids or dissolved organic matter to reduce toxicity to phototrophic and heterotrophic species.

As noted in section 2.1, one of the modes of action of atrazine in phototrophs is to increase the formation of ROS. Given that the formation of ROS is dependent on light intensity, it is plausible that increased turbidity (e.g. from increased suspended solids) could lead to a decrease in atrazine toxicity. Wilkinson et al. (2015) examined the combined effects of diuron, another PSII-inhibiting herbicide, and light intensity to the seagrass *Halophila ovalis* and found that the interaction was sub-additive (antagonistic) at low light intensity, additive at saturating light intensity, and additive or synergistic at elevated light intensity (Wilkinson et al. 2015). Wilkinson et al. (2017) also found that water temperatures greater or less than the thermal optima for *H. ovalis* tended to exert sub-additive effects when combined with diuron. However, these sub-additive effects were still greater than the effect of each stressor alone. As diuron and atrazine are both PSII-inhibiting herbicides, it is quite likely that the toxicity of atrazine will also be affected by light intensity and by water temperature, although quantitative relationships that demonstrate this have not been developed.

4 Default guideline value derivation

The DGVs were derived in accordance with the method described in Warne et al. (2018) and using Burrlioz 2.0 software.

4.1 Toxicity data used in derivation

An extensive search of the scientific literature was conducted to obtain data on the toxicity of atrazine to marine organisms. In addition, searches of the US EPA ECOTOX Knowledgebase (US EPA 2015), Australasian Ecotoxicology Database (Warne et al. 1998) and ANZECC and ARMCANZ (2000) toxicant database (Sunderam et al. 2000) were conducted. There are now sufficient data available on the chronic toxicity of atrazine, including data for both phototrophic species and heterotrophic species, to enable the derivation of DGVs in marine water based on chronic toxicity alone. All the toxicity data used to calculate the DGVs were determined from experiments using technical or higher grades of atrazine or with a minimum purity of 80% active ingredient (Warne et al. 2018).

Organisms classified only to genus level are not normally used to derive DGVs, as ambiguity at the genus level could result in more than one toxicity value being assigned to a single species. However, visual identification and classification of species within a genus, particularly for microalgae, can be difficult for some genera due to their lack of characteristic morphological features (Kessler and Huss 1992). Nonetheless, when there are no other data for species belonging to the same genus (i.e. there is no chance of duplicating a species) or when there are limited amounts of toxicity data available, such data could be included in the derivation of DGVs. In deriving the DGVs for atrazine in marine water, toxicity data for the green alga *Platymonas* sp. were included, as no other toxicity data for this genus were available.

There were acute and chronic marine toxicity data for 28 species from 8 phyla/clades that passed the screening and quality assessment processes. These consisted of 13 marine phototrophic species and 15 heterotrophic species. The phototrophic species consisted of 5 diatoms, 5 green algae, one brown macroalga, one red alga and one macrophyte. The 15 heterotrophic species consisted of 5 fish and 10 crustaceans. The represented phyla were Arthropoda, Bacillariophyta, Chlorophyta, Chordata, Haptophyta, Ochrophyta, Rhodophyta and Tracheophyta. Of this dataset, the chronic data for 18 species from 8 phyla were used in the DGV derivation.

While atrazine has a specific mode of action that targets phototrophs (inhibition of the PSII pathway), it also has a non-specific mode of action (formation of ROS). Reflecting this, there was no evidence of a difference in the sensitivities of phototrophs and heterotrophs to atrazine (Appendix A). The weight of evidence indicated that the sensitivity of marine species to atrazine is unimodal and, therefore, all available data of appropriate quality were used to derive the DGVs, as recommended by Warne et al. (2018).

Bejarano and Chandler (2003) conducted a multi-generational toxicity test exposing a copepod (*Amphiascus tenuiremis*) to atrazine. This resulted in the lowest tested concentration (3.5 µg/L) being significantly different to the control (i.e. it is a LOEC) for second generation (F₁) copepods. This results in an estimated NOEC value of 1.4 µg/L (i.e. the LOEC value of 3.5 µg/L divided by 2.5; Warne et al. 2018), which is more sensitive than other NOEC values reported in the same study for both, F₁ and F₂

generations. As multigenerational endpoints are considered a chronic response, they were included in the dataset to calculate the DGVs for atrazine in marine water. However, as this was the only study to report multigenerational toxicity data, the DGVs are unlikely to provide adequate protection to other organisms that are continuously exposed to atrazine over multiple generations.

There were chronic negligible-effect (EC10/NOEC/NOEL) and chronic estimated-negligible-effect (chronic LC50 values that were converted to chronic EC10/NOEC values) data for 18 marine species (13 phototrophs and 5 heterotrophs) belonging to 8 phyla and 14 classes that met the minimum data requirements (i.e. at least 5 species belonging to at least 4 phyla) to use a species sensitivity distribution (SSD) to derive DGVs (Warne et al. 2018). Details of the data-quality assessment and the data that passed the quality assessment are provided as supporting information.

A summary of the toxicity data (one value per species) used to derive the DGVs for atrazine in marine water is provided in Table 2. Further details of the water-quality parameters for each single species value used to calculate the DGVs are presented in Appendix B.

Table 2 Summary of the single chronic toxicity values for each species that were used to derive the default guideline values for atrazine in marine water

Taxonomic group	Species	Life stage	Duration (days)	Toxicity measure (endpoint) ^a	Toxicity value (µg/L)	Final toxicity value (µg/L)
Diatom	<i>Navicula incerta</i>	Not stated	3	EC50 (biomass yield, growth rate, AUC ^b)	460	92 ^c
	<i>Phaeodactylum tricornutum</i> *	Not stated	10	EC50 (biomass yield, growth rate, AUC ^b)	200	40 ^c
	<i>Rhizosolenia setigera</i> *	Exponential growth phase	12	NOEC (cell density)	61.2	61.2
	<i>Skeletonema costatum</i> *	Not stated	5	NOEL (biomass yield, growth rate, AUC ^b)	14	14
	<i>Thalassiosira fluviatilis</i>	Not stated	3	EC50 (biomass yield, growth rate, AUC ^b)	110	22 ^c
	<i>Thalassiosira weissflogii</i> *	Continuous growth phase	2	LOEC/EC50 (cell density)	20/42	8.2 ^c
Brown microalga	<i>Isochrysis galbana</i>	Not stated	5	EC50 (biomass yield, growth rate, AUC ^b)	22	4.4 ^c
Brown macroalga	<i>Monochrysis lutheri</i>	Not stated	3	EC50 (biomass yield, growth rate, AUC ^b)	77	15.4 ^c
Red microalga	<i>Porphyridium cruentum</i> *	Not stated	3	EC50 (biomass yield, growth rate, AUC ^b)	79	15.8 ^c
Green microalga	<i>Dunaliella tertiolecta</i>	Log growth phase	4	NOEC (cell density)	25	25
	<i>Nephroselmis pyriformis</i> *	Not stated	3	EC10 (cell density)	11	11
	<i>Platymonas</i> sp.	Not stated	3	EC50 (biomass yield, growth rate, AUC ^b)	100	20 ^c
Macrophyte	<i>Zostera marina</i>	Not stated	21	NOEC (number of leaves)	10	10
Crustacean (shrimp)	<i>Americamysis bahia</i>	Life cycle	28	NOEL (mortality)	260	260
Crustacean (copepod)	<i>Amphiascus tenuiremis</i>	(F ₁) stage 1 copepodite juvenile	26	LOEC (viable offspring production per female)	3.5 ^d	1.4 ^c
Fish	<i>Cyprinodon variegatus</i>	Early life stage	33	NOEL (mortality)	1,100	1,100
	<i>Gasterosteus aculeatus</i>	Larvae < 24 hour	42	NOEC (wet weight, length)	89.5	89.5
	<i>Sciaenops ocellatus</i>	Not stated	9	NOEC (length)	37.4	37.4

^a The measure of toxicity being estimated/determined – 10% effect concentration (EC10), no-observed-effect concentration (NOEC) and no-observed-effect level (NOEL) – require no conversion.

^b AUC = area under the growth curve.

^c Chronic LOEC and EC50 data were converted to chronic negligible-effect (EC10/NOEC) data by dividing by 2.5 and 5, respectively (Warne et al. 2018).

^d This value was preferentially chosen over other data points (including chronic NOEC values) as the F₁ generation was significantly impacted (reproduction; viable offspring per female) at 3.5 µg/L.

* Species that originated from/are distributed in Australia and/or New Zealand.

To identify species that were regionally relevant to Australia and New Zealand ecosystems, searches of Algaebase (Guiry and Guiry 2017), Atlas of Living Australia (ALA 2017), Catalogue of Life (Roskov et al. 2017), Integrated Taxonomic Information System (ITIS 2017) and the World Register of Marine Species (WoRMS 2017) were conducted. The dataset used in the guideline derivation process for atrazine in marine water (Table 2) includes toxicity data for 6 marine species that either originated from or are distributed within Australia or New Zealand.

4.2 Species sensitivity distribution

The cumulative frequency (species sensitivity) distribution of the 18 marine species that were used to derive the DGVs for atrazine in marine water is presented in

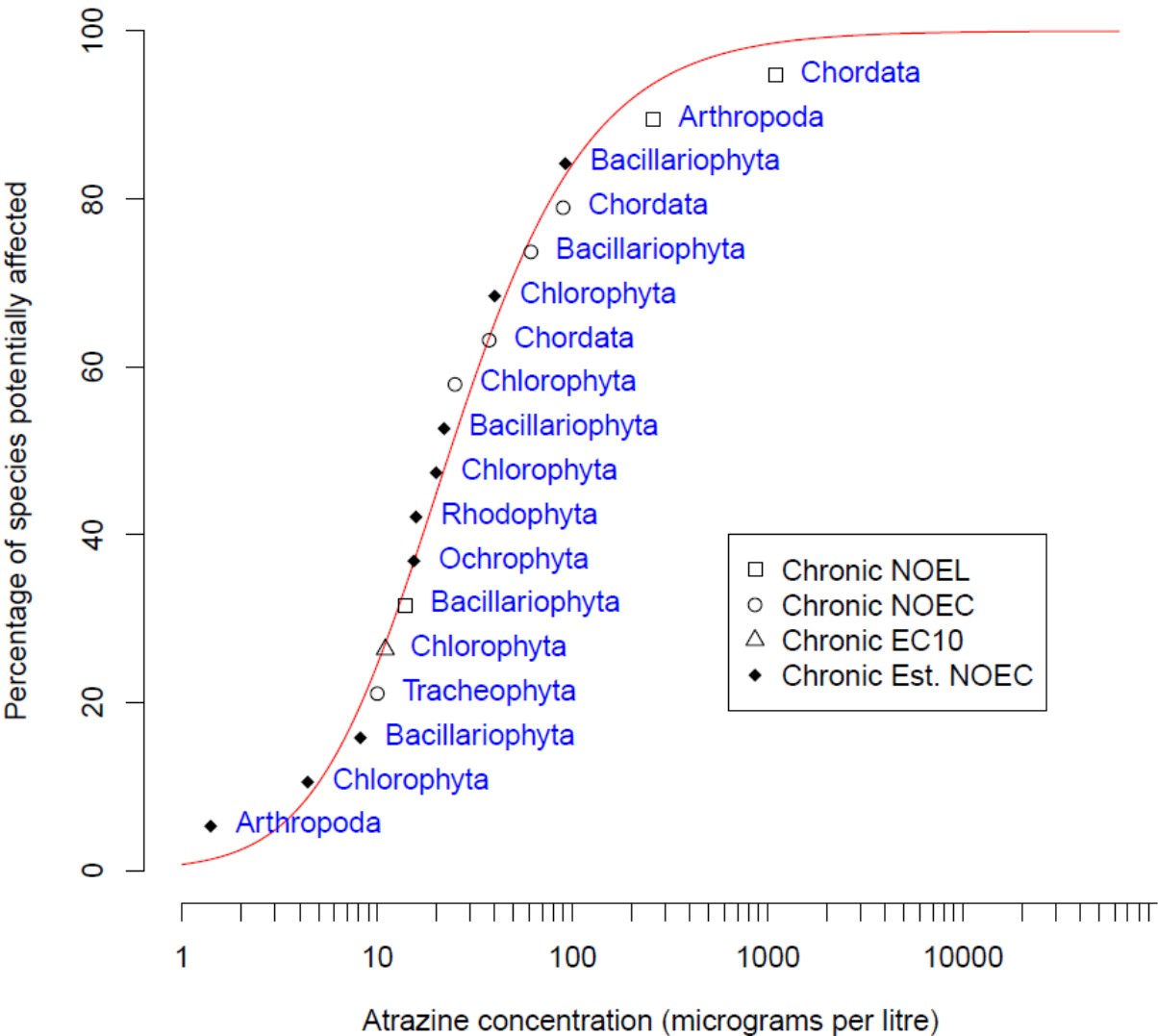


Figure 2 Species sensitivity distribution of atrazine in marine water

. The SSD was plotted using the BurrIioz 2.0 (2016) software. The model was judged to provide a good fit to the data (Figure 2).

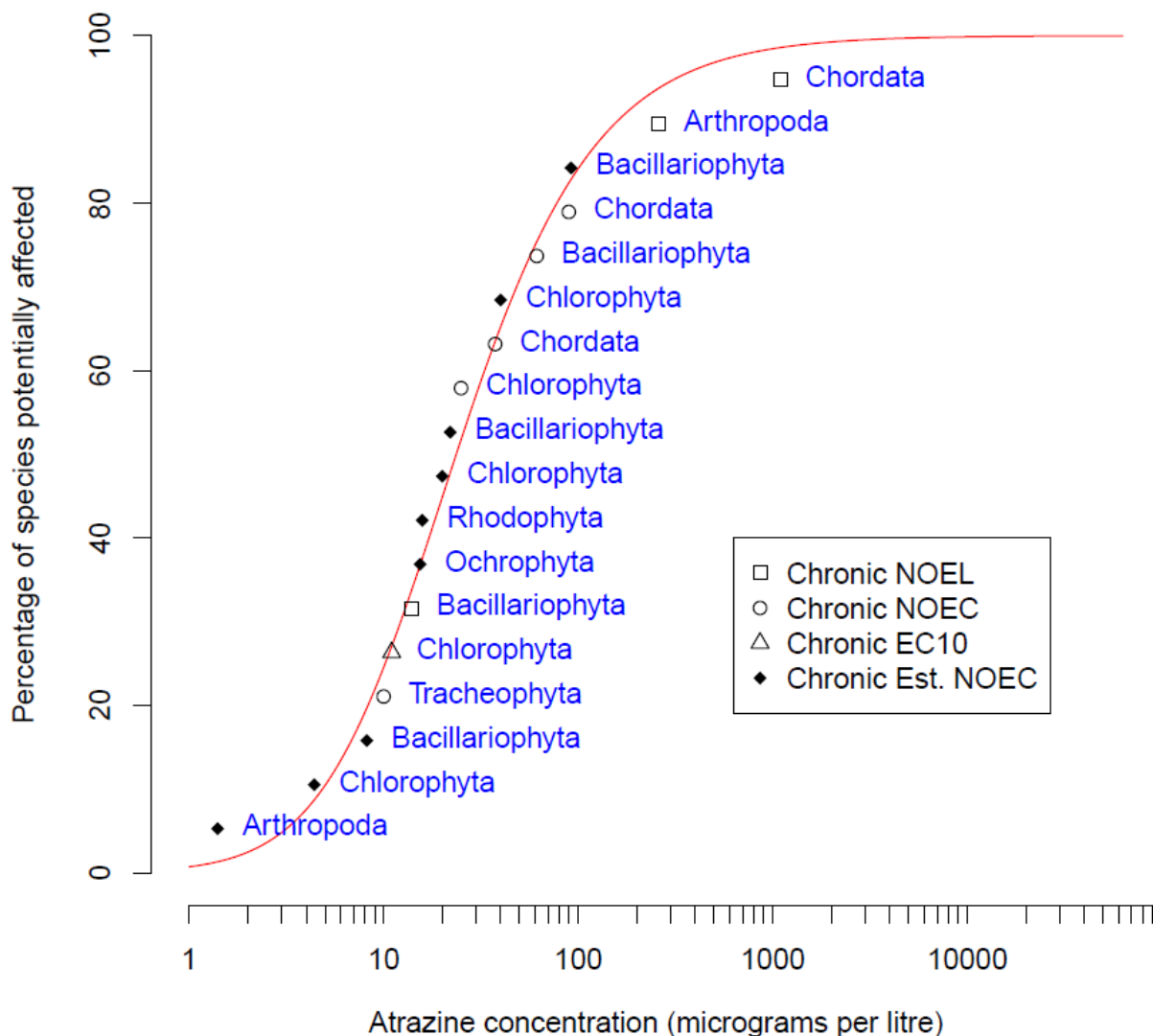


Figure 2 Species sensitivity distribution of atrazine in marine water

4.3 Default guideline values

It is important that the DGVs (Table 3) and associated information in this technical brief are used in accordance with the detailed guidance provided in the the [Australian and New Zealand Guidelines for Fresh and Marine Water Quality](#) website (ANZG 2018).

The derived Australian and New Zealand DGVs for atrazine in marine water are provided in Table 3. As with other pesticides, the DGVs for atrazine are expressed in terms of the concentration of the active ingredient. The DGVs relate to atrazine only, not to any of its breakdown products. The 95% species-protection DGV of 3.1 µg/L is recommended when assessing ecosystems that are slightly to moderate disturbed.

Measured logarithm of the bioconcentration factor (log-BCF) values for atrazine are low (Table 1) and below the threshold (log BCF = 4, Warne et al. 2018) at which secondary poisoning or bioconcentration must be considered. Therefore, the DGVs for atrazine do not need to account for secondary poisoning.

Based on the multi-generational study by Bejarano and Chandler (2003), these DGVs (at all levels of species protection) should be treated with caution as they may not provide adequate protection to organisms that are continuously exposed to atrazine for multiple generations.

Table 3 Default guideline values (µg/L) for atrazine in marine water

Level of species protection (%)	DGVs for atrazine in marine water (µg/L) ^a
99	1.2
95	3.1
90	4.8
80	8.3

¹ Default guideline values were derived using the BurrIioz 2.0 (2016) software and rounded to 2 significant figures.

4.4 Reliability classification

The atrazine marine DGVs have a very high reliability classification (Warne et al. 2018) based on the outcomes for the following 3 criteria:

- sample size – 18 (preferred)
- type of toxicity data – marine chronic data
- SSD model fit – good (burr type III).

Glossary and acronyms

Term	Definition
Acute toxicity	An adverse effect that occurs as the result of a short (relative to the organism's life span) exposure to a chemical. Refer to Warne et al. (2018) for examples of acute exposures.
ATP	Adenosine triphosphate, used for cellular metabolism.
Bimodal	When the distribution of the sensitivity of species to a toxicant has 2 modes. This typically occurs with chemicals with specific modes of action. For example, herbicides are designed to affect plants at low concentrations, but most animals are only affected at high concentrations.
Bioconcentration factor (BCF)	A ratio that measures how much of a chemical accumulates in an organism compared to how much is in its environment. Bioconcentration factors are used to assess the risk of chemical contaminants in the environment.
CAS no.	Chemical Abstracts Service number. Each chemical has a unique identifying number that is allocated to it by the American Chemical Society.
Chronic toxicity	A lethal or adverse sub-lethal effect that occurs as the result of exposure to a chemical for a period of time that is a substantial portion of the organism's life span or an adverse sub-lethal effect on a sensitive early life stage. Refer to Warne et al. (2018) for examples of chronic exposures.
Default guideline value (DGV)	A guideline value recommended for generic application in the absence of a more specific guideline value (e.g. site-specific value), in the <i>Australian and New Zealand Water Quality Guidelines</i> . Formerly known as 'trigger value'.
DNA	Deoxyribonucleic acid.
ECx	The concentration of a substance in water or sediment that is estimated to produce an x% effect on a sub-lethal endpoint. The magnitude of x can vary from 1 to 100; however, values between 5 and 50 are more typical. The ECx is usually expressed as a time-dependent value (e.g. 24-h or 96-h ECx).
Endpoint	The specific response of an organism that is measured in a toxicity test (e.g. mortality, growth, reproduction, a particular biomarker).
Guideline value (GV)	A measurable quantity (e.g. concentration) or condition of an indicator for a specific environmental value below which (or above which, in the case of stressors such as pH, dissolved oxygen and many biodiversity responses) there is considered to be a low risk of unacceptable effects occurring to that environmental value. Guideline values for more than one indicator should be used simultaneously in a multiple-lines-of-evidence approach.
ICx	The concentration of a substance in water or sediment that is estimated to produce an x% inhibition of the response being measured in test organisms relative to the control response, under specified conditions.
LCx	The concentration of a substance in water or sediment that is estimated to be lethal to x% of a group of test organisms relative to the control response, under specified conditions.
LOEC (lowest-observed-effect concentration)	The lowest concentration of a chemical used in a toxicity test that has a statistically significant ($p \leq 0.05$) adverse effect on the exposed population of test organisms as compared to the controls. All higher concentrations should also cause statistically significant effects.
Mode of action	The means by which a chemical exerts its toxic effects. For example, triazine herbicides inhibit the photosystem II component of the photosynthesis biochemical reaction in plants.
NADPH	Nicotinamide adenine dinucleotide phosphate, used in converting carbon dioxide to glucose.

NEC (no-effect concentration)	The highest concentration of a toxicant that does not have an adverse effect in a target organism. This is determined differently from a NOEC.
NOEC (no-observed-effect concentration)	The highest concentration of a toxicant used in a toxicity test that does not have a statistically significant ($p > 0.05$) effect on the exposed populations of test organisms as compared to the controls. The statistical significance is measured at the 95% confidence level.
NOEL (no-observed-effect level)	Synonymous with NOEC.
Octanol–water partition coefficient (K_{OW})	The ratio of a chemical's solubilities in <i>n</i> -octanol and water at equilibrium. The logarithm of K_{OW} is used as an indication of a chemical's propensity for bioaccumulation by aquatic organisms.
Organic carbon–water partition coefficient (K_{OC})	Adsorption coefficient normalised to the organic carbon content of the soil
Phototrophs	Organisms that photosynthesise as their main means of obtaining energy, e.g. plants, algae.
PSII	Photosystem II of the photosynthetic biochemical pathway.
RNA	Ribonucleic acid.
ROS	Reactive oxygen species.
Site-specific	Relating to something that is confined to, or valid for, a particular place. Site-specific guideline values are relevant to the location or conditions that are the focus of a given assessment.
Species	A group of organisms that resemble each other to a greater degree than members of other groups and that form a reproductively isolated group that will not produce viable offspring if bred with members of another group.
Species sensitivity distribution (SSD)	A method that plots the cumulative frequency of species sensitivity and fits the best possible statistical distribution to the data. The concentration that should theoretically protect a selected percentage of species can be determined from the distribution.
Toxicity	The inherent potential or capacity of a material to cause adverse effects in a living organism.
Toxicity test	The means by which the toxicity of a chemical or other test material is determined. A toxicity test is used to measure the degree of response produced by exposure to a specific level of stimulus (or concentration of chemical) for a specified test period.

Appendix A: modality assessment for atrazine toxicity to aquatic species

A modality assessment was undertaken for atrazine according to the weight-of-evidence approach and the 4 questions specified in Warne et al. (2018).

1. Is there a specific mode of action that could result in taxa-specific sensitivity?

Atrazine is a PS-II inhibiting herbicide that binds to the plastoquinone B (Q_B) protein-binding site on the D1 protein in PSII. This prevents the transport of electrons needed to synthesise ATP and NADPH and, therefore, prevents CO_2 fixation (Wilson et al. 2000).

In addition, atrazine can lead to increased concentrations of ROS (Halliwell 1991). In phototrophs, ROS are formed when the absorbed light energy exceeds the ability to convert CO_2 to organic molecules, thus accumulating oxygen (Chen et al. 2012). Normal concentrations of ROS are involved in a number of cellular processes (Chen et al. 2012). However, prolonged exposure to elevated concentrations of ROS can cause irreversible cell damage and ultimately lead to cell death (apoptosis). This indicates that atrazine would be expected to be toxic to phototrophs at lower concentrations than it is to heterotrophs.

Finally, atrazine is known to cause endocrine-disrupting effects (Mnif et al. 2011). However, endocrine-disrupting effects are generally not considered in the derivation of DGVs.

2. Does the data suggest bimodality?

Modality was assessed using a dataset that combined all freshwater and marine toxicity data for atrazine that passed the screening and quality assessment schemes ($n = 147$). This was done to increase the sample size of the dataset being assessed. All data that were not chronic negligible-effect values (e.g. EC5, EC10, NOEC) were first converted to this type of data using the methods recommended by Warne et al. (2018). A kernel-density plot of the data for freshwater and marine species data showed the 2 groups mostly overlapping, indicating that the dataset is unlikely to be bimodal (Figure A1). Therefore, the pooled freshwater and marine dataset was retained for the modality assessment. Calculation of the bimodality coefficient (BC) on log-transformed data yielded a value of 0.307. This is below the indicative threshold BC for bimodality of 0.55, suggesting the dataset does not exhibit bimodality.

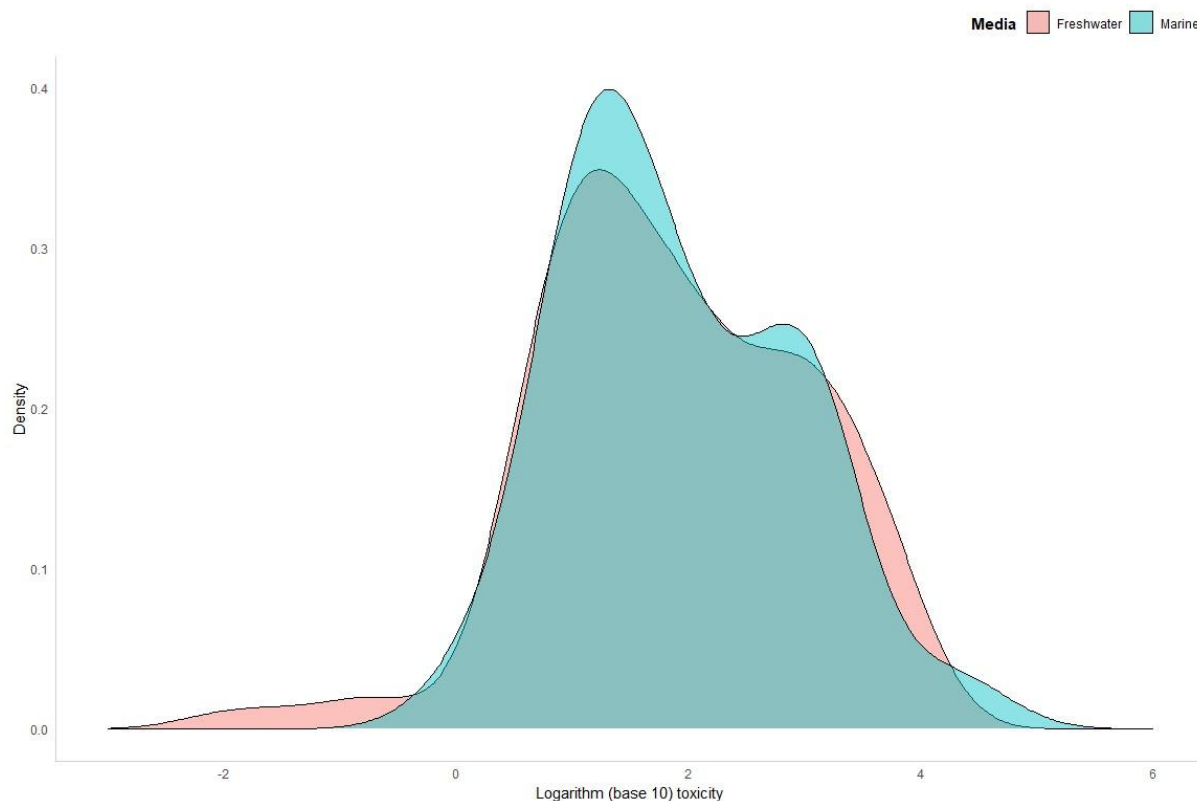


Figure A1 Kernel-density plot of the log-transformed atrazine ecotoxicity data for freshwater and marine species exposed to atrazine

3. Do data show taxa-specific sensitivity (i.e. through distinct groupings of different taxa types)?

The relative sensitivities of phototrophs and heterotrophs to atrazine were compared using a kernel-density plot (Figure A2) and an SSD (Figure A3). These figures indicate that phototrophs as a group appear to be generally more sensitive than heterotrophs. However, there is a large overlap between the 2 groups, supporting the results of the BC that the dataset is unimodal.

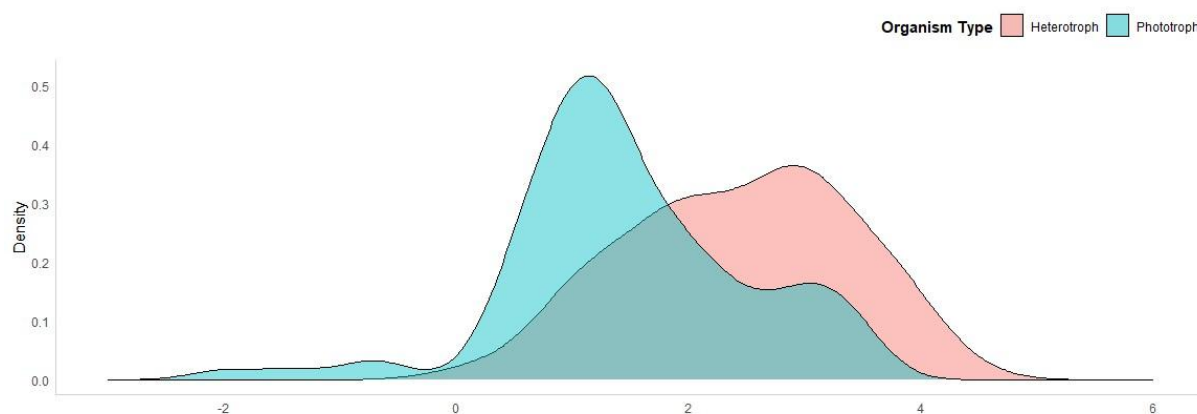


Figure A2 Kernel-density plot of the log-transformed toxicity data for heterotrophic (pink shaded area) and phototrophic (blue shaded area) freshwater and marine organisms exposed to atrazine

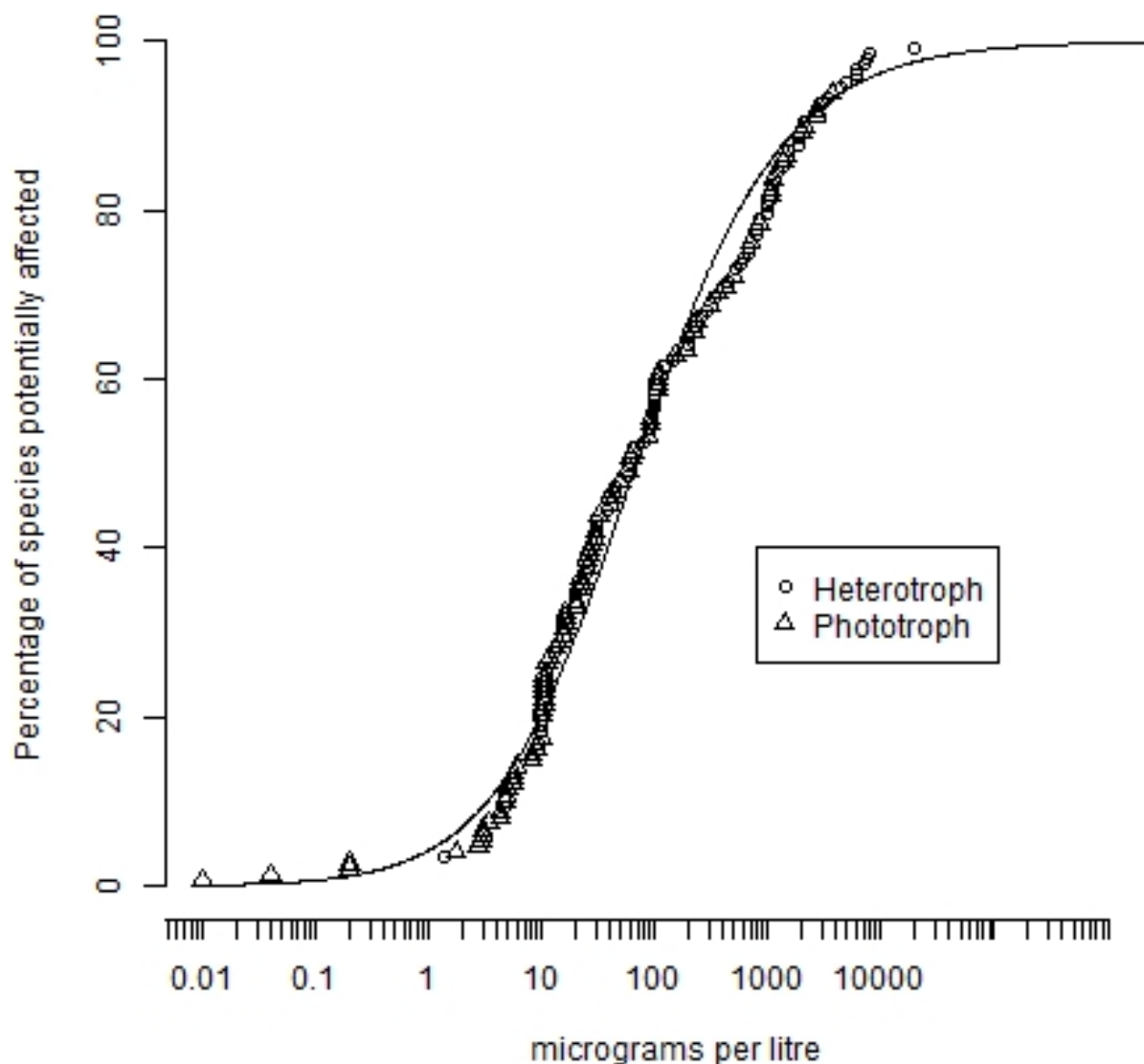


Figure A3 Species sensitivity distribution, generated by Burrlioz 2.0, using available ecotoxicity data for phototrophic and heterotrophic organisms exposed to atrazine

- 4. Is it likely that indications of bimodality or multimodality or distinct clustering of taxa groups are not due to artefacts of data selection, small sample size, test procedures or other reasons unrelated to a specific mode of action?**

Given that there are ecotoxicity data for 87 phototrophs and 60 heterotrophs (a total of 147 species), it is likely that the distributions are representative and that this large dataset does not show evidence of a difference in the sensitivities of phototrophic and heterotrophic species. The weight of evidence suggests that the sensitivity of aquatic species to atrazine is unimodal and, therefore, all the available highest quality data were used to derive the DGVs as recommended by Warne et al. (2018).

Appendix B: toxicity data used to derive the default guideline values for atrazine in marine water

Table B1 Summary of the toxicity data that passed the screening and quality-assurance processes for atrazine in marine water

Taxonomic group (phylum or clade)	Species	Life stage	Exposure duration (days)	Test type	Toxicity measure (test endpoint)	Salinity (‰)	Test medium	Temperature (°C)	pH	Concentration (µg/L)	Reference
Bacillariophyta (diatoms)	<i>Navicula incerta</i>	Not stated	3	Chronic	EC50 (biomass yield, growth rate, AUC ^a)	30 ± 5	Synthetic salt water or filtered natural salt water	20 ± 2	8.0 ± 0.1	460	US EPA (2015)
										92^b	Value used in SSD
	<i>Phaeodactylum tricornutum</i>	Not stated	10	Chronic	EC50 (biomass yield, growth rate, AUC ^a)	30 ± 5	Synthetic salt water or filtered natural salt water	20 ± 2	8.0 ± 0.1	200	US EPA (2015)
										40^b	Value used in SSD
<i>Rhizosolenia setigera</i>	Exponential growth phase	12	Chronic	NOEC (cell density)	36	F/2 medium	19 ± 1	7.8–8	61.2		Kalopesa et al. (2008)
										61.2	Value used in SSD
<i>Skeletonema costatum</i>	Not stated	5	Chronic	NOEL (biomass yield, growth rate, AUC ^a)	30 ± 5	Synthetic salt water or filtered natural salt water	20 ± 2	8.0 ± 0.1	14		US EPA (2015)
										14	Value used in SSD

Toxicant default guideline values for aquatic ecosystem protection: Atrazine in marine water

Taxonomic group (phylum or clade)	Species	Life stage	Exposure duration (days)	Test type	Toxicity measure (test endpoint)	Salinity (‰)	Test medium	Temperature (°C)	pH	Concentration (µg/L)	Reference
	<i>Thalassiosira fluviatilis</i>	Not stated	3	Chronic	EC50 (biomass yield, growth rate, AUC ^a)	30 ± 5	Synthetic salt water or filtered natural salt water	20 ± 2	8.0 ± 0.1	110	US EPA (2015)
										22 ^b	Value used in SSD
	<i>Thalassiosira weissflogii</i>	Continuous growth phase	2	Chronic	EC50 (cell density)	24	Artificial seawater with f/2 media	18 ± 1	Not stated	42	Doherty 1997
		Continuous growth phase	2	Chronic	LOEC (cell density)	24	Artificial seawater with f/2 media	18 ± 1	Not stated	20	Doherty 1997
										29	Geometric mean
										8.2 ^b	Value used in SSD
Haptophyta (brown microalgae)	<i>Isochrysis galbana</i>	Not stated	5	Chronic	EC50 (biomass yield, growth rate, AUC ^a)	30 ± 5	Synthetic salt water or filtered natural salt water	20 ± 2	8.0 ± 0.1	22	US EPA (2015)
										4.4 ^b	Value used in SSD
Ochrophyta (brown macroalgae)	<i>Monochrysis lutheri</i>	Not stated	3	Chronic	EC50 (biomass yield, growth rate, AUC ^a)	30 ± 5	Synthetic salt water or filtered natural salt water	20 ± 2	8.0 ± 0.1	77	US EPA (2015)
										15.4 ^b	Value used in SSD
Rhodophyta (red microalgae)	<i>Porphyridium cruentum</i>	Not stated	3	Chronic	EC50 (biomass yield, growth rate, AUC ^a)	30 ± 5	Synthetic salt water or filtered natural salt water	20 ± 2	8.0 ± 0.1	79	US EPA (2015)

Toxicant default guideline values for aquatic ecosystem protection: Atrazine in marine water

Taxonomic group (phylum or clade)	Species	Life stage	Exposure duration (days)	Test type	Toxicity measure (test endpoint)	Salinity (‰)	Test medium	Temperature (°C)	pH	Concentration (µg/L)	Reference
										15.8 ^b	Value used in SSD
Tracheophyta (vascular plants)	<i>Zostera marina</i>	Not stated	21	Chronic	NOEC (number of leaves)	Not stated	Marine water	Not stated	Not stated	10	Hershner et al. (1982)
Chlorophyta (green algae)	<i>Platymonas</i> sp.	Not stated	3	Chronic	EC50 (biomass yield, growth rate, AUC ^a)	30 ± 5	Synthetic salt water or filtered natural salt water	20 ± 2	8.0 ± 0.1	100	US EPA (2015)
										20 ^b	Value used in SSD
	<i>Dunaliella tertiolecta</i>	Log growth phase	4	Chronic	NOEC (cell density)	25	F/2 marine medium	Not stated	Not stated	25	DeLorenzo and Serrano (2003)
										25	Value used in SSD
	<i>Nephroselmis pyriformis</i>	Not stated	3	Chronic	EC10 (cell density)	Filtered seawater	Not stated	24	Not stated	11	Magnusson et al. (2008)
										11	Value used in SSD
Arthropoda	<i>Americamysis bahia</i> (shrimp)	Life cycle	28	Chronic	NOEC (mortality)	20 ± 3	Natural or artificial filtered seawater	25 ± 2	Not stated	260	US EPA (2015)
										260	Value used in species sensitivity distribution (SSD)
	<i>Amphiascus tenuiremis</i> (copepod)	(F ₁) stage 1 copepodite juvenile	26 ^c	Chronic	LOEC (viable offspring production per female)	35	Filtered and aerated seawater	20	8.25 ± 0.02	3.5	Bejarano and Chandler (2003)
										1.4 ^b	Value used in SSD

Toxicant default guideline values for aquatic ecosystem protection: Atrazine in marine water

Taxonomic group (phylum or clade)	Species	Life stage	Exposure duration (days)	Test type	Toxicity measure (test endpoint)	Salinity (‰)	Test medium	Temperature (°C)	pH	Concentration (µg/L)	Reference
Chordata (fish)	<i>Cyprinodon variegatus</i> (sheepshead minnow)	Early life stage	33	Chronic	NOEL (mortality)	Not stated	Dilution marine water	25 ± 2	Not stated	1,100	US EPA (2015)
										1,100	Value used in SSD
	<i>Gasterosteus aculeatus</i> (3-spined stickleback)	Larvae < 24 hour	42	Chronic	NOEC (wet weight, length)	18	Aerated filtered seawater	Not stated	Not stated	> 89 ^d	Le Mer et al. (2013)
		Larvae < 24 hour	42	Chronic	NOEC (wet weight, length)	18	Aerated filtered seawater	Not stated	Not stated	90	Le Mer et al. (2013)
										89.5	Geometric mean
										89.5	Value used in SSD
	<i>Sciaenops ocellatus</i> (red drum)	Not stated	9	Chronic	NOEC (growth rate)	27.1 ± 0.14	Seawater	28.4 ± 0.67	Not stated	37.4	Del carmen Alvarez (2005)
										37.4	Value used in SSD

^a AUC = area under the growth curve.

^b Chronic LOEC and EC50 data were converted to chronic negligible effect (EC10/NOEC) data by dividing by 2.5 and 5, respectively (Warne et al. 2018).

^c This is a multi-generational study. F₀ were exposed to atrazine for 13 days and F₁ were exposed to atrazine for another 13 days. Therefore, F₁ is noted as being exposed for 26 days to reflect exposure across multiple generations.

^d No significant effect observed up to and including the highest test concentration of 89 µg/L; thus, this concentration was assumed to be the NOEC, as per guidance in Warne et al. (2018).

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