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Toxicant default guideline values for aquatic ecosystem protection

Molybdenum in marine water

Technical brief

October 2026

Water Quality Guidelines is a joint initiative of the Australian and New Zealand governments, in partnership with the Australian states and territories.

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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 (www.waterquality.gov.au/anz-guidelines).

Molybdenum is a naturally occurring trace element in oxide or sulfide minerals. It is a micronutrient in plants and animals, and it is present in more than 30 enzymes.

The major sources of molybdenum for human use are through direct mining of molybdenum ore and as a by-product of copper and tungsten mining. Molybdenum is used across a wide variety of industries, and it is in metallurgical (e.g. heat resistant components, solar panels, wind turbines), nuclear medicine (e.g. imaging), mechanical (e.g. lubricant, corrosion inhibitor) and agricultural (e.g. fertilisers) products.

The primary source of molybdenum in marine water is from natural weathering of continental material (e.g. rocks, soils). However, anthropogenic sources also exist (e.g. fossil fuel combustion, leaching from fly ash, mining and mineral processing wastes).

Molybdenum exists in open marine water as molybdate oxyanion (MoO_4^{2-}) (Smedley and Kinniburgh 2017). Natural background concentrations of molybdenum in open (oxic) marine water are approximately 10 µg/L but can reduce to <1 µg/L under hypoxic conditions. However, there is a paucity of published data on nearshore and anthropogenically-elevated concentrations of molybdenum in marine water.

The previous DGV for molybdenum in marine water was a low reliability indicative interim working level of 23 µg/L based on the application of an assessment factor of 200 to the lowest of only two available toxicity values (ANZECC/ARMCANZ 2000). There are now sufficient data on the toxicity of molybdenum to marine species to derive moderate reliability DGVs. The DGVs in this technical brief build on the molybdenum marine guideline values derived by Heijerick and Carey (2017) and van Dam et al. (2018a), and they supersede the ANZECC/ARMCANZ (2000) DGVs.

The chronic toxicity of molybdenum to marine species appears to be low. Chronic toxicity values for marine species ranged from 4.4 mg/L for the mussel *Mytilus edulis* (48-h EC10, larval development) to 1 174 mg/L for the oyster *Crassostrea gigas* (48-h EC10, larval development). Molybdenum has a low potential to bioaccumulate in aquatic biota and does not biomagnify within the food chain.

Moderate reliability DGVs for dissolved molybdenum in marine water were derived based on chronic toxicity data for nine marine species from seven taxonomic groups, with a poor fit of the species sensitivity distribution (SSD) to the toxicity data.

The DGVs for 99%, 95%, 90% and 80% species protection levels are 0.6 mg/L, 5 mg/L, 10 mg/L and 40 mg/L, respectively. The DGVs relate to dissolved molybdenum, defined as the <0.45 µm-filtered measurement. The 95% species protection DGV of 5 mg/L is recommended for application to slightly-to-moderately disturbed ecosystems.

1 Introduction

Molybdenum is a naturally occurring trace element that comprises approximately 0.0015% of the earth's crust and can be found extensively in nature (CCME 1999; ATSDR 2020). It has five possible oxidation states: +2, +3, +4, +5 and +6 (Amuda et al. 2018). Molybdenum is a micronutrient in plants and animals, and it occurs in more than 30 enzymes, including nitrogenases and xanthine oxidase (Cotton et al. 1999; Kośla et al. 2019; ATSDR 2020). Molybdenum does not occur naturally as a free metal (Smedley and Kinniburgh 2017) but as oxide or sulfide minerals such as molybdenite, powellite, wulfenite, ferrimolybdite, and ilsemannite (Smedley and Kinniburgh 2017; ATSDR 2020).

Approximately a third of global molybdenum production occurs through the mining of molybdenum ore, with the remaining proportion mostly a by-product of copper and tungsten production (Amuda et al. 2018; BC Ministry 2021). Most of the world's molybdenum is mined in China, Chile, the United States, Peru, Mexico and Canada (Amuda et al. 2018; ATSDR 2020). Australia has numerous molybdenum deposits, particularly in Queensland and Western Australia (Austrade 2021; Senior et al. 2021).

Molybdenum is used widely across industries. It has many metallurgical applications, including in high temperature furnaces and other heat resistant components, the production of metal alloys, as a support wire for tungsten filaments in incandescent light bulbs, and as a component of steel used in solar panels and wind turbines (Amuda et al. 2018; ATSDR 2020). It is also used in nuclear medicine for imaging and as a lubricant additive, catalyst and corrosion inhibitor (Smedley and Kinniburgh 2017; Amuda et al. 2018). Molybdenum compounds are also in printing inks, lacquers, paints, rubbers, leathers and fertilisers (CCME 1999).

The major source of molybdenum in marine water is from the natural weathering of continental material (e.g. rocks, soil) (Smedley and Kinniburgh 2017). Anthropogenic sources of molybdenum in marine water include fossil fuel combustion, leaching from fly ash, and mining and mineral processing wastes (CCME 1999; Smedley and Kinniburgh 2017).

Molybdenum exists in open marine water as molybdate oxyanion (MoO_4^{2-}) (Smedley and Kinniburgh 2017). It is the most abundant transition metal in the oceans, with a concentration in open (oxic) water of approximately 10 µg/L, which can reduce to <1 µg/L in hypoxic conditions. It has a very long residence time in oceanic water and is lost to sediments at a very slow rate (Smedley and Kinniburgh 2017). In contrast, molybdenum behaves less conservatively in estuarine water with low to intermediate salinities, with formation of a small proportion of inorganic colloidal or organic forms of molybdenum that deposit in sediments (van den Berg 1993). Smedley and Kinniburgh (2017) summarised published molybdenum concentrations for estuarine water, reporting a range of 0.1–15 µg/L.

There are limited published data on anthropogenically-elevated concentrations of molybdenum in aquatic ecosystems, especially in marine systems of Australia and New Zealand. Some data exist in relation to the Gove alumina refinery in the Northern Territory. Molybdenum concentrations in the refinery wastewater discharge were 12–18 µg/L (Harford et al. 2011; Negri et al. 2011); however, receiving water column concentrations would most likely have been lower than this upon immediate dispersion and dilution of the discharge. For the same refinery, molybdenum concentrations in

marine sediments (total extractable metal) and porewater near the discharge location were 1–4 mg/kg and 30–300 µg/L, respectively, dropping to ≤1 mg/kg and 20–60 µg/L at sites 1–2 km offshore (Cornall et al. 2013; Neave et al. 2013).

Regoli et al. (2012) assessed the bioaccumulation of molybdenum in several fish species and reviewed data for other aquatic biota. As with many other metals, an inverse relationship between exposure concentration and bioconcentration or bioaccumulation factor was found. This indicates that internal molybdenum concentrations are well regulated in the presence of variable external molybdenum concentrations. Regoli et al. (2012) reported whole body concentrations of molybdenum in a range of aquatic biota to be <1 mg/kg dry weight at background sites or sites slightly contaminated with molybdenum (e.g. <300 µg/L) and <20 mg/kg dry weight at sites highly contaminated with molybdenum (e.g. 1 000–4 000 µg/L). Overall, the data indicate that molybdenum does not bioaccumulate or biomagnify; therefore, the potential for significant food web exposure to animals is low (EcoMetrix 2008; Regoli et al. 2012).

There are few formal guideline values for molybdenum in marine water. ANZECC/ARMCANZ (2000) did not derive a DGV for molybdenum in marine water due to insufficient data. Instead, a low reliability indicative interim working level of 23 µg/L was recommended based on the application of an assessment factor of 200 to the lowest of only two available toxicity values (ANZECC/ARMCANZ 2000). There are now sufficient chronic toxicity data available to derive improved DGVs for marine water in Australia and New Zealand. Heijerick et al. (2012a) derived a 95% hazardous concentration (equivalent to a 95% species protection guideline value) for molybdenum in marine water of 5.70 mg/L, which was updated by Heijerick and Carey (2017) to 6.85 mg/L. Subsequently, van Dam et al. (2018a) derived 99%, 95%, 90% and 80% species protection guideline values for molybdenum in marine water of 1.82 mg/L, 3.88 mg/L, 5.97 mg/L and 10.7 mg/L, respectively. Notably, a number of the available chronic toxicity data cited by Heijerick and Carey (2017) and van Dam et al. (2018a) are from Australian studies for Australasian species. The updated DGVs reported here build upon the guideline values for molybdenum derived by Heijerick and Carey (2017) and van Dam et al. (2018a) and supersede the ANZECC/ARMCANZ (2000) value.

2 Aquatic toxicology

2.1 Mechanisms of toxicity

Molybdenum is a component of numerous enzymes in plants and animals (Kośla et al. 2019; ATSDR 2020; BC Ministry 2021). However, molybdenum can be toxic at high concentrations.

According to ATSDR (2020), the mechanism of toxicity of molybdenum has not been established. Available evidence is generally restricted to mammalian toxicology, but can be used to infer potential mechanisms for aquatic biota. Molybdenum toxicity appears to involve an interaction with copper. Molybdenum induces the mobilisation of internal copper, and molybdenum exposure results in effects that are also observed in copper-deficient animals (e.g. haematological effects such as anaemia and neutropenia, impaired bone formation, oxidative stress and metabolic disturbances associated with inhibition of copper-dependent enzymes (Zatta and Frank 2007), while the administration of high levels of copper can reduce or reverse these effects (Crosby 1998; ATSDR 2020; BC Ministry 2021). Molybdenum also interacts with sulfate, forming thiomolybdates, which can

complex with copper and reduce its cellular uptake (Kosla et al. 2019; ATSDR 2020). Molybdenum has also been reported to induce oxidative stress (ATSDR 2020).

Ricketts et al. (2015) assessed the effects of acute molybdenum exposure of up to 1 000 mg/L on a range of physiological and cellular biomarkers of stress in rainbow trout, but found no responses in any of them.

2.2 Toxicity

Molybdenum exhibits low acute toxicity to marine organisms, with reported LC50s typically in the hundreds to thousands of milligrams per litre. Eisler (1989) reviewed the acute toxicity of molybdenum to marine species, with a summary of the findings as follows (reported to ≤3 significant figures): 96-h LC50 of 247 mg/L for the amphipod *Allorchestes compressa*; 48-h LC50 of 22 mg/L for the crab *Eupagurus bernhardus*; 48-h LC50 of 1 020 mg/L for the crab *Carcinus maenus*; 96-h EC50 (shell growth) of 1 380 mg/L for the oyster *Crassostrea virginica*; 96-h LC50 of 1 210 mg/L for the shrimp *Americamysis bahia* (formerly called *Mysidopsis bahia*); 96-h LC50 of 1 910 mg/L for the shrimp *Penaeus duorarum*; 24-h LC50 of 254 mg/L for the starfish *Asterias rubens*; and a 96-h LC50 of 3 060 mg/L for the minnow *Cyprinodon variegatus*.

The chronic toxicity of molybdenum is also low, with toxicity typically reported near or above 10 mg/L. The mussel *Mytilus edulis* is the most sensitive species, with a 48-h EC10 (larval development) of 4.4 mg/L (Morgan et al. 1986 as reported by Heijerick et al. 2012b). This is followed by the copepod *Acartia tonsa* (Heijerick et al. 2012b), with a 20-d EC10 (reproduction, development) of 8 mg/L. For four Australasian species, the golden microalga *Tisochrysis lutea* (Trenfield et al. 2015), snail *Nassarius dorsatus* (Trenfield et al. 2016), barnacle *Amphibalanus amphitrite* (van Dam et al. 2016) and hermit crab *Coenobita variabilis* (van Dam et al. 2018b), NOECs ranging from 7 mg/L to 10 mg/L were reported. However, these NOECs were unbounded; that is, no effects were observed up to and including the highest molybdenum concentration tested. Thus, the true sensitivities of these species to molybdenum are unknown.

Other species that have been tested are less sensitive to molybdenum, with NOECs and EC10s generally close to or above 100 mg/L. The chronic toxicity of molybdenum ranged from 84.1 mg/L to 326 mg/L for seven species (reported as EC10s or NOECs): the diatom *Phaeodactylum tricornutum* (72-h growth rate) (Heijerick et al. 2012b); the red macroalga *Ceramium tenuicorne* (7-d growth rate) (Heijerick et al. 2012b); the sea urchin *Strongylocentrotus purpuratus* (48-h larval development) (Heijerick et al. 2012b); the sand dollar *Dendraster excentricus* (48-h larval development) (Heijerick et al. 2012b); the mysid shrimp *A. bahia* (14-d growth) (Heijerick et al. 2012b); the minnow *C. variegatus* (28-d growth) (Heijerick et al. 2012b); and the silverside *Menidia beryllina* (37-d growth) (Heijerick and Carey 2017).

The green microalga *Dunaliella tertiolecta* (72-h growth rate EC10 of 881 mg/L) and the oyster *Crassostrea gigas* (48-h larval development EC10 of 1 170 mg/L) were the least sensitive species (Heijerick et al. 2012b).

Sensitivity does not appear to be related to taxonomic group or trophic level and, interestingly, bivalve molluscs represent the most and least sensitive species. The modality of the dataset is discussed in Section 4.1.

3 Factors affecting toxicity

There is limited knowledge on the factors that affect the toxicity of molybdenum to aquatic species. Above pH 6, molybdenum predominantly occurs as the stable MoO_4^{2-} oxyanion and, given the stable pH of seawater (pH ~8), pH does not play a significant role in molybdenum bioavailability for marine species. Sulfate has been reported to reduce molybdenum toxicity (ATSDR 2020). This may be due to competitive inhibition between molybdate and sulfate anions at uptake sites (ATSDR 2020). Also, sulfate inhibits molybdate assimilation by phytoplankton. Low concentrations of molybdenum in marine phytoplankton—despite the molybdenum concentration (10 µg/L) of the water—have been attributed to the very high sulfate concentrations in marine water (i.e. 2 000–3 000 mg/L) (Eisler 1989). Overall, the high sulfate concentrations in marine water may make molybdenum less bioavailable and toxic to marine biota than to freshwater biota. Under euxinic conditions (i.e. hypoxic and sulfidic), molybdenum is sequestered by sulfides (including iron sulfide (FeS)) or thiomolybdates (and potentially, organic-rich phases) (Smedley and Kinniburgh 2017), thus being removed from the water column.

4 Default guideline value derivation

The DGVs were derived in accordance with the method described by Warne et al. (2018), except that the shinyssdtools software (version 0.2.0) (Dalgarno 2018) was used instead of the Burrlioz 2.0 software, and the DGVs were rounded to the appropriate number of significant figures, according to the guidance in Warne et al. (2025).

4.1 Toxicity data used in derivation

Molybdenum toxicity data for marine species that were compiled by Heijerick and Carey (2017) and van Dam et al. (2018a) were used as the base dataset for the DGV derivation. A literature search was also undertaken using Google Scholar and the USEPA ECOTOX database (USEPA 2021) to identify additional toxicity data for molybdenum.

As there were sufficient chronic toxicity data to derive the DGVs based on the minimum requirements (i.e. five species from four taxonomic groups), acute toxicity data were not used in the derivation. Chronic toxicity data for molybdenum were available for 15 marine species from nine taxonomic groups (one green microalga, one golden microalga, one diatom, one red macroalga, two echinoderms, one gastropod mollusc, two bivalve molluscs, four crustaceans and two fish). All data passed the quality assessment and screening processes prescribed by Warne et al. (2018). For all but one species, the chronic toxicity data were reported as measured dissolved (<0.45 µm filtered) molybdenum concentrations. Although the toxicity value for the mussel *M. edulis* was reported as a nominal concentration, this was confirmed by quantitative analysis (Morgan et al. 1986). Moreover, use of nominal concentrations for highly soluble substances tested in the ‘mg/L’ range is of less concern than for other types of substances.

Heijerick et al. (2012b) summarised the results of molybdenum chronic toxicity data for nine species from results originally reported in various consultancy reports. The original consultancy reports were

obtained from the International Molybdenum Association so that the primary data sources could be checked. An assessment of the chronic toxicity data summarised by Heijerick et al. (2012b), including justification for the toxicity values selected for the DGVs derivation, is in Appendix A. Also, as the EC10 for *M. edulis* (4.4 mg/L) was estimated by Heijerick et al. (2012b) using the raw data reported by Morgan et al. (1986), the approach used by Heijerick et al. (2012b) (i.e. a log-normal distribution fitted to the larval development data) was reproduced as a cross-check, and was confirmed accurate.

The marine mysid *A. bahia* and the silverside *M. beryllina* were assessed for molybdenum toxicity at a salinity of 20 PSU (Heijerick et al. 2012b; Heijerick and Carey 2017). Warne et al. (2018) recommend a marine water salinity minimum threshold of 25 PSU for deriving marine guideline values. Given the likelihood that sulfate concentrations in seawater will reduce molybdenum toxicity (Section 3), a salinity of 20 PSU was considered too low to be suitable for inclusion in the DGV derivation. Thus, the recommended marine water salinity minimum threshold of 25 PSU was retained and neither *A. bahia* nor *M. beryllina* were included in the final dataset.

Chronic toxicity data included a range of temperate, tropical and subtropical species. Most of the tropical/subtropical species were in the lower 50th percentile of the dataset, suggesting that they might be more sensitive to molybdenum than temperate species. However, four of the tropical/subtropical species (*T. lutea*, *N. dorsatus*, *A. amphitrite* and *C. variabilis*) reported unbounded toxicity values (NOECs) for the highest concentration tested (i.e. no significant effects were observed up to the highest tested concentration). For these species, the highest test concentration was between 7 mg/L and 10 mg/L, which is low in the overall range of all the reported toxicity values (i.e. between 4.4 mg/L and 1 170 mg/L). Thus, it is unclear at which concentrations of molybdenum these species would be affected. According to Warne et al. (2018), NOECs expressed as '>' or '≥' values can be used if (i) they are not too far outside the existing data range, and/or (ii) do not have an overly large influence on the final guideline values. Although the unbounded NOECs met criterion (i), the author determined them to have an unacceptable influence on the SSD and associated DGVs (criterion (ii)); therefore, they were excluded from the final dataset (Appendix B). Further assessment of the data did not reveal any basis that would support splitting the data into temperate and tropical datasets.

Although there is no mechanistic evidence to indicate that molybdenum exhibits a bimodal toxicity relationship due to taxa sensitivity (Section 2), the acceptable molybdenum toxicity data did cluster into a sensitive subset (toxicity ≤10 mg/L, n = 2) and a less sensitive subset (toxicity ≥100 mg/L, n = 7). However, as can be seen in the species sensitivity distribution (SSD) for these data (Figure 1), there is no distinct taxonomic differentiation between the two subsets. Moreover, the dataset is too small to discriminate taxa-specific sensitivity with confidence. Thus, the full dataset of acceptable toxicity values was used to derive the DGVs.

A summary of the toxicity data used to derive the DGVs is provided in Table 1. The final dataset comprised chronic toxicity data for nine species from seven taxonomic groups, including one green microalga, one diatom, one red macroalga, two echinoderms, two bivalves, one crustacean and one fish. Four of the nine species in the dataset occur in Australasian temperate and/or tropical marine waters, although two of these (*C. gigas* and *M. edulis*) are not native to the region. The dataset comprised nine EC10s. Further details on the data that passed the quality assessment and screening

process and were used to derive the DGVs are in Appendix C. Details of the data quality assessment and the data that passed the quality assessment are provided as supporting information.

Table 1 Summary of single chronic toxicity values, all species used to derive default guideline values for molybdenum in marine water

Taxonomic group	Species	Life stage	Duration (d)	Toxicity measure [a] (endpoint)	Final toxicity value (mg/L)
Green microalga	*Dunaliella tertiolecta* [b, d]	Exponential growth phase	3	EC10 (growth rate)	881
Diatom	*Phaeodactylum tricornutum* [b, d]	Exponential growth phase	3	EC10 (growth rate)	170
Red macroalga	*Ceramium tenuicorne* [b]	Cut algal tips, 2 d old cultures	7	EC10 (growth rate)	274
Echinoderm	*Strongylocentrotus purpuratus* [b]	Embryo	2	EC10 (larval development)	326
Echinoderm	*Dendraster excentricus* [b]	Embryo	2	EC10 (larval development)	234
Bivalve	*Crassostrea gigas* [b, d]	Embryo	2	EC10 (larval development)	1 170
Bivalve	*Mytilus edulis* [b, d]	Embryo	2	EC10 (larval development)	4.4
Crustacean	*Acartia tonsa* [b]	Embryo	20	EC10 (reproduction, development)	7.96
Fish	*Cyprinodon variegatus* [b, c]	Embryo-larval	28	EC10 (growth)	84.1

a The measure of toxicity being estimated/determined. EC10: 10% effect concentration.
b Temperate species.
c Tropical species.
d Species known to occur in Australasian marine water.

4.2 Species sensitivity distribution

The cumulative frequency (species sensitivity) distribution (SSD) of the nine toxicity values reported in Table 1 is shown in Figure 1. The SSD was plotted using the shinyssdtools (version 0.2.0) software. The model provides a poor fit to the data (Figure 1). Although only one of the nine toxicity values did not sit close to the fitted model (crustacean *A. tonsa*), the model had little data available to inform the shape of the lower tail (i.e. below 100 mg/L), resulting in high uncertainty in this part of the SSD. Further details on the SSD fitting process are in Appendix D.

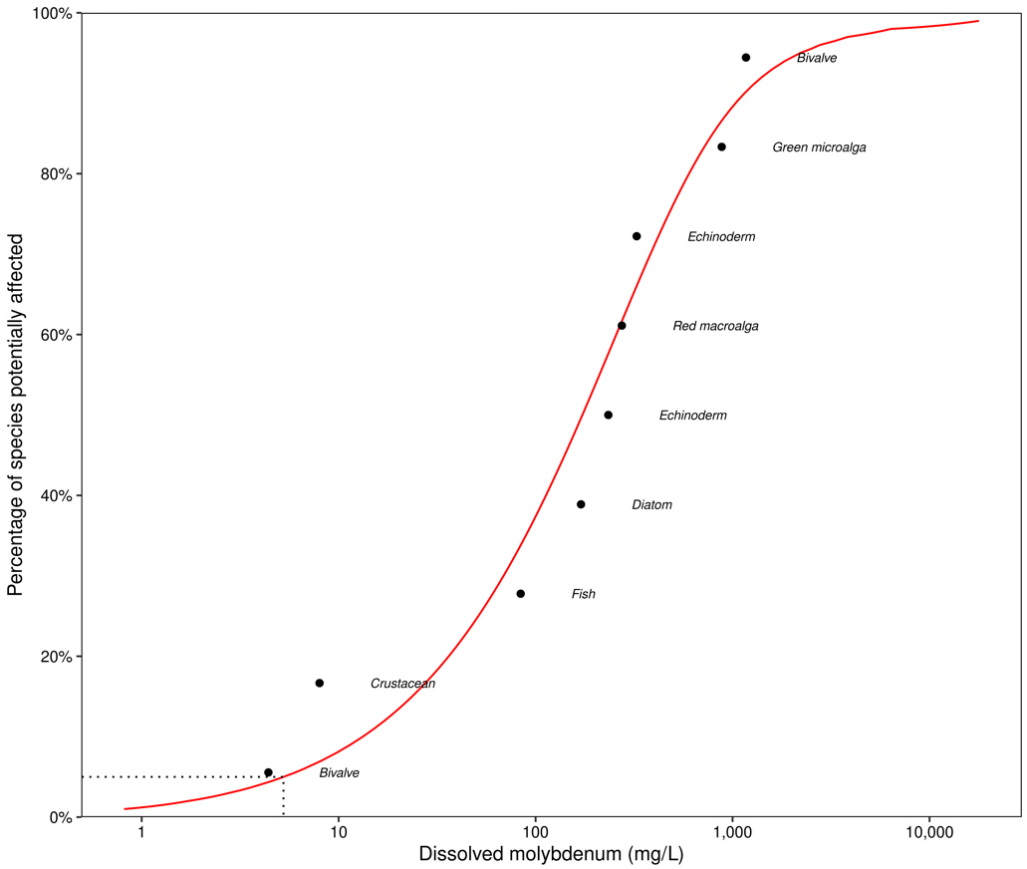


Figure 1 Species sensitivity distribution, molybdenum in marine water

4.3 Default guideline values

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

The DGVs for 99%, 95%, 90% and 80% species protection for molybdenum in marine water are in Table 2. The uncertainty associated with the DGVs means that they are only reported to one significant figure (Appendix E). The DGVs relate to dissolved molybdenum, defined as the <0.45 µm-filtered measurement. The 95% species protection DGV of 5 mg/L is recommended for application to slightly-to-moderately disturbed ecosystems.

The 95% species protection DGV is protective of the four Australasian tropical species for which the molybdenum toxicity data were deemed not acceptable for inclusion in the DGV derivation (Section 4.1 and Appendix B). Because there is insufficient evidence of regional/climatic differences in molybdenum toxicity, the DGVs are applicable to both temperate and tropical marine water. Guidance on the application of DGVs to estuarine water is in ANZG (2018).

The current DGVs differ from the guideline values derived by Heijerick and Carey (2017) and van Dam et al. (2018a) for the following key reasons.

- Heijerick and Carey (2017) used data for two species (*A. bahia* and *M. beryllina*) that were excluded from the current DGV derivation because the salinity (20 PSU) was too low.
- van Dam et al. (2018a) used the unbounded NOECs for the four Australasian species that were excluded from the current DGV derivation for the reasons detailed in Section 4.1 and Appendix B.
- Different SSD modelling approaches were used for all three derivations.

Environmental monitoring data for comparison with a DGV must be rounded according to the Australian Standard AS 2706-2003 (Standards Australia 2003) to the number of significant figures in the DGV.

Table 2 Default guideline values, molybdenum in marine water, moderate reliability

Level of species protection (%)	DGV for molybdenum in marine water (mg/L) [a]
99	0.6
95	5
90	10
80	40

a The DGVs were derived using the shinyssdtools (Version 0.2.0) software and rounded according to the details in Appendix E.

4.4 Reliability classification

The molybdenum marine water DGVs have a moderate reliability classification (Warne et al. 2018) based on the outcomes for the following three criteria:

- sample size—9 (good)
- type of toxicity data—chronic EC10, NOEC
- SSD model fit—poor.

Glossary

Term	Definition
acute toxicity	A lethal or adverse sub-lethal effect that occurs as the result of a short exposure period to a chemical relative to the organism's life span.
bioaccumulation	The process by which chemical substances are accumulated by aquatic organisms by all routes of exposures (dietary and the ambient environment).
chronic toxicity	A lethal or sublethal adverse effect that occurs after exposure to a chemical for a period of time that is a substantial portion of the organism's life span or an adverse effect on a sensitive early life stage.
default guideline value (DGV)	A guideline value recommended for generic application in the absence of a more specific guideline value (e.g. site-specific) in the Australian and New Zealand Guidelines for Fresh and Marine Water Quality.
EC10 (10% effect concentration)	The concentration of a substance in water or sediment that is estimated to produce a 10% change in the response being measured or a certain effect in 10% of the test organisms relative to the control response, under specified conditions.
EC50 (median effective concentration)	The concentration of a substance in water or sediment that is estimated to produce a 50% change in the response being measured or a certain effect in 50% of the test organisms relative to the control response, under specified conditions.
endpoint	The specific response of an organism that is measured in a toxicity test (e.g. mortality, growth, a particular biomarker).
guideline value	A measurable quantity (e.g. concentration) or condition of an indicator for a specific community 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 community value. Guideline values for more than one indicator should be used simultaneously in a multiple lines of evidence approach.
LC50 (median lethal concentration)	The concentration of a substance in water or sediment that is estimated to be lethal to 50% of a group of test organisms, relative to the control response, under specified conditions.
NOEC (no observed effect concentration)	The highest concentration of a material used in a toxicity test that has no statistically significant adverse effect on the exposed population of test organisms as compared with the controls.
PSU	Practical salinity units.
site-specific guideline value	A guideline value that is relevant to the specific location or conditions that are the focus of a given assessment or issue.
species (biological)	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.
SSD (species sensitivity distribution)	A method that plots the cumulative frequency of species' sensitivities to a toxicant and fits a statistical distribution to the data. From the distribution, the concentration that should theoretically protect a selected percentage of species can be determined.
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: Assessment of the chronic toxicity data summarised by Heijerick et al. (2012b)

Table A 1 Data assessment of species used by Heijerick et al. (2012b)

Species	Source study	Toxicity value (mg/L)		Assessment	Final value selected (mg/L)
		EC10 (95% CI)	NOEC		
Dunaliella tertiolecta	Le Page and Hayfield (2010)	*Growth rate:* 881 (not calculable) [a]	*Growth rate:* ≥938	*Growth rate:* Poor (non-monotonic) concentration–response relationship. Maximum growth rate per cent inhibition was 13% (not significant) at 356 mg/L, with 3% and 8% inhibition at 591 mg/L and 938 mg/L (highest test concentration), respectively. Overall, the reliability of the EC10 and the unbounded NOEC (≥938 mg/L) for growth rate is questionable. However, the EC10 is conservative relative to the NOEC; therefore, it is the preferred value. Notably, the choice of value does not change the DGVs when rounded to the appropriate number of significant figures.	881
		Biomass: 513 (432–725)	*Biomass:* ≥938	*Biomass:* This endpoint is less relevant than growth rate. Poor (non-monotonic) concentration–response relationship; therefore, it is not considered further.	
Phaeodactylum tricornutum	Kools and Vanagt (2009)	170 (144–191) [a]	150	Good concentration–response relationship. Data reliable. EC10 is the preferred value.	170
Ceramium tenuicorne	Le Page et al. (2010)	274 (<0–507)	641 [a]	Small concentration–response relationship, with a generally monotonic reduction in growth rate up to a 38% reduction at 1 190 mg/L (highest test concentration). Le Page et al. (2010) warned against using the EC10 due to high variability, instead suggesting the NOEC as a more reliable value. However, the effect at the NOEC corresponded to an almost 20% effect, whereas the EC10 of 274 mg/L lay between concentrations with effect sizes of 2% (215 mg/L) and 15% (328 mg/L). Therefore, despite the warning provided by Le Page et al. (2010), the EC10 is the preferred value as it is more representative of a negligible effect concentration.	274
Strongylocentrotus purpuratus	Parametrix (2010)	326 (269–394) [a]	265	Full concentration–response relationship with partial responses. Result is considered reliable, with the EC10 being the preferred value.	326

Species	Source study	Toxicity value (mg/L)		Assessment	Final value selected (mg/L)
		EC10 (95% CI)	NOEC		
Dendraster excentricus	Parametrix (2008)	234 (232–236) [a]	218	Full concentration–response relationship, although no partial responses. No significant effects were observed up to and including the second highest test concentration of 218 mg/L, followed by a 100% effect (i.e. 0% normal larvae) at the highest test concentration of 438 mg/L. Result is considered reliable, with the EC10 being the preferred value.	234
Crassostrea gigas	Kools and Vanagt (2009)	1 174 (577–1 534) [a]	1 100	Good concentration–response relationship. Data reliable. EC10 is the preferred value.	1 174
Mytilus edulis	Morgan et al. (1986)	4.4 (not reported) [a]	Not reported	The EC10 was based on re-analysis of the data from Morgan et al. (1986) by Heijerick et al. (2012b), using a log-normal distribution (Morgan et al. 1986 reported an EC50 only). The log-normal regression analysis was reproduced and the EC10 verified as accurate. The EC10 is the preferred value.	4.4
Americamysis bahia	Lehmann (2010)	Not calculable	≥116	The study was conducted at a salinity of 20 PSU, which is below the Warne et al. (2018) minimum salinity criterion for marine water of 25 PSU. Thus, the species was not included in the DGV derivation.	–
Acartia tonsa	Kools and Vanagt (2009)	*Reproduction, F0:* 4.2 (0.5–660)	*Reproduction, F0:* 270	*Reproduction, F0:* Unusual concentration–response relationship, with ~25–30% effect relative to controls at first four concentrations, followed by monotonic reduction in reproduction over final two concentrations. Resulted in an EC10 below the lowest concentration tested. Data indicate uncertainty in the reliability of this test, as noted by Heijerick et al. (2012b); therefore, not considered further.	7.96
		Development: 7.96 (0.14–27) [a]	*Development:* 26	*Development:* Reasonable concentration–response relationship. Data reliable. EC10 is the preferred value.	
		Reproduction, F1: 14.9 (13.9–16.8)	*Reproduction, F1:* 79	*Reproduction, F1:* Poor (non-monotonic) concentration–response relationship; therefore, not considered further.	
Cyprinodon variegatus	Parametrix (2009)	*Larval survival:* 485 (404–582)	*Larval survival:* 444	Incomplete concentration–response relationships for all endpoints, but with sufficient effects measured to estimate NOECs, EC10s and EC20s with confidence intervals. Higher growth was observed at the highest test concentration, but this was a density dependent effect due to high (~70%) mortality at this concentration. This test concentration was excluded from the analysis. The NOEC (dry weight) of ≤64 mg/L corresponded to an approximate 9% effect; thus, the EC10 (dry weight) of 84 mg/L is considered an appropriate estimate of a 10% effect and is the preferred value.	84.1
		Dry weight: 84 (36–199) [a]	*Dry weight:* ≤64		
		Biomass: 392 (309–498)	*Biomass:* 112		

Note: CI: confidence interval.

a Toxicity estimate used by Heijerick et al. (2012b) for deriving a predicted no effect concentration for molybdenum.

Appendix B: Assessment of unbounded NOEC inclusion

The reported NOECs for four species in the available dataset were unbounded, representing the highest concentration tested (i.e. no significant effects were observed up to the highest tested concentration) (Table B 1). For these species, the highest test concentration was between 7 mg/L and 10 mg/L, which is low in the overall range of all the reported toxicity values (i.e. between 4.4 mg/L and 1 170 mg/L). These unbounded NOECs are uncertain and may be unrepresentative of the true threshold of effects for the four species. According to Warne et al. (2018), NOECs expressed as '>' or '≥' values can be used if (i) they are not too far outside the existing data range, and/or (ii) do not have an overly large influence on the final GVs. This is assessed below.

Table B 1 Unbounded chronic toxicity values for molybdenum

Species	Toxicity measure (endpoint)	Reported toxicity value (mg/L)
Tisochrysis lutea	NOEC (growth rate)	9.5
Nassarius dorsatus	NOEC (growth rate)	7.0
Amphibalanus amphitrite	NOEC (larval development)	9.0
Coenobita variabilis	NOEC (larval development)	10.0

Location of unbounded data in the dataset

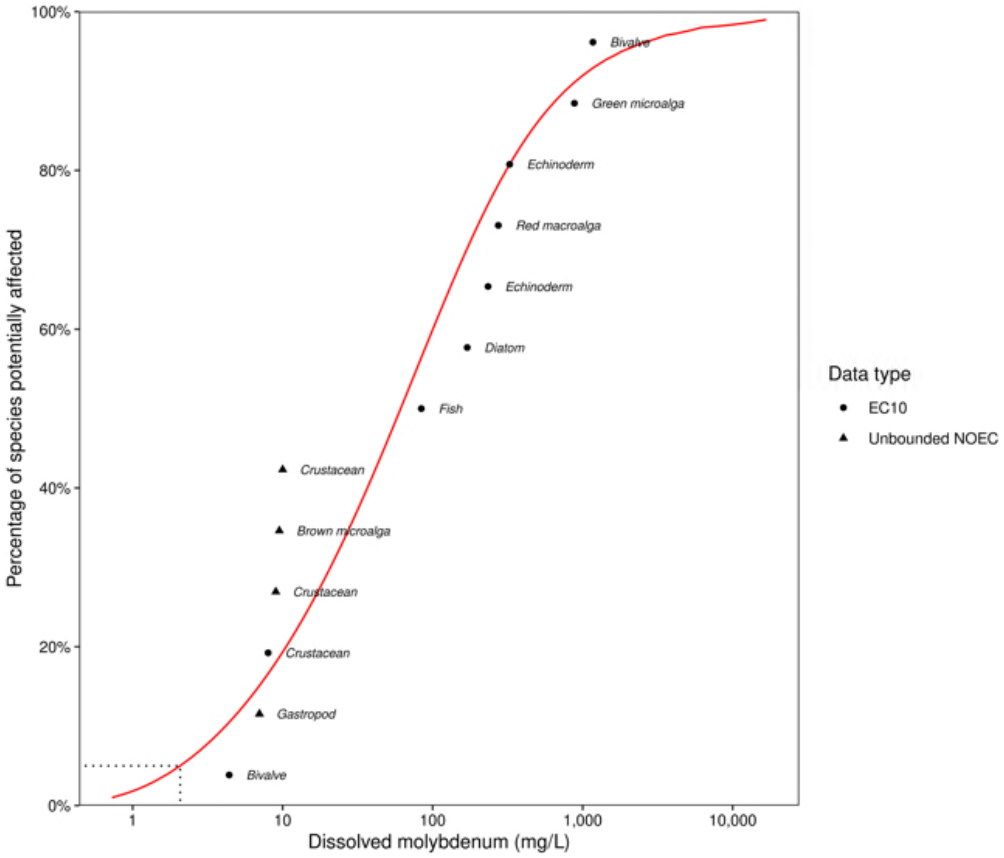
All the unbounded NOECs are within the data range for bounded values of 4.4 mg/L to 1 170 mg/L, which meets the Warne et al. (2018) criterion (i). However, the unbounded NOECs range from 7 mg/L to 10 mg/L, which is at the low end of the data range. While this is conservative (i.e. offers additional protection for these species), including these four values may over-represent the proportion of sensitive species, which could affect the DGVs (criterion (ii)).

Influence of unbounded NOECs on the default guideline values

To assess the influence of the unbounded NOECs on the DGVs, two datasets were examined:

- all available and acceptable chronic toxicity data, including the unbounded NOECs (dataset = 13 values)
- all available and acceptable chronic toxicity data, excluding the four unbounded NOECs (dataset = nine values).

Species sensitivity distributions (SSDs) were fitted to the datasets using shinyssdtools (version 0.2.0) software, and are shown in Figure B 1 and Figure B 2. The resultant 99%, 95%, 90% and 80% protective concentration (PC) values are in Table B 2. The unbounded NOECs affected the PC values. The effect was minor for the PC99 value (<2-fold difference), but was greater for the PC95 value (~2.5-fold difference), PC90 value (~3.5-fold difference) and PC80 value (~4-fold difference). For the last three cases, exclusion of the unbounded NOECs resulted in less conservative (i.e. higher) PC values, compared to the full dataset. This is attributed to the SSD for the full dataset being shifted to the left by the near-vertical stacking of five values between 7 mg/L and 10 mg/L, four of which are the unbounded NOECs, around the 10th to 40th percentiles (Figure B 1). This demonstrates that the unbounded NOECs influence the shape of the SSD and the PC values.



Note: The log-normal/log-normal mixture distribution was assigned the highest weight for the full dataset (data not shown), but this was an artefact of the inclusion of the four unbounded NOECs, which artificially created a bimodal dataset, as can be seen in Figure B 1. Consequently, this distribution was removed from the model averaging process for the full dataset. As described in Appendix D, the log-normal/log-normal mixture distribution was assigned a zero weight for the reduced dataset and thus had no influence on the resultant PC values.

Figure B 1 Species sensitivity distribution, chronic toxicity dataset including unbounded NOECS

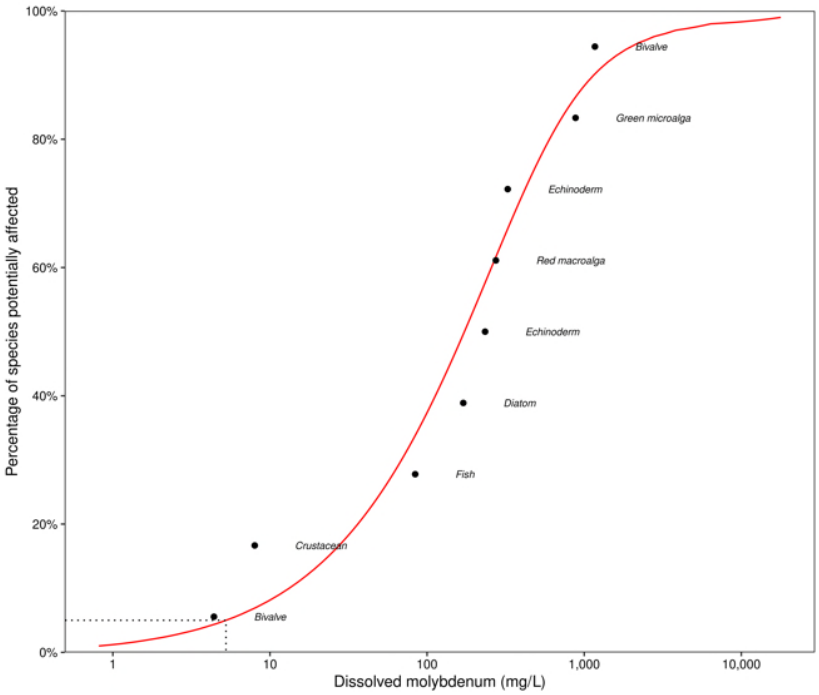


Figure B 2 Species sensitivity distribution, chronic toxicity dataset excluding unbounded NOECS

Table B 2 Protective concentration values, both datasets

Protective concentration value	Molybdenum (mg/L) [a]	
	Dataset including unbounded NOECs (n = 13)	**Dataset excluding unbounded NOECs (n = 9)**
PC99	0.73	0.59
PC95	2.1	5.2
PC90	4.2	13
PC80	11	35
Fit of SSD	Poor	Poor
Reliability of PC values	Moderate	Moderate

a Rounded to two significant figures.

The reliability of the PC values was also considered for each of the datasets, based on the reliability classification prescribed by Warne et al. (2018). The SSD of the dataset including the unbounded NOECS provided a poor fit across most of the dataset (Figure B 1). The SSD of the dataset excluding the unbounded NOECS provided a poor fit at the lower end of the dataset. As the sample size of both datasets is ≥8, the PC values have a *moderate* reliability.

Although there are benefits to including data for more species and taxonomic groups, the data must have sufficient certainty. Inclusion of uncertain values reduces confidence in the SSD and PC values, particularly when those values are influential in determining the shape of the SSD. Consequently, the unbounded NOECs were excluded from the dataset due to their uncertainty and the influence they had on the SSD and PC values.

Appendix C: Toxicity data that passed the screening and quality assessment and were used to derive the default guideline values

Table C 1 Summary, chronic toxicity data that passed the screening and quality assessment processes, molybdenum in marine water

Taxonomic group	Species	Life stage	Exposure duration (d)	Test medium	Toxicity measure [a] (test endpoint)	pH	Temp. (°C)	Salinity (PSU)	Toxicity value (mg/L) [b]	Reference
Green microalga	*Dunaliella tertiolecta*	Exponential growth phase, 10^4 cells/mL	3	MM/5 Medium, based on ISO 10253/2006	EC10 (Growth rate)	8.0–8.5	20 ± 2	32	881	Le Page and Hayfield (2010); Heijerick et al. (2012b)
	–								**881**	**Value used in SSD**
Diatom	*Phaeodactylum tricornutum*	Exponential growth phase, 10^4 cells/mL	3	Artificial seawater with nutrients	EC10 (Growth rate)	8.0–8.1	22.0–23.4	31	170	Kools and Vanagt (2009); Heijerick et al. (2012b)
	–								**170**	**Value used in SSD**
Red macroalga	*Ceramium tenuicorne*	Cut algal tips, 2 d old cultures	7	Natural seawater with added nutrients	EC10 (Growth rate (length))	8.1–8.3	21.8–21.9	30	274	Le Page et al. (2010); Heijerick et al. (2012b)
	–								**274**	**Value used in SSD**
Echinoderm	*Strongylocentrotus purpuratus*	Embryo (1 h post-fertilisation)	2	Natural seawater	EC10 (Larval development)	8.0–8.3	15.0 ± 1.0	29	326	Parametrix (2010); Heijerick et al. (2012b)
	–								**326**	**Value used in SSD**
	Dendraster excentricus	Embryo (2 h post-fertilisation)	2	Natural seawater	EC10 (Larval development)	8.0 ± 0.1	15.9 ± 0.1	30	234	Parametrix (2008); Heijerick et al. (2012b)
	–								**234**	**Value used in SSD**

Taxonomic group	Species	Life stage	Exposure duration (d)	Test medium	Toxicity measure [a] (test endpoint)	pH	Temp. (°C)	Salinity (PSU)	Toxicity value (mg/L) [b]	Reference
Bivalve	*Crassostrea gigas*	Embryo (freshly fertilised)	2	Natural filtered seawater	EC10 (Larval development)	7.9–8.1	19.7–20.9	33	1 174	Kools and Vanagt (2009); Heijerick et al. (2012b)
	–								**1 170**	**Value used in SSD**
	Mytilus edulis	Embryo (2 h post-fertilisation)	2	Natural filtered seawater	EC10 (Larval development)	8.4 ± 0.2	19 ± 1	26	4.4	Morgan et al. (1986); Heijerick et al. (2012b) [c]
	–								**4.4**	**Value used in SSD**
Crustacean	*Acartia tonsa*	Embryo	20	Natural filtered seawater	EC10 (Reproduction, development)	8.0–8.2	19.7–20.5	28	7.96	Kools and Vanagt (2009); Heijerick et al. (2012b)
	–								**7.96**	**Value used in SSD**
Fish	*Cyprinodon variegatus*	Embryo-larval	28	Reconstituted seawater	EC10 (Growth)	25.1 ± 0.4	7.6–8.0	28	84.1	Parametrix (2009); Heijerick et al. (2012b)
	–								**84.1**	**Value used in SSD**

a The measure of toxicity being estimated/determined. EC10: 10% effect concentration.

b Value used in the SSD rounded to three significant figures.

c The original study conducted by Morgan et al. (1986) reported a 48-h EC50 (development) of 147 mg/L. Heijerick et al. (2012b) re-analysed the raw data from Morgan et al. (1986) and reported a 48-h EC10 (development) of 4.4 mg/L.

Appendix D: Details of the shinyssdtools SSD fitting process for the molybdenum toxicity dataset

The SSD software package shinyssdtools (version 0.2.0) uses a model averaging approach to generating an SSD (described by Fox et al. 2021). Figure D 1 shows the full set of default distributions fitted to the molybdenum marine toxicity dataset, while Table D 1 provides the relevant goodness-of-fit and weighting estimates for each of the distributions. The log normal – log normal mixture distribution was weighted zero because it has five parameters that, when compared to the dataset of only nine values, represents over-fitting. The final model-averaged SSD is shown in Figure 1.

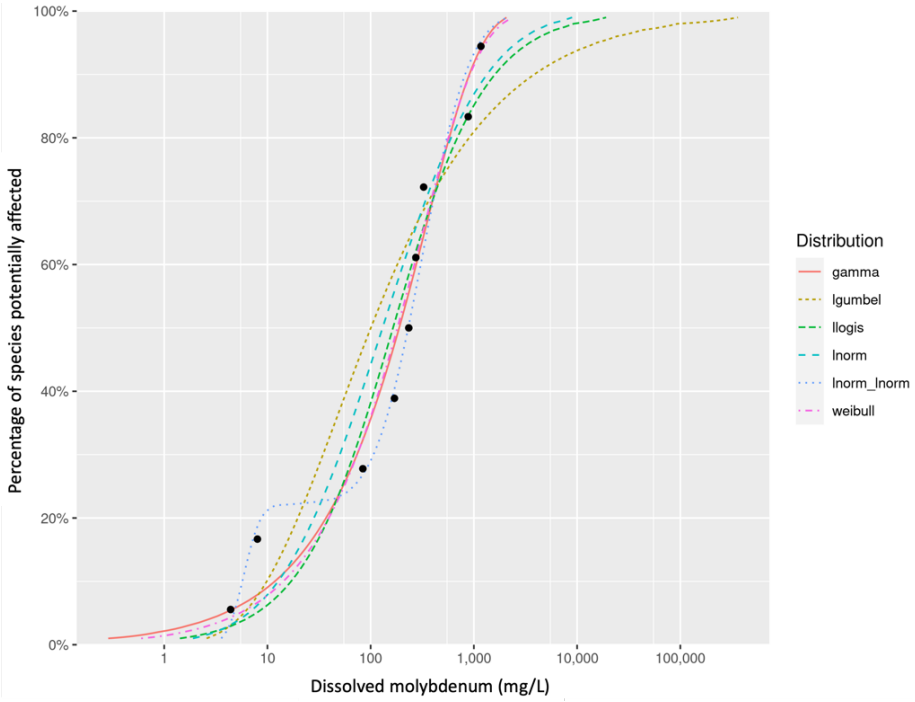


Figure D 1 Species sensitivity distributions, six default distributions used to model the molybdenum marine toxicity dataset

Table D 1 Goodness-of-fit and weighting estimates, six default distributions used in model averaging for the molybdenum marine toxicity dataset

Distribution	Akaike's Information Criterion	Corrected Akaike's Information Criterion	Delta	Weight
Gamma	-1.35	0.645	0	0.383
Weibull	-1.09	0.913	0.268	0.335
Log normal	0.789	2.79	2.14	0.131
Log logistic	1.06	3.06	2.41	0.115
Log gumbel	3.39	5.39	4.75	0.036
Log normal – log normal	-1.6	18.4	17.8	0

Appendix E: Assessment of significant figures for default guideline values

The number of significant figures to which DGVs are reported is determined by the degree of uncertainty in the values, based on their standard errors, according to the following rule:

The significant figure to which a DGV is reported must correspond to the place of the first significant figure in the standard error of the DGV. Where the standard error is greater than the DGV, the DGV must be reported to one significant figure.

For molybdenum in marine water DGVs, the raw PC values and their standard errors are shown in Table E 1. Standard errors were determined using shinyssdtools (version 0.2.0) with the default set of distributions (see Appendix D). For all PC values, the standard errors were greater than the raw PC values, dictating that all the DGVs are reported to one significant figure.

Table E 1 Assessment of number of significant figures, molybdenum in marine water

Level of species protection (%)	Raw PC value (mg/L)	Standard error	Interpretation of significant figures rule	Final DGV (mg/L)
99	0.589	8.12	SE > PCx value; therefore, report DGV to one significant figure	0.6
95	5.22	18.0	SE > PCx value; therefore, report DGV to one significant figure	5
90	13.1	28.3	SE > PCx value; therefore, report DGV to one significant figure	10
80	35.3	47.4	SE > PCx value; therefore, report DGV to one significant figure	40

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