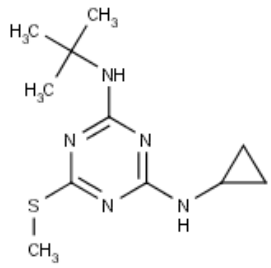
CYBUTRYNE (IRGAROL)

This EQS dossier was prepared by the Sub-Group on Review of the Priority Substances List (under Working Group E of the Common Implementation Strategy for the Water Framework Directive).

The dossier was reviewed by the Scientific Committee on Health and Environmental Risks (SCHER), which commented that the assessment factor of 8 for the MAC-QS from the SSD was not fully explained. Explanation has been added in section 7.

1 CHEMICAL IDENTITY

Common name	Cybutryne*
Chemical name (IUPAC)	N'-tert-butyl-N-cyclopropyl-6-(methylthio)-1,3,5-triazine-2,4-diamine
Synonym(s)†	Irgarol® 1051, Irgarol® 1071, Irgaguard® D 1071
Chemical class (when available/relevant)	Triazine
CAS number	28159-98-0
EU number	248-872-3
Molecular formula	C11H19N5S
Molecular structure	
Molecular weight ($g.mol^{-1}$)	253.37

2 EXISTING EVALUATIONS AND REGULATORY INFORMATION

Annex III EQS Dir. (2008/105/EC)	Not Included
Existing Substances Reg. (793/93/EC)	Not listed in a priority list
Pesticides (91/414/EEC)	Not included in Annex I
Biocides (98/8/EC)	Not included in Annex I (see below, "other relevant chemical regulation") Included in 2010/72/: Commission Decision of 8 February

* Irgarol 1051 is the trade name for an algicide used in antifouling coatings, CAS No. 28159-98-0. The name cybutryne is another name of this substance. Irgarol 1051/Irgarol will however be used in most cases in the following text due to the use of this name in the original studies.

† These are trade names rather than synonyms

	2010 concerning the non-inclusion of certain substances in Annex I, IA or IB to Directive 98/8/EC. regarding use in Product-type 9: Fibre, leather, rubber and polymerised materials preservatives.
PBT substances	Not investigated
Substances of Very High Concern (1907/2006/EC)	No Not listed in the ECHA Candidate List of Substances of Very High Concern for authorisation
POPs (Stockholm convention)	No
Other relevant chemical regulation (veterinary products, medicament, ...)	Listed in annex I of EC regulation 1451/2007 as an active substance identified as existing and in annex II, as a substance to be examined under the review programme.
Endocrine disrupter	Not evaluated[‡]

3 PROPOSED QUALITY STANDARDS (QS)

ENVIRONMENTAL QUALITY STANDARD (EQS)

QS for water is the "critical QS" for derivation of an Environmental Quality Standard

	Value	Comments
Proposed AA-EQS for [freshwater] [µg.l^{-1}] **Proposed AA-EQS for [marine water] [µg.l^{-1}]**	**0.0025**	**Critical QS is QS$_{water}$.** **See section 7**
Proposed MAC-EQS for [freshwater] [µg.L^{-1}] **Proposed MAC-EQS for [marine water] [µg.L^{-1}]**	**0.016**	**See section 0**

SPECIFIC QUALITY STANDARD (QS)

Protection objective[§]	Unit	Value	Comments
Pelagic community (freshwater)	[µg.l^{-1}]	0.0025	See section 0
Pelagic community (marine water)	[µg.l^{-1}]	0.0025	
Benthic community (freshwater)	[µg.kg^{-1} $_{dw}$]	0.18	EqP, see section 0
	[µg.l^{-1}]		
Benthic community (marine)	[µg.kg^{-1} $_{dw}$]	0.18	
	[µg.l^{-1}]	-	
Predators (secondary poisoning)	[µg.kg^{-1} $_{biota\ ww}$]	230	See section 7.2

[‡] Endocrine effects have been studied in snails. No effects were observed in the snail *Lymnaea stagnalis* up to and including the highest tested concentration (117 µg/l) (Habekost *et al.*, 2010) or in the snail *Ilyanassa obsoleta* (highest tested concentration 2.5 mg/l) (Finnegan *et al.*, (2009), while effects in ng/l concentrations were observed in *Radix balthica* in a mesocosm study (UBA Umweltbundesamt, 2007).

[§] Please note that as recommended in the Technical Guidance for deriving EQS (European Commission, 2011), "EQSs […] are not reported for 'transitional and marine waters', but either for freshwater or marine waters". If justified by substance properties or data available, QS for the different protection objectives are given independently for transitional waters or coastal and territorial waters.

	[µg.l^{-1}]	0.9 (fresh and marine waters)	
Human health via consumption of fishery products	[µg.kg$^{-1}_{\text{biota ww}}$]	1400	See section 7.3
	[µg.l^{-1}]	6,0 (fresh and marine waters)	
Human health via consumption of water	[µg.l^{-1}]	0.1	

4 MAJOR USES AND ENVIRONMENTAL EMISSIONS

4.1 USES AND QUANTITIES

Irgarol 1051 is an effective herbicidal biocide mainly used as an antifouling agent in paints for boats and vessels. It is applied at marine as well as at inland freshwater sites. Referring to the technical information provided by the former producer, an amount of Irgarol between 1 - 6 % (on weight-% binder solids) is recommended for marine coatings. Irgarol 1051 is often combined with copper or copper compounds in anti fouling paints. (Ciba, 2004a)

Cybutryne (N'-tert-butyl-N-cyclopropyl-6-(methylthio)-1,3,5-triazine-2,4-diamine) is a low production chemical (LPV), one producer is listed in ESIS (2009).

Irgarol® 1071 and Irgaguard® D 1071 have been designed for use in the manufacture of aqueous and solvent coating compositions: paints, coatings, stucco, stains and seals for outdoor uses to inhibit or control the growth of algae on coating surfaces. An amount of Irgarol between 0.1 - 1 % is recommended (on weight % binder solids Ciba (2004b).

4.2 ESTIMATED ENVIRONMENTAL EMISSIONS

The emission of Irgarol used as an antifouling agent on boats has been estimated to 1.89 µg/cm^2/day at steady state (KEMI, 2006).

5 ENVIRONMENTAL BEHAVIOUR

5.1 ENVIRONMENTAL DISTRIBUTION

Physical chemical data on Irgarol have been evaluated by the Swedish Chemicals Agency (KEMI, 1998). These data and data from a number of additional studies are listed in the table below.

		Master reference
Water solubility (mg.l^{-1})	7	(KEMI, 1998)
Volatilisation		
Vapour pressure (Pa)		
Henry's Law constant		

($Pa.m^3.mol^{-1}$)		
Adsorption	**The log K_{OC} = 3.15 is used for derivation of quality standards.** The K_{OC} is the geometric mean of K_{OC} from studies listed below with Kimlish code 1 or 2. Where a range was given the mean of the min and max was used.	
Organic carbon – water partition coefficient (K_{OC})	K_{OC} = 548 – 2590 (Log K_{OC}= 2.7-3.4) Kimlish code: 2 (validated by the Swedish Chemicals Agency but original data not available for assessment)	KEMI (1998)
	log K_{OC} = 3.3 ±0.72 Mean value from field studies in German marinas (n=7) in the Baltic Sea. Kimlish code: 3 (Partitioning of the substance in the field may be affected by other factors than the K_{OC})	Biselli *et al.* (2000)
	Log K_{OC} = 3.58-4.06 (4.36 assessed as an outlier). Adsorption coefficients in an indoor pond system, on day 147, at Irgarol concentrations between 0.04-5 µg/l. Kimlish code: 3 (Partitioning of the substance in the mesocosm may be affected by other factors than the K_{OC})	Umweltbundesamt UBA (2007)
	Log K_{OC} (±SD)= 2.16 ±0.03 Based on a triphasic SPME equilibrium model. Kimlish code: 3 (The reliability of this method in comparison to the standardised OECD tests is uncertain)	Lam *et al.* (2006)
	K_{OC} = 472-2158, mean 1106 (log K_{OC} = 2.7-3.3, mean 3.0) Adsorption Kimlish code: 2 (no description of experiment available but it is stated that US EPA Guideline 163-1 was followed)	Ciba (2006)
	Log K_{OC} = 2.41-3.65 Batch type equilibrium experiments on sediments; 20 and 200 g/l of suspended solids.	Comber *et al.* (2002)

	Kimlish code: 2 (Data from experiment with 1 g/l susp. excluded due to the remark by the author that there was analytical imprecision in this test) Log K_{OC} = 3.0 Dissolved and suspended phases in water from a marina. Kimlish code: 3 (Partitioning of the substance in the field may be affected by other factors than the K_{OC}) Log K_{OC}= 3.38 and 3.47 (direct and headspace, respectively) Partitioning to humic organic matter (Fluka humic acids) measured with solid-phase microextraction (SPME). Kimlish code: 2 Log K_{OC}: 2.7 QSAR for triazines and a log K_{OW} of 3.95. ($logK_{oc}=0.4*logK_{ow}+1.12$)	Tolosa *et al.* (1996) Lambropoulou *et al.* (2004) Calculated in accordance with the TGD for deriving EQS (European Commission, 2011)
Sediment – water partition coefficient ($K_{sed-water}$) **Suspended matter – water partition coefficient ($K_{susp-water}$)**	36 m^3 m^{-3}	
Bioaccumulation	**The BCF value 250 on fish is used for derivation of quality standards.**	
Octanol-water partition coefficient (Log Kow)	log K_{OW} = 3.95	Evaluated by KEMI (1998)
BCF (measured) Fish, *Lepomis macrochirus* Fish, *Cyprinodon variegatus* Algae and aquatic plants *Vaucheria* spp., *Potamogeton lucens, P.pectinus, Elodea nuttallii* *Myriophyllum verticillatum*	 160 240 (exposure conc. 36 mg/l) 250 (exposure conc. 3.6 mg/l) 30 000 (estimated) 744 - 1 520 (based on fresh weight)	 Dionne (1991) Dionne (1991) Evaluated by KEMI (1998) Mohr *et al.* (2009)

	6 790 - 10 560 (based on dry weight), time weighted average 150 d, pond study, single application, TWA: 0.006 - 0.211 µg/L	

5.2 ABIOTIC AND BIOTIC DEGRADATIONS

The major degradation product of Irgarol 1051 is M1 (2-methylthio-4-tert-butylamino-6-amino-s-triazine) (see *e.g.* Okamura *et al.*, 1999; Okamura *et al.*, 2000b; Liu *et al.*, 1997).

The Swedish Chemicals Agency has evaluated degradation studies regarding Irgarol 1051 and concluded that the substance is hydrolytically stable in waters with pH 5-9 (25ºC) and that photolysis is of minor importance in natural waters. Results from a modified Sturm test indicate that Irgarol 1051 is not readily biodegradable, in one study 17 % and 1 % were degraded in 28 days, at the concentrations 10 and 20 mg/l, respectively. In degradation studies in both freshwater and marine water it was observed that 1-4 % of Irgarol 1051 was transformed during 30 days at 25ºC during aerobic conditions. (KEMI, 1998)

Results from a modified OECD 302 Test indicated that Irgarol 1051 is not inherently biodegradable (<10 % were degraded in 28 days (Meinacke *et al.*, in prep).

In a 35-d estuarine mesocosm experiment the dissipation of Irgarol in water was about 7 d (± 3d). However, focussing on the total system (sum of water + sediment) the sum of Irgarol and its primary metabolite M1 at the end of the experiment was almost 100 % of the initial dose (Sapozhnikova *et al.*, 2009).

In a comprehensive mesocosm study, conducted by the UBA (Meinecke *et al.*, in prep), slow degradation rates of Irgarol were determined in fresh water. Irgarol was dosed once at 4 concentrations (range: 0.004 µg/l - 5 µg/l) to indoor pond systems (22 m^3 water volume; sand and soft sediment, macrophytes, zoobenthos and plankton community, artificial irradiation, analysis by GC-MS and SPE). After single dosing the dissipation in water followed a biphasic kinetic (double first order kinetic in parallel = DFOP). Thus, the dissipation DT50 in water depended on the concentration level as well as on the duration of the experiment. At the end of the experiment after 146 days, the total amount of Irgarol and M1 in water, sediment and macrophytes was between 30 and 46 % of the initial dosing.

Okamura *et al.* (1999) studied the photodegradation of Irgarol 1051 in river water, sea water, buffered solutions (pH 5, 7 and 9) and in ultra-pure water. After 15 weeks, more than 80 % of the substance had degraded in all solutions. In solutions kept in dark conditions 70-94 % of the substance remained after 6 months, with the exception of the salt water solution in which 52 % remained. Okamura also studied hydrolysis of Irgarol 1051 and concluded that the substance is hydrolytically stable.

Sakkas *et al.* (2002) investigated the photochemical degradation of Irgarol 1051 in natural water under natural solar irradiation and simulated solar irradiation (Suntest incubator, ATLAS) and the influence of humic and fulvic substances, The half life under natural solar irradiation was 52 d for lake water (Pamvotis lake, pH 7.67), 60 d for river water (Kalamas river, pH 7.9) and 56 d for sea water (Ionian sea, pH 7.72). The photodegradation half-live time decreased with the amount of humic and fulvic acids.

Lam *et al.* (2009) conducted a mechanistic study on the photodegradation of Irgarol 1051 in coastal seawater (Victoria Harbour, Hong Kong). Spiked samples were irradiated inside an environmental chamber (light intensity 29 $W*m^{-2}$. The first order kinetic rate constant for degradation of Irgarol was $4.02 * 10^{-4}$ h^{-1} (DT50: 72 d).

UBA (unpublished data, UBA Umweltbundesamt, 2010) studied the photodegradation of Irgarol in buffered and unbuffered pure water by use of a laboratory test system (Suntest CPS+, ATLAS). The spiked samples were irradiated with simulated solar irradiation (550 $W*m^{-2}$). The dissipation of Irgarol followed a single first order kinetic. Converted to average Europe irradiation, the calculated DT50 was between 52-59 d.

Degradation of Irgarol in fresh water sediment and marine water sediments has been reported to be 100-200 days during aerobic conditions and to be slower in anaerobic conditions (Ciba Geigy, 1988).

		Master reference
Hydrolysis	hydrolytically stable	Okamura *et al.*, 1999
Photolysis	DT_{50}= circa 2 weeks in natural waters	Okamura *et al.*, 1999
	DT_{50}: 52-60 d (natural water)	Sakkas *et al.*, 2002
	DT_{50}: 52-59 d (unbuffered pure und buffered artificial water)	UBA Umweltbundesamt, 2010
	DT_{50}: 72 d (natural sea water)	Lam *et al.*, 2009
Biodegradation	$DT_{50\ (type\ of\ water)}$= d	
	Not readily biodegradable	KEMI, 1998
	Not inherently biodegradable	Meinecke *et al.*, in prep.
	DT_{50} (water + sediment + freshwater) ca. 146 d	Meinecke *et al.*, in prep.

6 AQUATIC ENVIRONMENTAL CONCENTRATIONS

6.1 ESTIMATED CONCENTRATIONS

The Swedish Chemicals Agency (KEMI, 2006a) has estimated $PEC_{marine\ waters}$, relevant for Swedish conditions, to 0.0621 µg/l, using the programme MAMPEC (Marine Antifoulant Model to Predict Environmental Concentrations) and the estimated emission rates given above (section 0).

Compartment	**Predicted environmental concentration (PEC)**	**Master reference**
Freshwater		
Marine waters (coastal and/or transitional)	0.0621 µg/l	KEMI, 2006
Sediment		
Biota (freshwater)		
Biota (marine)		
Biota (marine predators)		

6.2 MEASURED CONCENTRATIONS

Konstantinou and Albanis (2004) have made a review of environmental levels of Irgarol 1051 in marine waters and freshwaters as well as sediments in a number of countries, as reported in the literature (European countries included in the review were: the United Kingdom, France, Spain, Greece, the Netherlands, Switzerland, Germany, Portugal and Sweden).

Furthermore, Irgarol 1051 has been measured in screening studies in the Swedish environment by Woldegiorgis *et al.* (2007) and Kaj *et al.* (2010). Irgarol 1051 has also been studied in the Swedish marina Bullandö, in this study it was shown that water concentrations of Irgarol 1051 were higher during the summer (KEMI, 2006b).

Screening and monitoring of Irgarol 1051, and its metabolite M1, have also been conducted by the German Federal Environment Agency (UBA Umweltbundesamt, 2010a). In this screening only single or few samples were taken at each location, mainly during the summer season. In the monitoring on the other hand, samples were taken over the year. Data from the freshwater and marine datasets are given in the table below. Irgarol concentrations (µg/l) in the whole dataset, including also 4 marine locations and 4 industrially influenced sites, were between 0.002 and 25.630 with a mean of 0.168 (n=218). Concentrations of the metabolite M1 were in the reduced dataset, *i.e.* freshwater locations and non-industrial influenced locations, between 0.002 and 0.604 with a mean of 0.022 (n=210). In the monitoring data, where measurements were made over the year, M1 mean concentrations were similar to Irgarol concentrations. The mean concentration of M1 in the whole dataset, including marine sites and industrially influenced sites was lower than Irgarol concentration (0.032 µg/l compared to 0.168 µg/l, n=218).

Compartment	**Measured environmental concentration (MEC)**	**Master reference**

Freshwater	<0.0003 – 0.0016 µg/l	Woldegiorgis *et al.* (2007)
	0.0025-0.26 µg/l	Konstantinou and Albanis (2004)
	0.002-1.725 µg/l (mean 0.041 n=210, samples from 86 locations)	UBA Umweltbundesamt (2010a)
	0.003-0.030 µg/l (mean values from eight locations, samples taken over the year, n=8-12/location)	UBA Umweltbundesamt (2010a)
	0.022 µg/l (maximum of the annual average by station) 0.058 µg/l (maximum of analyses)	UBA Umweltbundesamt (2010b)
Marine waters (coastal and/or transitional)	<0.006-0.17 µg/l In the marina <0.005-0.014 µg/l In the bay, outside the marina <0.004-0.042 µg/l Natural harbour <LOQ (0.006-0.015 µg/l) Background location	KEMI (2006b)
	<0.001-1.7 µg/l Marinas, ports, estuaries and beaches	Konstantinou and Albanis (2004)
	0.095 - 0.296 µg/l 4 marinas at the German Baltic Sea coast	UBA Umweltbundesamt (2010a)
WWTP effluent	<0.0003 – 0.011 µg/l	Woldegiorgis *et al.* (2007)
Sediment	<0.001-20 µg/kg dw	Woldegiorgis *et al.* (2007)
	<0.2- 1011 µg/kg dw	Konstantinou and Albanis (2004)

	Swedish lakes and rivers: 0.26-9.1 µg/kg dw, median: 2.3 above LOQ (0.05 µg/kg dw) in 7/12 samples Swedish Baltic and west coasts - marinas, coastal areas and open sea background stations: 0.07-42 µg/kg dw, median: 0.46 above LOQ (0.05-0.07 µg/kg dw) in 56/87 samples	Kaj *et al.*, 2010
Biota	< 1 ng/g ww fish and mussels	Woldegiorgis *et al.* (2007)
	< 2 - 96 µg/kg dw bladderwrack	KEMI (2006b)
Biota (marine predators)		

7 EFFECTS AND QUALITY STANDARDS

7.1 ACUTE AND CHRONIC AQUATIC ECOTOXICITY

Validated acute toxicity data relevant for the EQS derivation. Primary producers.

	Taxa	Species	Duration	Endpoint	EC50 (µg/l)	Val.	Reference
Freshwater	algae	*Chlamydomonas intermediata*	6 d	growth	0.5	2	Berard *et al.* (2003)
	algae	*Chlorella vulgaris*	4 d	growth	1.5	2	Berard *et al*. (2003)
	algae	*Chlorella vulgaris*	4 d	growth	1.45	2	Nyström *et al.* (2002)
	algae	*Closterium ehrenbergii*	5 d	growth	2.5	2	Okamura *et al.* (2000b)
	algae	*Closterium ehrenbergii*	5 d	embryogenesis	3.6	2	Okamura *et al.* (2000b)
	algae	*Navicula accomoda*	4 d	growth	0.5	2	Berard *et al.* (2003)
	algae	*Navicula accomoda*	4 d	growth	0.45	2	Nyström *et al*. (2002)
	algae	*Navicula pelliculosa*	5 d	growth	0.0957	1	Hughes and Alexander (1993a)*
	algae	*Nitszchia sp.*	4 d	growth	0.8	2	Berard *et al*. (2003)
	algae	*Nitszchia sp.*	4 d	growth	0.75	2	Nyström *et al.* (2002)
	algae	*Pseudokirchneriella subcapitata*	4 d	growth	3.3	2	Berard *et al.* (2003)
	algae	*Scenedesmus acutus*	4 d	growth	5.1	2	Berard *et al.* (2003)
	algae	*Scenedesmus vacuolatus*	24 h	reproduction	5.57	2	Arrhenius *et al*. (2006)
	algae	*Scenedesmus vacuolatus*	24 h	reproduction	12.903	2	Neuwoehner *et al.* (2008)
	algae	*Scenedesmus vacuolatus*	24 h	photosynthesis	6.072	2	Neuwoehner *et al.* (2008)
	algae	*Selenastrum capricornutum*	3 d	growth	10.8	2	Fernandez-Alba *et al.* (2002)
	algae	*Selenastrum capricornutum*	3 d	growth	1.6	2	Okamura *et al.* (2003)
	algae	*Selenastrum capricornutum*	72 h	cell number-area	1.6	2	Okamura *et al.* (2000a)
	algae	*Selenastrum capricornutum*	72 h	cell number-growth rate	2.3	2	Okamura *et al.* (2000a)
	algae	*Staurastrum sebaldii*	6 d	growth	2.5	2	Berard *et al.* (2003)
	macrophyte	*Lemna gibba*	7 d	growth	11	2	Okamura *et al.* (2000b)
	macrophyte	*Lemna gibba*	14 d	growth	1.65	1	Hughes and Alexander (1993e)*
	macrophyte	*Lemna minor*	7 d	growth	8.1	2	Okamura *et al.* (2000b)
Marine Water	algae	*Ceramium tenuicorne*	7 d	growth	0.96	2	Karlsson *et al.* (2006)
	algae	*Chaetocerus gracilis*	3 d	growth	1.1	2	Koutsaftis *et al.* (2006)
	algae	*Dunaliella tertiolecta*	4 d	growth	0.73	2	DeLorenzo and Serano (2006)
	algae	*Dunaliella tertiolecta*	3 d	growth	1.1	2	Gatidou and Thomaidis (2007).
	algae	*Eisena bicyclis*	4 d	growth	5.9	2	Okamura *et al.* (2000b)
	algae	*Eisena bicyclis*	7 d	cell division	2.2	2	Okamura *et al.* (2000b)
	algae	*Eisena bicyclis*	7 d	growth	2	2	Okamura *et al.* (2000b)
	algae	*Eisena bicyclis*	7 d	growth	2.1	2	Okamura *et al.* (2000b)
	algae	*Emiliana huxleyi*	3 d	growth	0.406	2	Buma *et al.* (2009)
	algae	*Emiliana huxleyi*	3 d	growth	0.25	2	Devilla *et al.* (2005)
	algae	*Enteromorpha intestinalis*	6 d	growth	5.4	2	Scarlett *et al.* (1997)
	algae	*Enteromorpha intestinalis*	72 h	photosynthesis	2.5	2	Scarlett *et al.* (1997)
	algae	*Fibrocapsa japonica*	3 d	growth	0.618	2	Buma *et al.* (2009)
	algae	*Fucus vesiculosus*	3 d	fertilization	0.325	2	Andersson (1995)*

	algae	*Hormosira banksii*	2 h	photosynthesis	0.17	2	Seery *et al.* (2006)
	algae	*Navicula forcipata*	3 d	growth	1.1	2	Gatidou and Thomaidis (2007)
	algae	*Porphyra yezoensis*	4 d	growth	0.6	2	Okamura *et al.* (2000b)
	algae	*Porphyra yezoensis*	4 d	lethality	5000	2	Okamura *et al.* (2000b)
	algae	*Porphyra yezoensis*	4 d	germination	4.1	2	Okamura *et al.* (2000b)
	algae	*Skeletonema costatum*	96 h	growth	0.17	2	Zhang *et al.* (2008)**
	algae	*Skeletonema costatum*	5 d	growth	0.452	1	Hughes and Alexander (1993b)*
	algae	*Tetraselmis sp.*	3 d	growth	0.116	2	Buma *et al.* (2009)
	algae	*Thalassiosira pseudonana*	4 d	growth	0.27	2	Zhang *et al.* (2008)**
	algae	*Thalassiosira weissflogii*	3 d	growth	0.303	2	Buma *et al.* (2009)
	cyanobacteria	*Synechococcus sp.*	72 h	growth	0.16	2	Devilla *et al.* (2005)
	macrophyte	*Potamogeton pectinatus*	28 d	dry weight	6.115	2	Hall *et al.* (1999a)*
	macrophyte	*Ruppia maritima*	28 d	growth	0.843	2	Hall *et al.* (1999a)*
	macrophyte	*Zostera marina*	10 d	photosynthesis	1.1	2	Chesworth *et al.* (2004)
	macrophyte	*Zostera marina*	10 d	photosynthesis	2.5	2	Scarlett *et al.* (1999)

*Industry studies not publicly available.

**The values are derived based on results for the exposure concentrations up to 1 µg/l.

Validated acute toxicity data relevant for the EQS derivation. Invertebrates and fish.

	Taxa	**Species**	**Duration**	**Endpoint**	**E/LC50** (µg/l)	**Val.**	**Reference**
Freshwater	Crustacea	*Daphnia magna*	48 h	immobilisation	7300	2	Fernandez-Alba *et al.* (2002)
	Crustacea	*Daphnia magna*	48 h	immobilisation	7300	2	Hernando *et al.* (2005)
	Crustacea	*Daphnia magna*	48 h	mortality	8300	2	Okamura *et al.* (2000a)
	Crustacea	*Daphnia magna*	48 h	mortality	2400	1	Vial (1990)*
	Crustacea	*Thamnocepharus platyurus*	24 h	mortality	12000	2	Okamura *et al.* (2000a)
	Fish	*Oncorhynchus mykiss*	7 d	mortality	25000	2	Okamura *et al.* (2002)
	Fish	*Oncorhynchus mykiss*	96 h	mortality	860	2	Rufli (1985)*
Marine water	Ascidia	*Ciona intestinalis*	24 h	embryogenesis	2110	2	Bellas (2006)
	Cnidaria	*Acropora formosa*	10 h	photosynthesis of symbiotic dinoflagellates	0.9	2	Jones and Kerswell (2003)
	Cnidaria	*Seriatophora hystrix*	10 h	photosynthesis of symbiotic dinoflagellates	0.7	2	Jones and Kerswell (2003)
	Crustacea	*Nitocra spinipes*	96 h	mortality	4500	2	Karlsson *et al.* (2006)
	Crustacea	*Palaemonetes pugio*	96 h	larval mortality	1520	2	Key *et al.* (2008)
	Crustacea	*Palaemonetes pugio*	96 h	adult mortality	2460	2	Key *et al.* (2008)
	Crustacea	*Balanus albicostatus*	48 h	mortality	556	2	Khandeparker *et al.* (2005)
	Crustacea	*Artemia salina*	24 h	mortality	1620	2	Bakoulia *et al.* (2002)
	Crustacea	*Mysidopsis bahia*	96 h	mortality	400	2	Hoberg (1986)*
	Echinodermata	*Paracentrotus lividus*	48 h	embryogenesis	4020	2	Bellas (2006)
	Echinodermata	*Paracentrotus lividus*	48 h	growth	6030	2	Bellas (2006)
	Mollusca	*Mytilus edulis*	48 h	embryogenesis	1540	2	Bellas (2006)
	Mollusca	*Ilyanassa obsoleta*	96 h	adult mortality	3730	2	Finnegan *et al.* (2009)
	Mollusca	*Ilyanassa obsoleta*	96 h	larval mortality	3160	2	Finnegan *et al.* (2009)

	Fish	*Fundulus heteroclitus*	96 h	mortality	3220	2	Key *et al.* (2009)
	Fish	*Menidia beryllina*	96 h	mortality	1760	1	Chandler (1989)*
Marine sediment	Crustacea	*Monoporeia affinis*	24 h	Avoidance response	0.04 (µg g^{-1}dw)	2	Eriksson Wiklund *et al.* (2009)

*Industry studies not publicly available.

Validated chronic toxicity data relevant for the EQS derivation. Primary producers.

	Taxa	Species	Duration	Endpoint	NOEC (µg/l)	Val.	Original reference
Freshwater	algae	*Scenedesmus vacuolatus*	24 h	reproduction	0.507	2	Arrhenius *et al.* (2006)
	algae	*Navicula pelliculosa*	5 d	growth	0.017**	1	Hughes and Alexander (1993a)*
	algae	*Nitszchia sp.*	4 d	growth	0.1	2	Nyström *et al.* (2002)
	macrophyte	*Lemna gibba*	14 d	growth	0.671	1	Hughes and Alexander (1993e)*
Marine water	algae	*Dunaliella tertiolecta*	4 d	growth	0.09	2	DeLorenzo and Serrano (2006)
	algae	*Eisena bicyclis*	4 d	growth (gametophyte)	3.2	2	Okamura *et al.* (2000b)
	algae	*Eisena bicyclis*	7 d	cell division	0.32	2	Okamura *et al.* (2000b)
	algae	*Eisena bicyclis*	7 d	growth	1	2	Okamura *et al.* (2000b)
	algae	*Eisena bicyclis*	7 d	growth	0.32	2	Okamura *et al.* (2000b)
	algae	*Porphyra yezoensis*	4 d	lethality	1500	2	Okamura *et al.* (2000b)
	algae	*Porphyra yezoensis*	4 d	germination	1.2	2	Okamura *et al.* (2000b)
	algae	*Enteromorpha intestinalis*	144 h	growth	0.05	2	Scarlett *et al.* (1997)
	algae	*Skeletonema costatum*	4 d	growth	0.022	2	Zhang *et al.* (2008)***
	algae	*Skeletonema costatum*	5 d	growth	0.146	1	Hughes and Alexander (1993b)*
	algae	*Thalassiosira pseudonana*	4 d	growth	0.047	2	Zhang *et al.* (2008)***
	algae	*Fucus serratus*	72 h	zygote germination (area)	8	2	Braithwaite and Fletcher (2005)
	macrophyte	*Zostera marina*	10 d	photosynthesis	0.5	2	Scarlett *et al.* (1999)
	macrophyte	*Zostera marina*	10 d	growth	0.5	2	Scarlett *et al.* (1999)

*Industry studies not publicly available.

**No NOEC given in the robust study summary. The value represents the EC10 presented for the study by van Wezel and van Vlaardingen (2001).

***The values represent EC10 derived on results for the exposure concentrations up to 1 µg/l.

Validated chronic toxicity data relevant for the EQS derivation. Invertebrates and fish.

	Taxa	Species	Duration	Endpoint	NOEC (µg/l)	Val.	Original reference
Freshwater	fish	*Oncorhynchus mykiss*	60 d	growth	4.0	1	Cohle and Veltri (1994)*
Freshwater sediment	insect	*Chironomus riparius*	10 d	development/emergence	100	3	Desmares-Koopmans (1997)* evaluated by KEMI (1998)
Marine water	crustacea	*Mysidopsis bahia*	28 d	growth	110	1	Boeri and Ward (1991)*
	mollusc	*Ilyanassa obsoleta*	45 d	mortality	1500	2	Finnegan *et al.* (2009)
	fish	*Cyprinidon variegatus*	33 d	growth	170	1	Sousa (2001)*

*Industry studies not publicly available.

Micro/mesocosm studies

	Water	Species	Duration	Lowest value (µg/l)		Endpoint	Val.	Reference
Acute	Marine	Periphyton	45 min	EC50	1.04	photosynthesis	2	Arrhenius *et al.* (2006)
	Marine	Periphyton	45 min	EC50	1.292	photosynthesis	2	Dahl and Blanck (1996)
	Marine	Phytoplankton community	3 d	EC50	0.070	reduction in pigment content and cell numbers	2	Readman *et al.* (2004)
Chronic	Fresh	Phytoplankton	24 d	NOEC	0.004	Bray-Curtis index	2	Nyström *et al.* (2002)
	Fresh	Chlorophytes	135 d	EC10	nominal: 0.01 TWA : 0.001	biomass	2	UBA Umweltbundesamt (2007), study also partly presented in Mohr *et al.* (2008) and Mohr *et al.* (2009)
		Cyclopoid copepodites	78 d	EC10	nominal: 0.01 TWA : 0.002	biomass		
		Myriophyllum verticillatum	150 d	EC10	nominal: 0.06 TWA : 0.01	biomass		
		Radix baltica	60 d	EC10	Nominal: 0.032 TWA : 0.014	spermatogenesis		
	Marine	Plankton, macrophytes and macro-invertebrates	12 w	NOEC	TWA : 186	Biomass and abundance	2	Giddings (2002)*, **
	Marine	Periphyton	21 d	NOEC	0.016	photosynthesis	2	Dahl and Blanck (1996)
	Marine	Eel grass and phytoplankton	70 d	NOEC	TWA : 0.323	biomass, photosynthesis and taxonomic abundance of phytoplankton	1	Hoberg (2004)*
	Marine	*Mercenaria mercenaria*	35 d	NOEC	0.100	Growth (dry weight and shell size)	2	DeLorenzo *et al.* (2009)

*Industry study not publicly available.

**Pilot study. Only one exposure concentration and two replicates.

The validated acute toxicity data set consists of E/LC50 values for 49 species belonging to nine taxonomic groups; algae, macrophytes, cyanobacteria, cnidarians (corals), crustaceans, ascidians, molluscs, echinoderms and fish, see above.

The validated chronic toxicity data set consists of NOEC values for 13 species of algae, cyanobacteria, macrophytes, and molluscs, see above.

Irgarol 1051 affects the photosynthesis in primary producers by inhibiting photosystem II (PSII) in the chloroplasts (Moreland, 1980; Mets and Thiel, 1989; Holt, 1993). Also the metabolite M1 is toxic to aquatic plants and algae (see *e.g.* Okamura *et al.*, 2000b; Gatidou and Thomaidis, 2007; Lambert *et al.*, 2006).

Validated acute toxicity data for primary producers are in the range 0.0957-8.1 µg/l, whereas the data for fish and invertebrates span the range 400-25000 µg/l. The data data distribution for validated acute toxicity data is presented in Figure 1 below. For the chronic toxicity data set NOEC/EC_{10} values for primary producers are in the range 0.01-8 µg/l (most sensitive endpoint/species), whereas the data for fish and invertebrates span the range 4.0-1500 µg/l.

In a mesocosm study (UBA Umweltbundesamt, 2007) low EC10 values (0.032 µg/l based on nominal concentrations, 0.014 µg/l TWA based on measured concentrations) on endocrine effects for the snail *Radix baltica*. However, no endocrine effects were seen for the snail *Ilyanassa obsoleta* in the laboratory study by Finnegan *et al.* (2009), nor in the laboratory study on *Lymnea stagnalis* by Habekost *et al.* (2010, Abstract).

It should be noticed that the AA-QSs derived based on toxicity data for primary producers result in values lower compared to the toxicity value given for *Radix baltica*, see below.

Acute toxicity

Assessment factor method

An AF of 10 is used to derive the MAC-QS to the lowest credible datum. The lowest EC50 value found, 95.7 ng/l, is for the freshwater algae *Navicula pelliculosa* (Hughes and Alexander (1993a).**This results in a MAC-QS (AF) of 9.6 ng/l.**

SSD method

A SSD was first constructed using the entire validated data set emploing the program ETX 2.0 (van Vlaardingen *et al.*, 2004). For species with more than one toxicity value, the geometric means were calculated. The resulting SSD showed a clear break, see Figure 1 below, and the data histogram a skewed distribution (Figure A1 and Table A1 in Appendix). The toxicity values for primary producers vary between 0.0957-8.1 µg/l, whereas the toxicity values for invertebrates and fish are in the range 556-25000 µg/l. The EC50 values for the two cnidarian species, *Seriatophora hystrix* and *Acropora formosa*, are 0.7 and 0.9 µg/l respectively (Jones and Kerswell, 2003). However, these toxicity values refer to the photosynthesis of the symbiotic dinoflagellates (algae). Inhibition of photosynthesis has also been shown for the coral species *Madractis mirabilis* after exposure to 1 µg/l of Irgarol, and for zooxanthellae isolated from the same species effects was seen already at a concentration of 63 ng/l (Owen *et al.*, 2002). Effects on isolated zooxanthellae have also been shown by Owen *et al.* (2003). Zooxanthellae isolated from the coral species *M. mirabilis*, *Diploria strigosa* and *Favia framum* were affected after exposure to 2 µg/l Irgarol. No toxicity values related to the cnidarian hosts relevant for the EQS derivation is avaiable. However, a reduction of calcification of the coral species *Galaxea fascicularis* has been shown after exposure to 10 µg/l (photosynthesis affected at 1 µg/l) (Sheikh *et al.*, 2009), and for *M. mirabilis*, Downs and Downs (2007) showed changes in expressions of proteins related to the cnidarian after exposure to 10 µg/l.

In order to determine if the toxicity data for the freshwater and marine primary producers differ or can be combined, the data were log-transformed and compared using an F-test and a two-tailed t-test. The F-test revealed equal variances ($p = 0.17$), however according to the t-test the freshwater and marine data can not be considered to belong to the same population ($p = 0.013$). The mean of the marine toxicity data is slightly lower (a factor of two) compared to the freshwater data, but the lowest toxicity value refers to freshwater algal species. Further, for the chronic toxicity data, no difference in sensitivity between freshwater and marine species is seen, see below. A SSD based on the combined validated acute toxicity data for primary producers, including data for the two cnidarians related to photosynthesis of the symbiotic dinoflagellates, was thus constructed. The data set comprises EC50 values for 34 species of algae (including the symbiotic dinoflagellates), macrophytes and cyanobacteria. The resulting SSD is shown in Figure 2 below. The tests for goodness of fit revealed normal distribution of the data (Figure A2 and Table A2 in Appendix), and the SSD resulted in a HC5 of 129 ng/l (Table A3 in Appendix).

According to the TGD for deriving EQS (European Commission, 2011), a default AF of 10 is recommended for a SSD derived on acute E/LC50 values. However, the SSD is constructed for the primary producers shown to be the most sensitive group, is based on a large number of data points (34) and show a good fit. Hence the AF is reduced to 8. **This results in a MAC-QS (SSD) of 16 ng/l.**

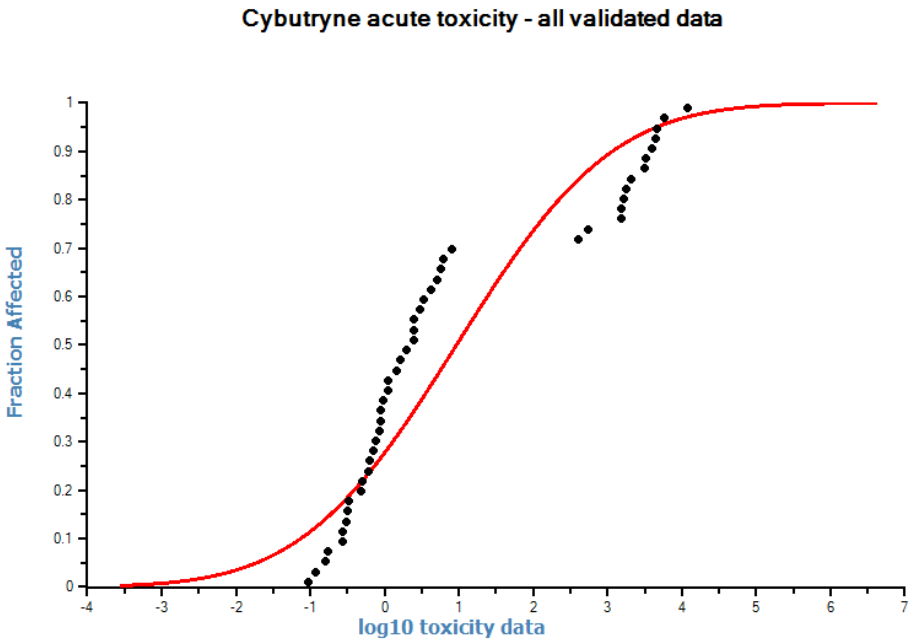


Figure 1. SSD with E/LC50 (µg/l) values for the entire validated data set calculated with the program ETX 2.0 (van Vlaardingen *et al.*, 2004).

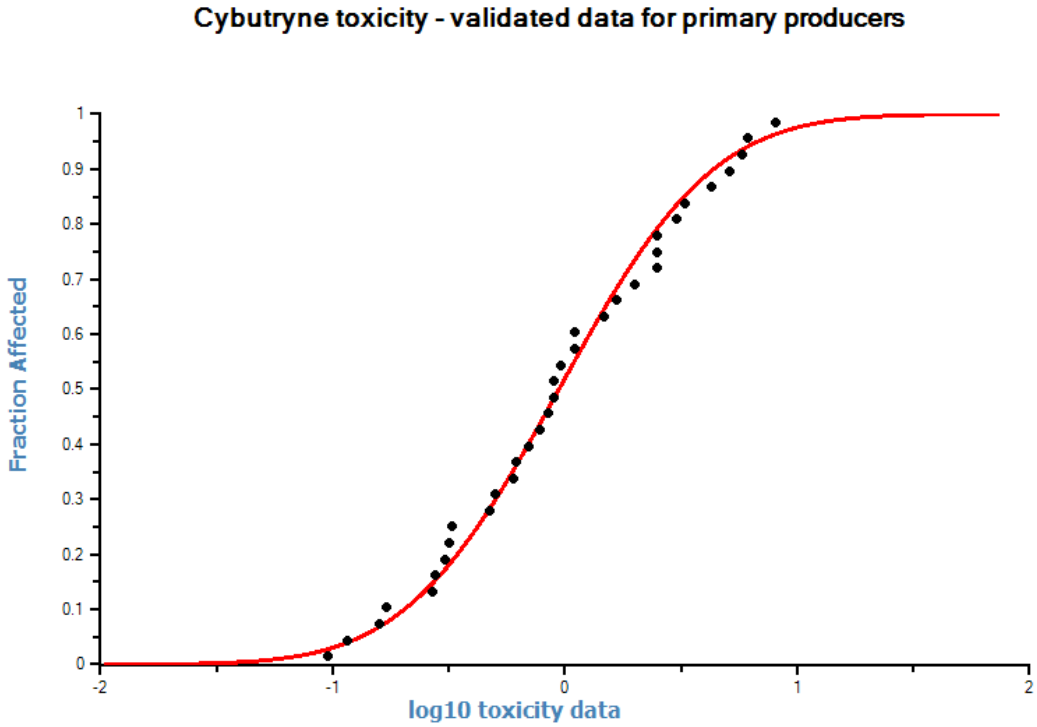


Figure 2. SSD derived from validated EC50 values (µg/l) for primary producers (marine and freshwater, including symbiontic dinoflagellates) with the program ETX 2.0 (van Vlaardingen *et al.*, 2004).

Micro-/ Mesocosm studies

Three short-term marine microcosm studies were found. Arrhenius *et al.* (2006) determined an EC50 of 1.04 µg/l and Dahl and Blanck (1996) determined an EC50 value of 1.29 µg/l for marine periphyton, whereas Readman *et al.* (2004) determined an EC50 value of 70 ng/l for marine phytoplankton. The EC50 determined by Readman *et al.* (2004) is used to derive the MAC-QS(Micro-/ Mesocosm). Since no short-term micro-/mesocosm studies on freshwater species, nor studies covering effects on macro algae and macrophytes, are available, an assessment factor of 5 is suggested. **This results in a MAC-QS(Micro-/ Mesocosm) of 14 n/l.**

The EC50 value reported by Readman *et al.* (2004) is below the HC5 value, 129 ng/l, calculated for the SSD. Therefore, it is not recommended to further reduce the AF of 8 used to derive the MAC-QS(SSD).

Conclusion and MAC-QS-proposal

The assessment factor method, the SSD method, and the microcosm studies result in MAC-QSs of 9.6 ng/l, 16 ng/l, and 14 ng/l, respectively. The EQS derived with the SSD method is considered to be the most reliable. Therefore, it is suggested to base the MAC-QS on the HC5 of 129 ng/l. With the proposed AF of 8 the following MAC-QS results:

MAC-EQS = 129 ng/l (HC5-SSD)/ 8 = 16 ng/l

Chronic toxicity

Considering only the validated chronic toxicity data, the base set is not complete and the requirements for deriving an SSD not met. However, considering the toxic mode of action and the data distributions for the entire acute and chronic data sets, it is proposed to use an AF of 10 to derive the AA-QS(AF) and to derive an AA-QS(SSD) based on the available chronic toxicity data for primary producers.

Assessment Factor method

An AF of 10 is used to derive the AA-QS to the lowest credible datum. The lowest NOEC found, 17 ng/l, has been reported for the freshwater algae *Navicula pelliculosa,* by van Wezel and van Vlaardingen (2001) based on a study by Hughes and Alexander (1993a). **Applying an AF of 10 to the lowest NOEC results in a AA-QS(AF) of 1.7 ng/l.**

SSD method

In order to determine if the toxicity data for the freshwater and marine primary producers differ or can be combined, the data were log-transformed and compared using an F-test and a two-tailed t-test. The F-test revealed equal variances ($p = 0.78$), and according to the t-test the freshwater and marine data can be considered to belong to the same population ($p = 0.81$).

A SSD for the chronic NOEC values for primary producers was calculated with the program ETX 2.0 (van Vlaardingen *et al.*, 2004), see Figure 3 below. Data showed a normal distribution and normality according to the tests for goodness of fit (Figure A3 and Table A5 in Appendix). The data set comprises 12 NOEC values for cyanobacteria, algae and macrophytes.

The SSD results in a HC5 of 7.61 ng/l (Table A6 in Appendix). According to the TGD-EQS a default assessment factor of 1-5 has to be applied on the SSD. An assessment factor of 3 is chosen. The reason for this is that although the SSD was made for the most sensitive taxonomic group, and the data distribution is very even (Figure A3 and Table A5 in Appendix A), the SSD consists of less than the recommended 15 data points (Commission of the European Communities 2010). Hence, the statistical uncertainty should be judged higher than the statistical fit suggests. Based on the HC5 of 7.61 ng/l and an assessment factor of 3, an **AA-QS(SSD)** of **2.5 ng/l** results.

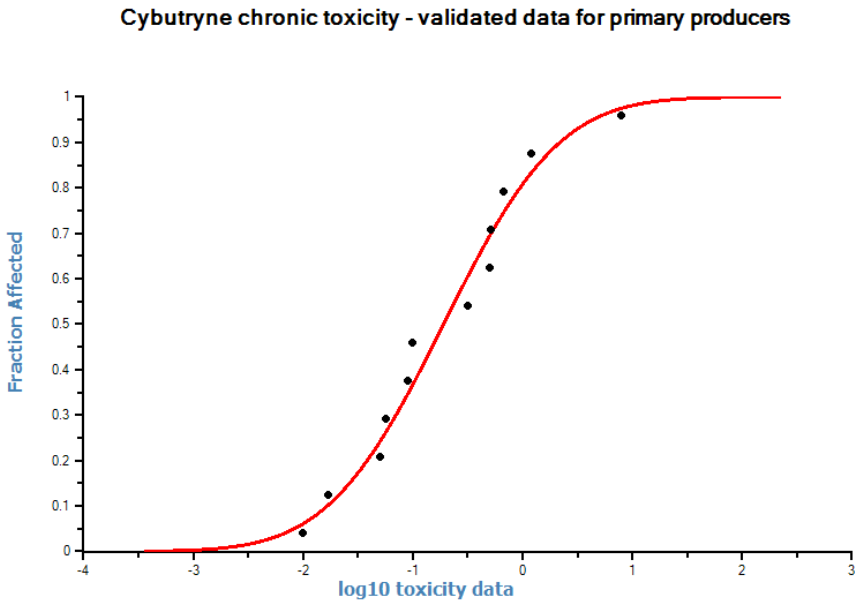


Figure 3. SSD derived from validated NOEC values (µg/l) for primary producers (with the program ETX 2.0 (van Vlaardingen *et al.*, 2004).

Micro-/ Mesocosm studies

Data on six mesocosm studies were found and the most sensitive endpoints are listed above. In the study by UBA Umweltbundesamt (2007) partly also presented by Mohr *et al.* (2008; 2009), cybutryne was only applied once and the concentrations dropped significantly (13-22 times compared to the nominal concentrations) during the experiment. EC10 values based both on nominal and time weighted average (TWA) concentrations are presented. In the study by DeLorenzo *et al.* (2009) concentrations were not measured. These studies do thus not fulfil the requirements according to the TGD-EQS (European Commission, 2011), but are used as supportive information. The pilot study conducted by Giddings (2002) consisted of only two replicates and one exposure concentration. Further, growth of introduced macrophytes was poor and marsh grass absent in both controls but not in the treatment replicates at the end of the study. This study is not considered in the QS derivation.

The EC10 and NOEC values range from 4-323 ng/l. However, it should be noted that for one of the studies used as supporting data (UBA Umweltbundesamt, 2007) the TWA EC10 values were lower compared to this range. The lowest valid NOEC, 4 ng/l, is used to derive the AA-QS(Micro-/ Mesocosm). Since the available mesocosm studies cover both marine and freshwater, and include several taxa of primary producers, an assessment factor of 2 is suggested.

This would result in an AA-QS(Micro-/Mesocosm) of 2 ng/l.

Conclusion and AA-QS-proposal

The EQS derived range between 1.7 ng/l and 2.5 ng/l. The EQS derived with the SSD method is the most reliable. Therefore, it is suggested to base the AA-QS on the HC5 of 7.61 ng/l. With the proposed AF of 3 the following AA-QS results:

AA-EQS = 8.42 ng/l (HC5-SSD)/3 = 2.5 ng/l

Sediment toxicity

The only chronic sediment toxicity study found, on development and emergence of *Chironomus riparius*, is not considered valid. There is a recent acute toxicity study on the crustacean *Monoporeia affinis* (Eriksson Wiklund *et al.*, 2009). An avoidance response (reduced burial in sediment) EC50 of 40 µg kg^{-1} d.w. was found. If only acute toxicity data is available, an assessment factor of 1000 should be applied to the lowest reliable value according to the TGD for deriving EQS (European Commission, 2011).

This would result in a QS_{sed}(AF) of 0.040 µg kg^{-1} d.w.

Log K_{oc} values are in the range 2.41-3.65, which mean that the trigger value for assessment of a sediment standard is met. This is further supported by studies showing that 60-80 % of the substance partitions to the sediment (KEMI, 1998). Therefore AA-QS_{sed} was also predicted with the equilibrium partitioning method (EqP) using the AA-QS(SSD), the Koc 1404 (geometric mean of valid Koc) and the default values outlined in the TGD.

This results in a QS_{sed}(EqP) of 0.18 µg kg^{-1} d.w.

Conclusion and QS_{sed}-proposal

The QSs for sediment derived by the deterministic approach and with the equilibrium partitioning method differ by a factor of five. For the deterministic approach only one toxicity study is available. It is short term but the endpoint is sub-lethal. In this study, the test organism preferred the contaminated sediment, which had a higher organic matter content. For the equilibrium partitioning method the AA-QS(SSD) have been used. The AA-QS(SSD) is derived for the most sensitive organism group and based on a large number of data points. Therefore it is suggested to use the QS_{sed} derived with the equilibrium partitioning method, 0.18 µg kg^{-1} d.w.

7.2 SECONDARY POISONING

Secondary poisoning of top predators		Master reference
Mammalian oral toxicity	rat / teratogenicity NOEL : 50 mg.kg$^{-1}_{bw}$.d^{-1} (maternal toxicity) *NOEC: 500 mg.kg$^{-1}_{biota\ ww}$ (CF=10)* NOEL : 300 mg.kg$^{-1}_{bw}$.d^{-1} (embryo toxicity and teratogenicity; highest dose tested)	Evaluated by KEMI, 1998
	rat / oral / 28 d / changes in the spleen NOEC : 100 mg.kg$^{-1}_{biota\ ww}$ NOAEL : 7.62 and 7.32 mg.kg$^{-1}_{bw}$.d^{-1} (males and females, respectively)	Evaluated by KEMI, 2006
	rat / oral / 28 d / changes in the liver NOEL : 8 and 7 mg.kg$^{-1}_{bw}$.d^{-1} (males and females, respectively) *NOEC: 70 mg.kg$^{-1}_{biota\ ww}$ (CF=10)*	Evaluated by KEMI, 1998
	rat / oral / 90 d / changes in the liver NOEL : 10 mg.kg$^{-1}_{bw}$.d^{-1} *NOEC: 100 mg.kg$^{-1}_{biota\ ww}$ (CF=10)*	Evaluated by KEMI, 1998
Avian oral toxicity	Bobwhite quail (*Colinus virginianus*) / time not stated NOEC : 1780 mg.kg$^{-1}_{feed\ ww}$	Evaluated by KEMI, 1998
	Mallard duck *(Anas platyrhynchos)* / *time not stated* NOEC: 1000 mg.kg$^{-1}_{feed\ ww}$	Evaluated by KEMI, 1998

A number of subchronic toxicity studies on rats have been evaluated by the Swedish Chemicals Agency (see KEMI, 1998; KEMI, 2006) and these are listed in the table above. Only a few mammalian toxicity studies on ecotoxicologically relevant endpoints, as described in the TGD for deriving EQS (European Commission, 2011) have been found in the literature. Therefore all studies are listed above.

The lowest NOEC from the mammalian and bird studies was used to derive a biota standard using assessment factors. The assessment factor 300 is given in the TGD for deriving EQS (European Commission, 2011) when the NOEC is from a 28 day mammalian oral study.

Due to the small dataset regarding bioconcentration, the corresponding QS in water was calculated with the highest BCF, using the formula below. BMF_1 and BMF_2 were set to 1 as the given default values in the TGD for deriving EQS (European Commission, 2011).

$$QS_{water\_biota}(\mu g.l^{-1}) = \frac{QS_{biota}(230\ \mu g.kg^{-1}\ ww)}{BCF(250\ l.kg^{-1}) \times BMF_1(1) \times BMF_2(1)}$$

Tentative QS_{biota}	Relevant study for derivation of QS	Assessment factor	Tentative QS
Biota	rat / oral / 28 d / changes in the liver NOEL : 8 and 7 $mg.kg^{-1}_{bw}.d^{-1}$ (males and females, respectively) *NOEC: 70 $mg.kg^{-1}_{biota\ ww}$ (CF=10)*	300	0.23 $mg.kg^{-1}_{biota\ ww}$ corresponding to 0.9 $\mu g.L^{-1}$ (fresh water and marine waters)

7.3 HUMAN HEALTH

Human health via consumption of fishery products		Master reference
Mammalian oral toxicity	rat / teratogenicity NOEL : 50 $mg.kg^{-1}_{bw}.d^{-1}$ (maternal toxicity) *NOEC: 500 $mg.kg^{-1}_{biota\ ww}$ (CF=10)* NOEL : 300 $mg.kg^{-1}_{bw}.d^{-1}$ (embryo toxicity and teratogenicity; highest dose tested)	Evaluated by KEMI (1998)
	rat / oral / 28 d / changes in the spleen NOEC : 100 $mg.kg^{-1}_{biota\ ww}$ NOAEL : 7.62 and 7.32 $mg.kg^{-1}_{bw}.d^{-1}$ (males and females, respectively)	Evaluated by KEMI (2006)
	rat / oral / 28 d / changes in the liver NOEL : 8 and 7 $mg.kg^{-1}_{bw}.d^{-1}$ (males and females, respectively) *NOEC: 70 $mg.kg^{-1}_{biota\ ww}$ (CF=10)*	Evaluated by KEMI (1998)
	rat / oral / 90 d / changes in the liver NOEL : 10 $mg.kg^{-1}_{bw}.d^{-1}$ *NOEC: 100 $mg.kg^{-1}_{biota\ ww}$ (CF=10)*	Evaluated by KEMI (1998)
CMR		

The lowest NOAEL from the mammalian toxicity study was used to calculate the $QS_{biota,hh}$ using the formula given below. Standard weight for human and fishery product consumption were used. The threshold level (TL) was calculated from the NOAEL with an assessment factor of 300.

$$QS_{biota,hh}\,(\mathrm{mg.kg^{-1}\ ww}) = \frac{0.1 \times \mathrm{TL}\ (0.023\,\mathrm{mg.kg^{-1}\ bw.d^{-1}}) \times \mathrm{bw}\ (70\,\mathrm{kg})}{\mathrm{cons.\,fishery\ prod.}\ (0.115\,\mathrm{kg.d^{-1}})}$$

The corresponding QS in water was calculated using the same method as described above.

Tentative $QS_{biota, hh}$	**Relevant study for derivation of $QS_{biota, hh}$**	**Assessment Factor**	**Tentative $QS_{biota, hh}$**
Human health	rat / oral / 28 d / changes in the liver NOEL : 8 and 7 $mg.kg^{-1}_{bw}.d^{-1}$ (males and females, respectively) *NOEC: 70 $mg.kg^{-1}_{biota\ ww}$ (CF=10)*	300	1.4 $mg.kg^{-1}_{biota\ ww}$ (6.0 $\mu g.L^{-1}$)

Human health via consumption of drinking water		**Master reference**
Existing drinking water standard(s)	0.1 $\mu g.L^{-1}$ (preferred regulatory standard)	Directive 98/83/EC
Provisional drinking-water standard		

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APPENDIX A

MAC-EQS

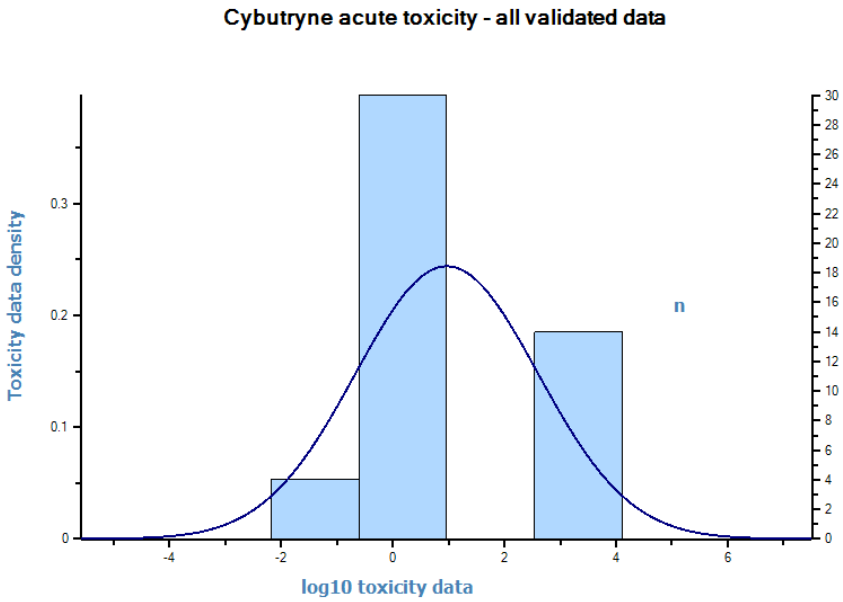

Figure A1: Distribution of all validated acute toxicity data.

Table A1: Goodness of fit for the SSD on all validated acute toxicity values calculated with the program ETX 2.0.

Anderson-Darling test for normality				
Sign. level	Critical	Normal?		
0.1	0.631	Rejected		
0.05	0.752	Rejected	AD Statistic:	3.734523
0.025	0.873	Rejected	n:	48
0.01	1.035	Rejected		
Kolmogorov-Smirnov test for normality				
Sign. level	Critical	Normal?		
0.1	0.819	Rejected		
0.05	0.895	Rejected	KS Statistic:	1.628034
0.025	0.995	Rejected	n:	48
0.01	1.035	Rejected		
Cramer von Mises test for normality				
Sign. level	Critical	Normal?		
0.1	0.104	Rejected		
0.05	0.126	Rejected	CM Statistic:	0.667534
0.025	0.148	Rejected	n:	48
0.01	0.179	Rejected		

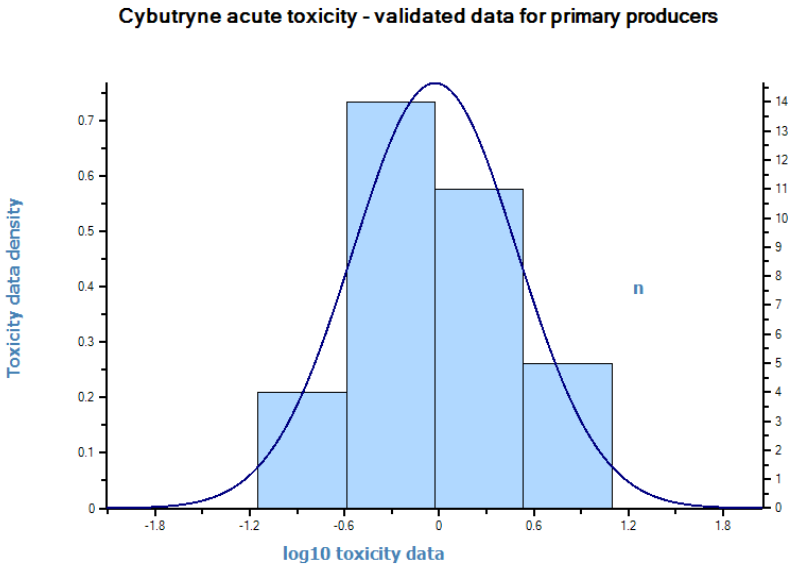

Figure A2: Distribution of validated acute toxicity data for primary producers.

Table A2: Goodness of fit for the SSD on validated acute toxicity values for primary producers as calculated with the program ETX 2.0.

Anderson-Darling test for normality				
Sign. level	Critical	Normal?		
0.1	0.631	Accepted		
0.05	0.752	Accepted	AD Statistic:	0.212345
0.025	0.873	Accepted	n:	34
0.01	1.035	Accepted		
Kolmogorov-Smirnov test for normality				
Sign. level	Critical	Normal?		
0.1	0.819	Accepted		
0.05	0.895	Accepted	KS Statistic:	0.519178
0.025	0.995	Accepted	n:	34
0.01	1.035	Accepted		
Cramer von Mises test for normality				
Sign. level	Critical	Normal?		
0.1	0.104	Accepted		
0.05	0.126	Accepted	CM Statistic:	0.026238
0.025	0.148	Accepted	n:	34
0.01	0.179	Accepted		

Table A3: Results for the SSD on validated acute toxicity data for primary producers calculated with the program ETX 2.0.

Parameters of the normal distribution		
Name	Value	Description
mean	-0.02631	mean of the log toxicity values
s.d.	0.519598	sample standard deviation
n	34	sample size

HC5 results			
Name	Value	log10(Value)	Description
LL HC5	0.06965	-1.15708	lower estimate of the HC5
HC5	**0.129187**	-0.88878	median estimate of the HC5
UL HC5	0.205771	-0.68662	upper estimate of the HC5
sprHC5	2.954363	0.470464	spread of the HC5 estimate

FA At HC5 results		
Name	Value	Description
FA lower	1.808	5% confidence limit of the FA at standardised median logHC5
FA median	5	50% confidence limit of the FA at standardised median logHC5
FA upper	9.471	95% confidence limit of the FA at standardised median logHC5

HC50 results			
Name	Value	log10(Value)	Description
LL HC50	0.665088	-0.17712	lower estimate of the HC50
HC50	0.941208	-0.02631	median estimate of the HC50
UL HC50	1.331963	0.124492	upper estimate of the HC50
sprHC50	2.002688	0.301613	spread of the HC50 estimate

FA At HC50 results		
Name	Value	Description
FA lower	38.879	5% confidence limit of the FA at standardised median logHC50
FA median	50	50% confidence limit of the FA at standardised median logHC50
FA upper	61.121	95% confidence limit of the FA at standardised median logHC50

AA-EQS

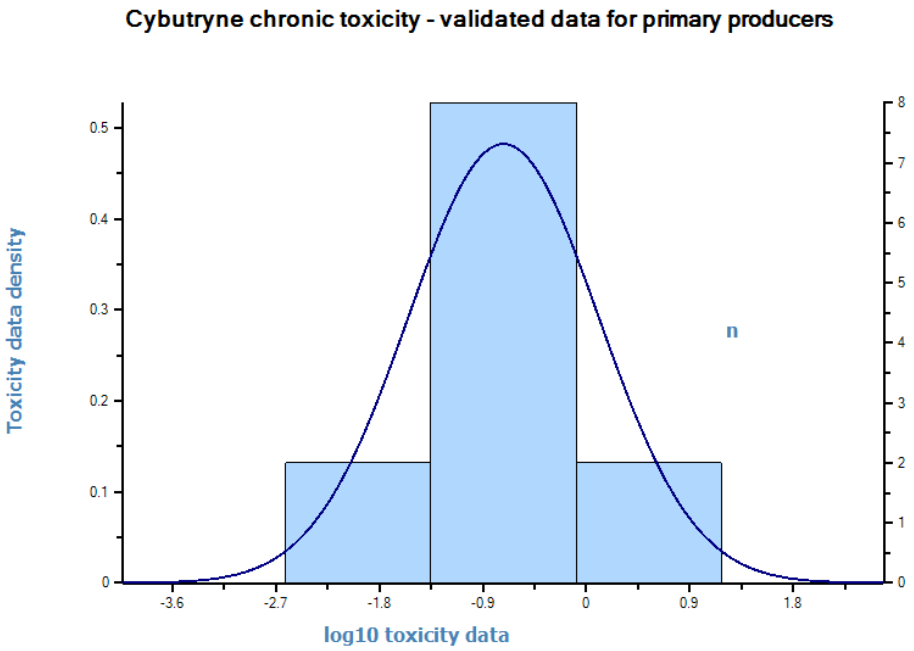

Figure A3: Histogram of the validated chronic data for primary producers.

Table A5: Goodness of fit for the SSD on validated chronic toxicity values for primary producers as calculated with the program ETX 2.0.

Anderson-Darling test for normality				
Sign. level	Critical	Normal?		
0.1	0.631	Accepted		
0.05	0.752	Accepted	AD Statistic:	0.218017
0.025	0.873	Accepted	n:	12
0.01	1.035	Accepted		
Kolmogorov-Smirnov test for normality				
Sign. level	Critical	Normal?		
0.1	0.819	Accepted		
0.05	0.895	Accepted	KS Statistic:	0.489784
0.025	0.995	Accepted	n:	12
0.01	1.035	Accepted		
Cramer von Mises test for normality				
Sign. level	Critical	Normal?		
0.1	0.104	Accepted		
0.05	0.126	Accepted	CM Statistic:	0.026257
0.025	0.148	Accepted	n:	12
0.01	0.179	Accepted		

Table A6: Results for the SSD on validated chronic toxicity data for primary producers calculated with the program ETX 2.0.

Parameters of the normal distribution			
Name	Value		Description
mean	-0.720402425		mean of the log toxicity values
s.d.	0.826727788		sample standard deviation
n	12		sample size
HC5 results			
Name	Value	log10(Value)	Description
LL HC5	0.001040847	-2.98261	lower estimate of the HC5
HC5	**0.007614382**	-2.11837	median estimate of the HC5
UL HC5	0.025189868	-1.59877	upper estimate of the HC5
sprHC5	24.20130659	1.383839	spread of the HC5 estimate
FA At HC5 results			
Name	Value		Description
FA lower	0.774		5% confidence limit of the FA at standardised median logHC5
FA median	5		50% confidence limit of the FA at standardised median logHC5
FA upper	18.064		95% confidence limit of the FA at standardised median logHC5
HC50 results			
Name	Value	log10(Value)	Description
LL HC50	0.070957667	-1.149	lower estimate of the HC50
HC50	0.19036959	-0.7204	median estimate of the HC50
UL HC50	0.510735238	-0.2918	upper estimate of the HC50
sprHC50	7.197745663	0.857196	spread of the HC50 estimate
FA At HC50 results			
Name	Value		Description
FA lower	31.74546726		5% confidence limit of the FA at standardised median logHC50
FA median	49.99999998		50% confidence limit of the FA at standardised median logHC50
FA upper	68.25453275		95% confidence limit of the FA at standardised median logHC50