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Environmental risk limits for monochloroanilines

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This investigation has been performed by order and for the account of Directorate-General for Environmental Protection, Sustainable Production Directorate (DP), within the framework of the project “Standard setting for other relevant substances within the WFD”.

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Abstract

Environmental risk limits for monochloroanilines

The RIVM has derived environmental risk limits (ERLs) for three monochloroanilines in water and groundwater. This group of substances contains 2-, 3-, and 4-chloroaniline. Monochloroanilines are used for the production of azo dyes, pigments, pharmaceutical and cosmetic products, and pesticides. 4-Chloroaniline was selected by the International Commission for the Protection of the Rhine (ICPR) as a Rhine relevant substance within the Water Framework Directive. The other substances, 2- and 3-chloroaniline, are selected for environmental risk limit derivation in the scope of the 'other relevant substances' for the Water Framework Directive because of their concentrations in surface water.

For deriving the environmental risk limits, RIVM used the most up-to-date ecotoxicological data in combination with the most recent methodology, as required by the European Water Framework Directive. No risk limits were derived for the sediment compartment, because sorption to sediment is assumed to be negligible.

Environmental risk limits, as derived in this report, are scientifically derived values, based on (eco)toxicological, fate and physico-chemical data. They serve as advisory values for the Dutch Steering Committee for Substances, which is appointed to set the Environmental Quality Standards (EQSs). ERLs are thus preliminary values that do not have any official status. Four different ERLs are distinguished: negligible concentrations (NC); the concentration at which no harmful effects are to be expected (maximum permissible concentration, MPC); the maximum acceptable concentration for ecosystems specifically for short-term exposure (MAC_{eco}), and the concentration at which possible serious effects are to be expected (serious risk concentration, $SRC_{eco,\ water}$).

Monitoring data from surface waters, from 1990 and for one location also from 2000, revealed that average concentrations measured in the field always exceeded the NC_{water} when the detection limit was exceeded. The annual average and maximum concentrations did not exceed MPC_{water} and $MAC_{eco,water}$ for all three compounds at any location. At one location (Schaar van Ouden Doel), the annual average concentration exceeded the MPC_{dw}.

Key words:

environmental risk limits, monochloroanilines, maximum permissible concentration

Rapport in het kort

Milieurisicogrenzen voor monochlooranilines

Het RIVM heeft milieurisicogrenzen afgeleid voor drie monochlooranilines in zoet en zout water, en grondwater. Monochlooranilines zijn stoffen die vrijkomen bij de productie van bijvoorbeeld (azo)verf, pigmenten, bestrijdingsmiddelen en farmaceutische en cosmetische producten. De stoffen zijn in verband met de Kaderrichtlijn Water door de Internationale Commissie voor Bescherming van de Rijn (ICBR) geselecteerd als Rijnrelevante stof (4-chlooraniline) of door Nederland als ‘overig relevante stof’ (2- en 3-chlooraniline) op grond van de concentraties waarin ze worden aangetroffen in het oppervlaktewater.

Voor de afleiding van de milieurisicogrenzen heeft het RIVM de meest actuele toxicologische gegevens gebruikt, gecombineerd met de meest recente methodiek. Deze methodiek is voorgeschreven door de Europese Kaderrichtlijn Water. Voor het sediment, de waterbodem, zijn geen milieurisicogrenzen afgeleid. Dat komt doordat de mate waarin de stoffen aan sediment binden, verwaarloosbaar wordt geacht.

Milieurisicogrenzen, zoals afgeleid in dit rapport, zijn wetenschappelijk afgeleide waarden, gebaseerd op (eco)toxicologische, milieuchemische en fysisch-chemische gegevens. Milieurisicogrenzen dienen als advieswaarden voor de Nederlandse interdepartementale Stuurgroep Stoffen, die de uiteindelijke milieukwaliteitsnormen vaststelt. Milieurisicogrenzen zijn dus voorlopige waarden zonder enige officiële status. Er bestaan vier verschillende niveaus voor milieurisicogrenzen: een verwaarloosbaar risiconiveau (VR), een niveau waarbij geen schadelijke effecten zijn te verwachten (MTR), het maximaal aanvaardbare niveau voor ecosystemen, specifiek voor kortdurende blootstelling (MAC_{eco}) en een niveau waarbij mogelijk ernstige effecten voor ecosystemen zijn te verwachten (ER_{eco}).

Monitoring data uit 1990 en 2000 laten zien dat op alle vijf meetlocaties het VR_{water} werd overschreden wanneer de detectielimiet werd gehaald. Wanneer echter wordt gekeken naar jaargemiddelde concentraties, dan werd het MTR_{water} niet overschreden en de MTR_{dw} voor drinkwater op één locatie. Maximumconcentraties waren altijd beneden de $MAC_{eco, water}$.

Trefwoorden: milieurisicogrenzen, monochlooranilines, maximaal toelaatbaar risiconiveau

Preface

The goal of this report is to derive risk limits for three chloroanilines that protect both man and the environment. This is done in accordance with the methodology of the Water Framewerk Directive (WFD) that is incorporated in the methodology for the project 'International and National Environmental Quality Standards for Substances in the Netherlands' (INS), following the Guidance for the derivation of environmental risk limits within the INS framework (Van Vlaardingen and Verbruggen, 2007). The three monochloroanilines have been evaluated by Reuther et al. in 1998, but only on an ecotoxicological basis. For the present evaluation, toxicity data are searched and are assessed again, following the present INS methodology (Van Vlaardingen and Verbruggen, 2007).

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Acknowledgements

Thanks are due to dr. T. Crommentuijn and ir. J.M.C. Appelman, who were contact persons at the Ministry of Housing, Spatial Planning and the Environment (VROM-DP) and to dr. M.P.M. Janssen who is program coordinator for the derivation of ERLs within the RIVM.

The results of the present report have been discussed in the scientific advisory group INS (WK-INS). The members of this group are acknowledged for their contribution.

Thanks are due to drs. L.C. van Leeuwen, dr. ir. C.T.A. Moermond and ing. P.L.A. van Vlaardingen for helpful discussions and commenting on the report.

Contents

Summary

Environmental risk limits (ERLs) are derived using ecotoxicological, physicochemical, and human toxicological data. They represent environmental concentrations of a substance offering different levels of protection to man and ecosystems. It should be noted that the ERLs are scientifically derived values. They serve as advisory values for the Dutch Steering committee for Substances, which is appointed to set the Environmental Quality Standards (EQSs) from these ERLs. ERLs should thus be considered as preliminary values that do not have any official status.

In this report, the risk limits negligible concentration (NC), maximum permissible concentration (MPC), maximum acceptable concentration for ecosystems (MAC_{eco}), and serious risk concentration for ecosystems (SRC_{eco}) are derived for three monochloroanilines in water. No risk limits were derived for the sediment compartment because sorption to sediment was assumed to be negligible.

For the derivation of the MPC and MAC_{eco} for water, the methodology used is in accordance with the Water Framework Directive (Lepper, 2005). This methodology is based on the Technical Guidance Document on risk assessment for new and existing substances and biocides (European Commission (Joint Research Centre), 2003). For the NC and the SRC_{eco}, the guidance developed for the project 'International and National Environmental Quality Standards for Substances in the Netherlands' was used (Van Vlaardingen and Verbruggen, 2007). An overview of the derived environmental risk limits is given in Table 1.

Monitoring data from surface waters, from 1990 and for one location also from 2000, revealed that average concentrations measured in the field always exceeded the NC_{water} when the detection limit was exceeded. The annual average and maximum concentrations did not exceed MPC_{water} and $MAC_{eco,water}$ for all three compounds at any location. At one location (Schaar van Ouden Doel), the annual average concentration exceeded the MPC_{dw}.

Table 1. Derived MPC, NC, MAC_{eco}, and $SRC_{eco, water}$ values for three chloroanilines (in µg/L).

Environmental risk limit[1]	2-chloroaniline	3-chloroaniline	4-chloroaniline
MPC_{water}	0.20	0.41	0.22
$MPC_{dw, water}$	3.2×10^{-2}	3.2×10^{-2}	3.2×10^{-2}
MPC_{gw}	3.2×10^{-2}	3.2×10^{-2}	3.2×10^{-2}
MPC_{marine}	3.2×10^{-2}	6.5×10^{-2}	5.7×10^{-2}
NC_{water}	2.0×10^{-3}	4.1×10^{-3}	2.2×10^{-3}
NC_{marine}	3.2×10^{-4}	6.5×10^{-4}	5.7×10^{-4}
$MAC_{eco, water}$	10	4.6	1.2
$MAC_{eco, marine}$	1.0	0.46	0.12
$SRC_{eco, water}$	1.3×10^{3}	1.8×10^{3}	5.5×10^{2}

[1] subscripts: water = freshwater; dw = drinking water; gw = groundwater; marine = marine waters
$MPC_{dw, water,}$ = MPC based on human consumption of drinking water.

Samenvatting

Milieurisicogrenzen worden afgeleid met gebruik van ecotoxicologische, fysisch-chemische en humaan-toxicologische gegevens en representeren de milieuconcentraties van stoffen waarbij verschillende niveaus van bescherming voor mens en milieu worden gegeven. De milieurisicogrenzen zijn wetenschappelijk afgeleide waarden, die dienen als basis voor de Stuurgroep Stoffen, die de milieukwaliteitsnormen vaststelt op basis van deze milieurisicogrenzen. Milieurisicogrenzen zijn dus voorlopige waarden zonder officiële status. In dit rapport zijn de milieurisicogrenzen verwaarloosbaar risiconiveau (VR), maximaal toelaatbaar risiconiveau (MTR), maximaal acceptabele concentratie voor ecosystemen (MAC_{eco}) en ernstig risiconiveau voor ecosystemen (ER_{eco}) afgeleid voor drie monochlooranilines in water. Voor het sediment zijn geen risicogrenzen afgeleid omdat de sorptie aan sediment verwaarloosbaar wordt geacht.

Voor het afleiden van het MTR en de MAC_{eco} voor water is gebruikgemaakt van de methodiek in overeenstemming met de Kaderrichtlijn Water (Lepper, 2005). Deze methodiek is gebaseerd op het EU richtsnoer voor de risicobeoordeling van nieuwe stoffen, bestaande stoffen en biociden (European Commission (Joint Research Centre), 2003). Voor ER_{eco} en VR is de handleiding voor het project (Inter)Nationale Normstelling Stoffen (INS) gebruikt (Van Vlaardingen and Verbruggen, 2007). Een overzicht van de afgeleide milieurisicogrenzen wordt in Tabel 2 gegeven.

Monitoring data uit 1990 en 2000 laten zien dat op alle vijf meetlocaties het VR_{water} werd overschreden wanneer de detectielimiet werd gehaald. Wanneer echter wordt gekeken naar jaargemiddelde concentraties, dan werd het MTR_{water} niet overschreden en de MTR_{dw} voor drinkwater op één locatie. Maximumconcentraties waren altijd beneden de $MAC_{eco, water}$.

Tabel 2. Afgeleide MTR, MAC_{eco}, VR en $ER_{eco, water}$ waarden voor drie chlooranilines (in µg/L).

Milieurisicogrens[1]	2-chlooraniline	3-chlooraniline	4-chlooraniline
MTR_{water}	0,20	0,41	0,22
$MTR_{dw, water}$	$3,2 \times 10^{-2}$	$3,2 \times 10^{-2}$	$3,2 \times 10^{-2}$
MTR_{gw}	$3,2 \times 10^{-2}$	$3,2 \times 10^{-2}$	$3,2 \times 10^{-2}$
MTR_{marine}	$3,2 \times 10^{-2}$	$6,5 \times 10^{-2}$	$5,7 \times 10^{-2}$
VR_{water}	$2,0 \times 10^{-3}$	$4,1 \times 10^{-3}$	$2,2 \times 10^{-3}$
VR_{marine}	$3,2 \times 10^{-4}$	$6,5 \times 10^{-4}$	$5,7 \times 10^{-4}$
$MAC_{eco, water}$	10	4,6	1,2
$MAC_{eco, marine}$	1,0	0,46	0,12
$ER_{eco, water}$	$1,3 \times 10^{3}$	$1,8 \times 10^{3}$	$5,5 \times 10^{2}$

[1] subscript: water = zoetwater; dw = drinkwater; gw = grondwater; marien = mariene wateren
$MTR_{dw,water}$ = MTR gebaseerd op humane consumptie van drinkwater.

1 Introduction

1.1 Project framework

In this report, environmental risk limits (ERLs) for surface water (freshwater and marine) and groundwater are derived for 2-, 3-, and 4-chloroaniline. The following ERLs are considered:

- negligible concentration (NC) – concentration at which effects to ecosystems are expected to be negligible and functional properties of ecosystems must be safeguarded fully. It defines a safety margin which should exclude combination toxicity. The NC is derived by dividing the MPC (see next bullet) by a factor of 100.
- maximum permissible concentration (MPC) – concentration in an environmental compartment at which:
  1 no effect to be rated as negative is to be expected for ecosystems;
  2a no effect to be rated as negative is to be expected for humans (for non-carcinogenic substances);
  2b for humans no more than a probability of 10^{-6} per year of death can be calculated (for carcinogenic substances). Within the scope of the Water Framework Directive, a probability of 10^{-6} on a life-time basis is used.

  Within the scope of the Water Framework Directive the MPC is specifically referring to long-term exposure.
- maximum acceptable concentration (MAC_{eco}) – concentration protecting aquatic ecosystems for effects due to short-term exposure or concentration peaks.
- serious risk concentration (SRC_{eco}) – concentration at which possibly serious ecotoxicological effects are to be expected.

The results presented in this report have been discussed by the members of the scientific advisory group for the INS-project (WK-INS). It should be noted that the Environmental Risk Limits (ERLs) in this report are scientifically derived values, based on (eco)toxicological, fate and physico-chemical data. They serve as advisory values for the Dutch Steering Committee for Substances, which is appointed to set the Environmental Quality Standards (EQSs). ERLs should thus be considered as preliminary values that do not have any official status.

1.2 Selection of substances

ERLs are derived for 2-, 3-, and 4-chloroaniline. The International Commission for the Protection of the Rhine (ICPR) has selected 4-chloroaniline as a Rhine relevant substance. The other substances, 2- and 3-chloroaniline, are selected by the Netherlands in scope of the Water Framework Directive (WFD, 2000/60/EC), because of their concentrations in surface water.

2 Methods

The methodology for the data selection and derivation of ERLs is described in detail in Van Vlaardingen and Verbruggen (2007), further referred to as the ‘INS-Guidance’. This guidance is in accordance with the guidance of the Fraunhofer Institute (FHI; Lepper, 2005) and prepared within the context of the WFD.

The process of ERL-derivation contains the following steps: data collection, data evaluation and selection, and derivation of the ERLs on the basis of the selected data. Specific items will be discussed below.

2.1 Data collection, evaluation and selection

In accordance with the WFD, data of existing evaluations were used as a starting point. An on-line literature search was performed on TOXLINE (literature from 1985 to 2001) and Current Contents (literature from 1997 to 2007). In addition to this, all potentially relevant references in the RIVM e-tox base and EPA’s ECOTOX database were checked.

Ecotoxicity studies were screened for relevant endpoints (i.e. those endpoints that have consequences at the population level of the test species). All ecotoxicity and bioaccumulation tests were then thoroughly evaluated with respect to the validity (scientific reliability) of the study. A detailed description of the evaluation procedure is given in the INS-Guidance (see section 2.2.2 and 2.3.2).

After data collection and validation, toxicity data were combined into an aggregated data table with one effect value per species according to section 2.2.6 of the INS-Guidance. When for a species several effect data were available, the geometric mean of multiple values for the same endpoint was calculated where possible. Subsequently, when several endpoints were available for one species, the lowest of these endpoints (per species) is reported in the aggregated data table.

2.2 Derivation of ERLs

2.2.1 Drinking water

The INS-Guidance includes the MPC for surface waters intended for the abstraction of drinking water ($MPC_{dw, water}$) as one of the MPCs from which the lowest value should be selected as the general MPC_{water} (see INS-Guidance, section 3.1.6 and 3.1.7). According to the proposal for the daughter directive Priority Substances, however, the derivation of the AA-EQS (= MPC) should be based on direct exposure, secondary poisoning, and human exposure due to the consumption of fish. Drinking water was not included in the proposal and is thus not guiding for the general MPC_{water} value. The exact way of implementation of the $MPC_{dw, water}$ in the Netherlands is at present under discussion within the framework of the ‘AMvB Kwaliteitseisen en Monitoring Water’. No policy decision has been taken yet, and the $MPC_{dw, water}$ is therefore presented as a separate value in this report. The MPC_{water} is thus derived considering the individual MPCs based on direct exposure ($MPC_{eco, water}$), secondary poisoning ($MPC_{sp, water}$) or human consumption of fishery products ($MPC_{hh food, water}$); the need to derive the latter two depends on the characteristics of the compound. Although the $MPC_{dw, water}$ is not taken into account for the derivation of the MPC_{water}, it is used for the derivation of the groundwater risk limit, MPC_{gw}.

2.2.2 $MAC_{eco, marine}$

In this report, the $MAC_{eco, marine}$ value is based on the $MAC_{eco,water}$ value when acute toxicity data for at least two specific marine taxa are available, using an additional assessment factor (analogous to the derivation of the MPC according to Van Vlaardingen and Verbruggen, 2007) of 5 when acute toxicity data for only one specific marine taxon is available and an additional assessment factor of 10 when no acute toxicity data is available for specific marine taxa. It has to be noted that this procedure is currently not agreed upon. Therefore, the $MAC_{eco, marine}$ value needs to be re-evaluated once an agreed procedure is availabe.

3 Substance identification, physico-chemical properties, bioconcentration, and human toxicological data

3.1 2-Chloroaniline

3.1.1 Identity

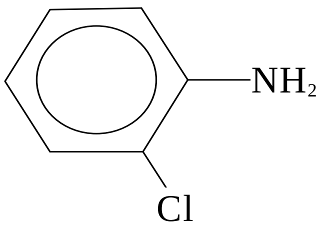

Figure 1. Structural formula of 2-chloroaniline.

Table 3. Identification of 2-chloroaniline.

Parameter	Name or nr.	Source
Chemical name	2-chloroaniline	
Common/trival/other name	1-amino-2-chlorobenzene 2-amino-1-chlorobenzene 2-chlorobenzenamine 2-chlorophenylamine Fast Yellow GC Base *o*-aminochlorobenzene *o*-chloroaniline OCA orthochloroaniline	IUCLID (European Commission, 2000), Mackay et al. (2000)
CAS nr.	95-51-2	
EC nr.	202-426-4	
SMILES code	Nc(c(ccc1)CL)c1	Epiwin 3.12 (US EPA, 2000)

3.1.2 Physico-chemical properties

Physico-chemical properties of 2-chloroaniline are shown in Table 4. Bold values indicate values used in calculations.

Table 4. Selected physico-chemical properties of 2-chloroaniline.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	**127.57**		Mackay et al. (2000) EPI Suite 3.12 (US EPA, 2000)
Water solubility	[mg/L]	**3800**	value selected by Mackay et al. (2000), 25 °C	Mackay et al. (2000)
		8760		Dreisbach (1955)[a]
		3765	20 °C, shake-flask, GC	Chiou (1981)[a] Chiou and Schmedding (1981)[a] Chiou et al. (1982)[a]
		2241	calculated, estimate from log K_{ow} (Bioloom value), 25 °C	EPI Suite 3.12 (US EPA, 2000)
		5232.4	calculated, estimate from fragments	
		12400	calculated, 25 °C	SPARC (Karickhoff et al., 2007)
		± 5130	20 °C	Bayer AG Leverkusen (IUCLID;
		5600	20 °C	EC, 2000)
pK_a	[-]	**2.661**[b]	value selected by Mackay et al. (2000)	Perrin (1972)[a]
		2.64	experimental	Bioloom (BioByte, 2004)
		2.67	calculated	SPARC (Karickhoff et al., 2007)
log K_{ow}	[-]	1.91	calculated	Bioloom (BioByte, 2004)
		1.90	experimental, value selected by Bioloom and Mackay et al. (2000)	Bioloom (BioByte, 2004) Mackay et al. (2000)
		1.92	shake-flask	Tichy and Bocek (private communication)[c]
		1.90	shake-flask	Glave and Hansch (unpublished)[c]
		1.93	slow-stirring-GC	De Bruijn et al. (1989)[a,c]
		1.74	HPLC	Könemann et al. (1979)[a,c]
		1.70	HPLC	Tsantili-Kakoulidou et al. (1987)[c]
		1.94	HPLC	Ahlers et al. (1988)[c]
		1.81	shake-flask	Fujita et al. (1964)[a]
		1.92	experimental	Leo et al. (1971)[a] Rekker et al. (1977)[a]
		1.92	HPLC	Carlson et al. (1975)[a] Sangster (1993)[a]
		1.91	experimental	Rekker (1977)[a]
		1.73	calculated	Rekker (1977)[a]
		1.90	shake-flask	Hansch and Leo (1979)[a]
		1.92	shake-flask	Hansch and Leo (1979)[a]
		1.76	HPLC	Könemann et al. (1979)[a]
		1.91	HPLC	Hammers et al. (1982)[a]
		1.99	HPLC	Hammers et al. (1982)[a]
		1.72	calculated	EPI Suite 3.12 (US EPA, 2000)
		1.57	calculated	SPARC (Karickhoff et al., 2007)
		1.9		Bayer AG Leverkusen (IUCLID (European Commission, 2000))

Parameter	Unit	Value	Remark	Reference
log K_{oc}	[-]	**2.03**	calculated, QSAR for anilines: log K_{oc} = 0.62 * log K_{ow} + 0.85 (Value of 1.90 for log K_{ow} was used)	Sabljic et al. (1995)
		1.869	Calculated	EPI Suite 3.12 (US EPA, 2000)
Vapour pressure	[Pa]	**22.66**	solid and liquid, value selected by Mackay et al., 25 °C	Mackay et al. (2000)
		35.30	torsion-weighing effusion	Piacente et al. (1985)[a]
		21	calculated, 25 °C	EPI Suite 3.12 (US EPA, 2000)
		59.79	calculated, 25 °C	SPARC (Karickhoff et al., 2007)
		13	20 °C	IUCLID (European Commission, 2000)
		36	30 °C	
		170	50 °C	
Melting point	[°C]	**-14**	value selected by Mackay et al. (2000)	Verschueren (1983)[a] Howard (1989)[a]
		-1.94		Dreisbach (1955)[a]
		24.41	calculated	EPI Suite 3.12 (US EPA, 2000)
		-3		IUCLID (European Commission, 2000)
Boiling point	[°C]	**208.84**	value selected by Mackay et al. (2000)	Kahlbaum (1898)[a] Stull (1947)[a] Dreisbach (1955)[a] Verschueren (1983)[a] Riddick et al. (1986)[a] Howard (1989)[a]
		209.0		Banerjee et al. (1990)[a]
		216.05	calculated	EPI Suite 3.12 (US EPA, 2000)
		202.9	calculated	SPARC (Karickhoff et al., 2007)
		208.8		IUCLID (European Commission, 2000)
		ca. 209	initial boiling point, decomposition	
Henry's law constant	[Pa.m^3/mol]	**0.761**	calculated (P/C), value selected by Mackay et al. (2000), 25 °C	Howard (1989)[a]
		0.143	calculated, bond method, 25 °C	EPI Suite 3.12 (US EPA, 2000)
		0.188	calculated, group method, 25 °C	
		1.21	vapour pressure / water solubility using EPI values; calculated using log K_{ow} = 1.90; 25 °C	
		0.62		SPARC (Karickhoff et al., 2007)

[a] Cited in Mackay et al. (2000).
[b] At pH 7, almost all 2-chloroaniline is present in unprotonated (neutral) form.
[c] Data obtained from Bioloom database (BioByte, 2004).

3.1.3 Bioconcentration and biomagnification

The structural analogue of 2-chloroaniline, 4-chloroaniline, has an R45 classification. Following Janssen et al. (1998), it may be assumed that 2-chloroaniline is carcinogenic as well. For this reason, the literature was searched for experimental bioconcentration data. The BCF data and experimental details are given in Table A1.1 of Appendix 1. BCF values were determined in whole fish and are 2.0 and 3.7 L/kg (Tsuda et al., 1993). Using the QSAR given in the INS guidance (Van Vlaardingen and Verbruggen (2007), applicable for substances with a log K_{ow} of 2 – 6) the BCF is calculated to be 8.22 L/kg. The geometric mean of the experimentally determined BCF values is 2.72 L/kg, which is used in the derivation of ERLs. The potential for biomagnification is expected to be low (log K_{ow} < 3).

3.1.4 Carcinogenicity

2-Chloroaniline is not classified in Annex I of Directive 67/548/EEC or by the International Agency for Research on Cancer (IARC). However, the structural analogue 4-chloroaniline has an R45 classification (may cause cancer).

3.1.5 Human toxicological treshold limits

Although 2-chloroaniline is not classified as possibly carcinogenic to humans, its structural analogue 4-chloroaniline has an R45 classification. For this reason, it may be assumed that 2-chloroaniline is carcinogenic as well. This approach is in accordance with the RIVM evaluation of monochloroanilines by Janssen et al. (1998). In this evaluation, an MPC_{oral} of 0.9 µg/kg_{bw}/d was derived, based on a lifetime cancer risk of 1 : 10^4. As the WFD guidance prefers to base risk limits on a 1 : 10^6 lifetime cancer risk, the TL_{hh} is calculated as MPC_{oral} / 100 = 9 ng/kg_{bw}/d. More details on the evaluation of the monochloroanilines with respect to human toxicology are given in section 3.3.5.

3.2 3-Chloroaniline

3.2.1 Identity

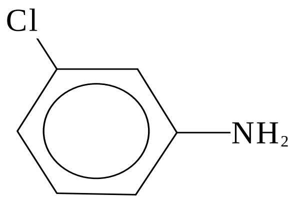

Figure 2. Structural formula of 3-chloroaniline.

Table 5. Identification of 3-chloroaniline.

Parameter	Name or nr.	Source
Chemical name	3-chloroaniline	
Common/trival/other name	1-amino-3-chlorobenzene *m*-chloroaniline 3-chlorophenylamine	Mackay et al. (2000)
CAS nr.	108-42-9	
EC nr.	203-581-0	
SMILES code	Nc(cccc1CL)c1	Epiwin 3.12 (US EPA, 2000)

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3.2.2 Physico-chemical properties

Physico-chemical properties of 3-chloroaniline are shown in Table 6. Bold values indicate values used in calculations.

Table 6. Selected physico-chemical properties of 3-chloroaniline.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	**127.57**		Mackay et al. (2000) EPI Suite 3.12 (US EPA, 2000)
Water solubility	[mg/L]	**5440**	value selected by Mackay et al. (2000), 25 °C	Mackay et al. (2000)
		5442	shake-flask-GC, 20 °C	Chiou (1981)[a] Chiou and Schmedding (1981)[a] Chiou et al. (1982)[a]
		2331	calculated, estimate from log K_{ow} (Bioloom value), 25 °C	EPI Suite 3.12 (US EPA, 2000)
		5232.4	calculated, estimate from fragments	
		11400	calculated, 25 °C	SPARC (Karickhoff et al., 2007)
pK_a	[-]	**3.5**[b]	value selected by Mackay et al. (2000)	Perrin (1972)[a]
		3.52	experimental	Bioloom (BioByte, 2004)
		3.73	calculated	SPARC (Karickhoff et al., 2007)
log K_{ow}	[-]	1.91	calculated	Bioloom (BioByte, 2004)
		1.88	experimental, value selected by Bioloom	Bioloom (BioByte, 2004)
		1.88		Fujita et al. (1964)[c]
		1.91	slow-stirring-GC	De Bruijn et al. (1989)[a,c]
		1.90		Tichy and Bocek (private communication)[c]
		1.57	HPLC	Könemann et al. (1979)[a,c]
		1.78	HPLC	Tsantili-Kakoulidou (1979)[c]
		1.82	HPLC	Ahlers et al. (1988)
		1.88	value selected by Mackay et al. (2000)	Mackay et al. (2000)
		1.88	shake-flask-AS	Fujita et al. (1964)[a]
		1.90	Experimental	Leo et al. (1971)[a] Rekker (1977)[a]
		1.90	shake flask	Hansch and Leo (1979)[a]
		1.88	shake flask	Hansch and Leo (1979)[a]
		1.76	HPLC	Könemann et al. (1979)[a]
		1.89	HPLC	Hammer et al. (1982)[a]
		2.00	HPLC	Hammer et al. (1982)[a]
		1.72	Calculated	EPI Suite 3.12 (US EPA, 2000)
		1.77	Calculated	SPARC (Karickhoff et al., 2007)
log K_{oc}	[-]	**2.02**	calculated, QSAR for anilines: log K_{oc} = 0.62 * log K_{ow} + 0.85 (Value of 1.88 for log K_{ow} was used)	Sabljic et al. (1995)
		1.861	Calculated	EPI Suite 3.12 (US EPA, 2000)
Vapour pressure	[Pa]	**9.53**	calculated (extrapolated from Antoine equation), solid and liquid, value selected by Mackay et al. (2000), 25 °C	Stephenson and Malanowski (1987)[a]
		15.60	torsion-weighing effusion	Piacente et al. (1985)[a]

Parameter	Unit	Value	Remark	Reference
		21	calculated, 25 °C	EPI Suite 3.12 (US EPA, 2000)
		24.13	calculated, 25 °C	SPARC (Karickhoff et al., 2007)
Melting point	[°C]	-11 – -9	value selected by Mackay et al. (2000)	Mackay et al. (2000)
		- 9.9	geometric mean	Mackay et al. (2000)
		-10.40		Stull (1947)[a] Dean (1985)[a] Verschueren (1983)[a] Budavari (1989)[a]
		-10.29		Dreibach (1955)[a]
		24.41	Calculated	EPI Suite 3.12 (US EPA, 2000)
Boiling point	[°C]	**229**	value selected by Mackay et al. (2000)	Mackay et al. (2000)
		228.5		Kahlbaum (1898)[a] Stull (1947)[a]
		229.9		Dreisbach (1955)[a]
		229.8		Verschueren (1983)[a]
		230.5		Dean (1985)[a] Budavari (1989)[a]
		216.05	Calculated	EPI Suite 3.12 (US EPA, 2000)\
		216.1	Calculated	SPARC (Karickhoff et al., 2007)
Henry's law constant	[Pa.m^3/mol]	**0.223**	calculated (P/C), value selected by Mackay et al. (2000), 25 °C	Mackay et al. (2000)
		0.143	calculated, bond method, 25 °C	EPI Suite 3.12 (US EPA, 2000)
		0.188	calculated, group method, 25 °C	EPI Suite 3.12 (US EPA, 2000)
		1.17	vapour pressure / water solubility using EPI values; calculated using log K_{ow} = 1.88; 25 °C	EPI Suite 3.12 (US EPA, 2000)
		0.27	calculated, 25 °C	SPARC (Karickhoff et al., 2007)

[a] Cited in Mackay et al. (2000).
[b] At pH 7, almost all 3-chloroaniline is present in unprotonated (neutral) form.
[c] Data obtained from Bioloom database (BioByte, 2004).

3.2.3 Bioconcentration and biomagnification

Although not experimentally confirmed, 3-chloroaniline is assumed to be carcinogenic based on the R45 classification of its structural analogue, 4-chloroaniline (in accordance with Janssen et al., 1998). Therefore, a literature search was conducted to obtain experimentally determined bioconcentration data. The BCF data and experimental details are given in Table A1.2 of Appendix 1. BCF values were determined in whole fish and are 0.8 and 2.2 L/kg (Tsuda et al., 1993). Using the QSAR given in the INS guidance (Van Vlaardingen and Verbruggen (2007), applicable to substances with a log K_{ow} of 2 - 6) results in a BCF of 7.91 L/kg. The geometric mean of the BCF values is 1.33 L/kg, which is used in the derivation of ERLs. Biomagnification is not considered relevant because log K_{ow} < 3.

3.2.4 Carcinogenicity

3-Chloroaniline is not classified in Annex I of Directive 67/548/EEC or by the International Agency for Research on Cancer (IARC). However, the structural analogue 4-chloroaniline has an R45 classification (may cause cancer).

3.2.5 Human toxicological threshold limits

3-Chloroaniline is not classified as a possibly carcinogenic to humans. However, based on the R45 classification of its structural analogue 4-chloroaniline, it may be assumed that 3-chloroaniline is carcinogenic as well. This approach is in accordance with the RIVM evaluation of monochloroanilines by Janssen et al. (1998). In this evaluation, an MPC_{oral} of 0.9 µg/kg_{bw}/d was derived, based on a lifetime cancer risk of 1 : 10^4. As the WFD guidance prefers to base risk limits on a 1 : 10^6 lifetime cancer risk, the TL_{hh} is calculated as MPC_{oral} / 100 = 9 ng/kg_{bw}/d. More details on the evaluation of the monochloroanilines with respect to human toxicology are given in section 3.3.5.

3.3 4-Chloroaniline

3.3.1 Identity

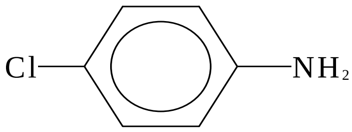

Figure 3. Structural formula of 4-chloroaniline.

Table 7. Identification of 4-chloroaniline.

Parameter	Name or nr.	Source
Chemical name	4-chloroaniline	
Common/trival/other name	1-amino-4-chlorobenzene *p*-chloroaniline 4-chlorophenylamine	Mackay et al. (2000)
CAS nr.	106-47-8	
EC nr.	203-401-0	
SMILES code	Nc(ccc(c1)Cl)c1	Epiwin 3.12 (US EPA, 2000)

3.3.2 Physico-chemical properties

Physico-chemical properties of 4-chloroaniline are shown in Table 8. Bold values indicate values used in calculations.

Table 8. Selected physico-chemical properties of 4-chloroaniline.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	**127.57**		Mackay et al. 2000 EPI Suite 3.12 (US EPA, 2000)
Water solubility	[mg/L]	**3000**	value selected by Mackay et al. (2000), 25 °C	Philpot et al. (1940)[a]
		2331	calculated, estimate from log K_{ow} (Bioloom value), 25 °C	EPI Suite 3.12 (US EPA, 2000)
		5232.4	estimate from fragments	EPI Suite 3.12 (US EPA, 2000)
		5090	calculated, 25 °C, melting point set at 70.0 °C	SPARC (Karickhoff et al., 2007)
pK_a	[-]	**3.982**[b]	value selected by Mackay et al. (2000)	Mackay et al. (2000)
		3.98	Experimental	Bioloom (BioByte, 2004)
		4.06	Calculated	SPARC (Karickhoff et al., 2007)
log K_{ow}	[-]	1.91	Calculated	Bioloom (BioByte, 2004)
		1.88	experimental, value selected by Bioloom	Bioloom (BioByte, 2004)
		1.88	slow-stirring-GC	De Bruijn et al. (1989)[a,c]
		1.83		Hanna et al. (1998)[c]
		1.83		Tichy and Bocek (private communication)[c]
		1.76	HPLC	Ahlers et al. (1988)[c]
		1.75	HPLC	Tsantili-Kakoulidou et al. (1987)[c]
		1.57	HPLC	Könemann et al. 1979[a,c]
		1.83	pH 7.4	Kishida et al. (1980)[c]
		2.01	centrifugal partition chromatography	El Tayar et al. (1991)[c]
		1.84	pH 7.4	Hitzel et al. (2000)[c]
		1.83	value selected by Mackay et al. (2000)	Garst and Wilson (1984)[a]
		1.83	HPLC	Carlson et al. (1975)[a]
		1.83	shake-flask	Hansch and Leo (1979)[a]
		1.76	HPLC	Könemann et al. (1979)[a]
		1.83	HPLC	Hammers et al. (1982)[a]
		2.02	HPLC	Hammers et al. (1982)[a]
		1.64	interlaboratory HPLC average	Eadsforth and Moser (1983)[a]
		1.88	experimental, ALPM	Garst and Wilson (1984)[a]
		2.78	shake-flask	Geyer et al. (1984)[a]
		1.83	RP-HPLC-capacity ratio	Minick et al. (1988)[a]
		1.72	Calculated	EPI Suite 3.12 (US EPA, 2000)
		1.64	Calculated	SPARC (Karickhoff et al., 2007)
log K_{oc}	[-]	2.36 – 2.67	5 Belgium soils	Van Bladel and Moreale (1977)[a]
		1.98 – 3.18	5 German soils	Rott et al. (1982)[a]
		3.74	colloidal organic matter in ground water	Means (1983)[a]
		1.96	soil, experimental	Meylan et al. (1992)[a]
		2.02	calculated, QSAR for anilines: log K_{oc} = 0.62 * log K_{ow} + 0.85 (Value of 1.88 for log K_{ow} was used)	Sabljic et al.(1995)

Parameter	Unit	Value	Remark	Reference
		2.56	geometric mean of values above	
		1.86	Calculated	Sabljic (1987)[a]
		1.86	Calculated	Meylan et al. (1992)[a]
		1.61	calculated	Mackay et al. (2000)
		1.861	Calculated	EPI Suite 3.12 (US EPA, 2000)
Vapour pressure	[Pa]	**2.33**	solid, value selected by Mackay et al. (2000), 25 °C	Mackay et al. (2000)
		6.873	liquid, value selected by Mackay et al. (2000), 25 °C	
		1.636	torsion-weighing effusion	Piacente et al. (1985)
		21	calculated, 25 °C	EPI Suite 3.12 (US EPA, 2000)
		7.29	calculated, 25 °C	SPARC (Karickhoff et al.*I*, 2007)
Melting point	[°C]	**70.0**	value selected by Mackay et al. (2000)	Mackay et al. (2000)
		70.50		Stull (1947)[a]
		69.85		Tsonopoulos and Prausnitz (1982)[a]
		69.90		Schmidt-Bleek et al. (1982)[a]
		70 - 72		Verschueren (1983)[a]
		24.41	Calculated	EPI Suite 3.12 (US EPA, 2000)
Boiling point	[°C]	**232**	value selected by Mackay et al. (2000)	Verschueren (1983)[a] Howard (1989)[a] Banerjee et al. (1990)[a]
		230.5		Stull (1947)[a]
		231.0		Schmidt-Bleek et al. (1982)[a] Verschueren (1983)[a]
		216.05	Calculated	EPI Suite 3.12 (US EPA, 2000)
		220.4	Calculated	SPARC (Karickhoff et al., 2007)
Henry's law constant	[Pa.m^3./mol]	**0.099**	calculated, value selected by Mackay et al. (2000), 25 °C	Mackay et al. (2000)
		0.143	calculated, bond method, 25 °C	EPI Suite 3.12 (US EPA, 2000)
		0.188	calculated, group method, 25 °C	EPI Suite 3.12 (US EPA, 2000)
		1.167	vapour pressure / water solubility using EPI values; calculated using log K_{ow} = 1.88, 25 °C	EPI Suite 3.12 (US EPA, 2000)
		0.00256	calculated, 25 °C	SPARC (Karickhoff et al., 2007)

[a] Cited in Mackay et al. (2000).
[b] At pH 7, almost all 4-chloroaniline is present in unprotonated (neutral) form.
[c] Data obtained from Bioloom database (BioByte, 2004).

3.3.3 Bioconcentration and biomagnification

4-Chloroaniline is classified with R45 and therefore, the literature was searched for experimentally determined BCF values. The available BCF data and details of the experiments are given in Table A1.3 of Appendix 1. The experimentally determined BCF values for 4-chloroanline in fish are 7 and 4 L/kg (not reported which part of fish, Ballhorn (1984), cited in Gesellschaft Deutscher Chemiker (1993)) and 0.8 and 1.7 L/kg (whole fish, Tsuda et al. (1993)). A value of 7.91 L/kg was calculated using the QSAR put forward in the INS guidance (Van Vlaardingen and Verbruggen (2007)), applicable for substances with a log K_{ow} of 2 – 6). The geometric mean of the experimentally determined BCF values is 2.48 L/kg, which is used in the derivation of ERLs. Biomagnification is not expected to be relevant as log K_{ow} is < 3.

3.3.4 Carcinogenicity

4-Chloroaniline is a potential human carcinogen, it is categorised as a class 2B carcinogen in the International Agency for Research on Cancer (IARC) monograph (IARC, 1997). The substance is also classified carcinogenic (category 2) in Annex I of Directive 67/548/EEC.

3.3.5 Human toxicological threshold levels

4-Chloroaniline is classified as possibly carcinogenic to humans and has an R45 classification. The US EPA (1995) derived an RfD of 4 µg/kg_{bw}/d. This value is less reliable, because it is based on a LOAEL without any supportive reproductive and toxicity data. Monochloroanilines were also evaluated by RIVM (Janssen et al., 1998) and more recently IPCS published an evaluation for 4-chloroaniline (WHO, 2003). Both reviews point out the carcinogenic action by the compound, as found in NTP-bioassays dating back to the 1980s. A typical pattern was found of splenic tumorigenicity, which is possibly related to toxic effects in the same organ. Note that aniline produces the same effects. Based on all data, including the available genotoxicity results, Janssen et al. (1998) concluded that the 4-chloroaniline-induced tumorigenic process may include genotoxic events, for which reason a non-threshold approach was deemed appropriate. This led to a risk-specific dose for one in ten thousand of 0.9 µg/kg_{bw}/d (MPC_{oral}). The higher value (TDI) of 2 µg/kg_{bw}/d as proposed by WHO (2003) results from applying a safety factor of 1000 to a LOAEL of 2 mg/kg_{bw}/d for fibrotic changes in the spleen and increased methemoglobin in blood as seen in rat studies. Within the Dutch approach, in case a chemical exerts a genotoxic action, a non-threshold approach is chosen. Considering the fact that the data set reviewed by WHO (2003) is practically identical to the data reviewed by Janssen et al. (1998), preference is given to the value of 0.9 µg/kg_{bw}/d. Note further that within the scope of EU Existing Substances (EU-RAR) it was concluded that aniline has a genotoxic action (European Commission, 2004). This lends support to the approach chosen by Janssen et al. (1998) for 4-chloroaniline.

As was already mentioned above, the MPC_{oral} of 0.9 µg/kg_{bw}/d derived by Janssen et al. (1998) is based on a lifetime cancer risk of $1 : 10^4$. As the WFD guidance prefers to base risk limits on a $1 : 10^6$ lifetime cancer risk, the TL_{hh} is calculated as MPC_{oral} / 100 = 9 ng/kg_{bw}/d.

rivm

4 Trigger values

This section reports on the trigger values for ERLwater derivation (as demanded in WFD framework).

4.1 2-Chloroaniline

Table 9. 2-Chloroaniline: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/source (if applicable)
log $K_{p, susp-water}$	1.03	[-]	$K_{p, susp-water} = K_{oc} \times f_{oc, susp}$[1]
BCF	2.72	[L/kg]	
BMF	1	[kg/kg]	default value for compounds with BCF < 2000 L/kg
log K_{ow}	1.90	[-]	
R-phrases	Not classified	[-]	Annex I of Directive 67/548/EEC
A1 value	n.a.		
DW standard	n.a.		

[1] $f_{oc, susp}$ = 0.1 kg_{oc}/kg_{solid} (European Commission (Joint Research Centre), 2003).
n.a. = not available.

- 2-Chloroaniline has a log $K_{p, susp-water}$ < 3; derivation of $MPC_{sediment}$ is not triggered.
- 2-Chloroaniline has a log $K_{p, susp-water}$ < 3; expression of the MPC_{water} as MPC_{water} in suspended particulate matter is not required.
- 2-Chloroaniline has a BCF < 100 L/kg; assessment of secondary poisoning is not triggered.
- Based on the classification of 4-chloroaniline (R45), it may be assumed that 2-chloroaniline is carcinogenic as well. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) is required.
- For 2-chloroaniline, no A1 and no Drinking Water value are available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, a provisional DWS needs to be derived.

4.2 3-Chloroaniline

Table 10. 3-Chloroaniline: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/source (if applicable)
log $K_{p, susp-water}$	1.02	[-]	$K_{p, susp-water} = K_{oc} \times f_{oc, susp}$[1]
BCF	1.33	[L/kg]	
BMF	1	[kg/kg]	default value for compounds with BCF < 2000 L/kg
log K_{ow}	1.88	[-]	
R-phrases	Not classified	[-]	Annex I of Directive 67/548/EEC
A1 value	n.a.		
DW standard	n.a.		

[1] $f_{oc, susp}$ = 0.1 kg_{oc}/kg_{solid} (European Commission (Joint Research Centre), 2003).
n.a. = not available.

- 3-Chloroaniline has a log $K_{p, susp-water}$ < 3; derivation of $MPC_{sediment}$ is not triggered.
- 3-Chloroaniline has a log $K_{p, susp-water}$ < 3; expression of the MPC_{water} as MPC_{water} in suspended particulate matter is not required.
- 3-Chloroaniline has a BCF < 100 L/kg; assessment of secondary poisoning is not triggered.
- Based on the classification of 4-chloroaniline (R45), it may be assumed that 3-chloroaniline is carcinogenic as well. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh food, water}$) is required.
- For 3-chloroaniline, no A1 and no Drinking Water value are available from Council Directives 75/440/EEC and 98/83/EC, respectively. Therefore, a provisional DWS needs to be derived.

4.3 4-Chloroaniline

Table 11. 4-Chloroaniline: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/source (if applicable)
log $K_{p, susp-water}$	1.56	[-]	$K_{p, susp-water} = K_{oc} \times f_{oc, susp}$ [1]
BCF	2.48	[L/kg]	
BMF	1	[kg/kg]	default value for compounds with BCF < 2000 L/kg
log K_{ow}	1.88	[-]	
R-phrases	Carc. Cat. 2, R45,23,24,25,43,50,53	[-]	Annex I of Directive 67/548/EEC
A1 value	n.a.		
DW standard	0.10	[µg/L]	Council Directive 98/83/EC (relevant metabolite of pesticide)

[1] $f_{oc, susp}$ = 0.1 kg_{oc}/kg_{solid} (European Commission (Joint Research Centre), 2003).
n.a. = not available.

- 4-Chloroaniline has a log $K_{p, susp-water}$ < 3; derivation of $MPC_{sediment}$ is not triggered.
- 4-Chloroaniline has a log $K_{p, susp-water}$ < 3; expression of the MPC_{water} as MPC_{water} in suspended particulate matter is not required.
- 4-Chloroaniline has a BCF < 100 L/kg; assessment of secondary poisoning is not triggered.
- 4-Chloroaniline has an R45 classification. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh food, water}$) should be derived.
- For 4-chloroaniline, no A1 is available from Council Directives 75/440, EEC, but there is a Drinking Water value from 98/83/EC. Therefore, a provisional DWS is not needed.

5 Derivation of Environmental Risk Limits

5.1 ERLs for water

5.1.1 2-Chloroaniline

5.1.1.1 Toxicity data

An overview of the available toxicity data for 2-chloroaniline (both for freshwater and marine organisms) is given in Table A2.1 – A2.4 in Appendix 2. The data selected for ERL derivation are tabulated in Table 12 for freshwater data and in Table 13 for marine data.

As there is no reason to assume that the toxicity of 2-chloroaniline in freshwater differs from that in salt water, the derivation of risk limits is based on the combined datasets for both compartments.

Table 12. 2-Chloroaniline: selected freshwater ecotoxicity data for ERL derivation (in mg/L).

Acute Taxonomic group	NOEC/EC10	Chronic Taxonomic group	L(E)C50
Bacteria		Protozoa	
Pseudomonas putida	55[a]	*Tetrahymena pyriformis*	188[d]
Algae		Algae	
Pseudokirchneriella subcapitata	32[b]	*Chlorella pyrenoidosa*	32
Scenedesmus subspicatus	25[c]	*Pseudokirchneriella subcapitata*	57[b]
Crustacea		*Scenedesmus subspicatus*	150[b]
Daphnia magna	0.032	Crustacea	
		Daphnia magna	1.25[e]
		Gammarus fasciatus	5.4
		Pisces	
		Carassius auratus	65.4
		Danio rerio	5.23
		Oncorhynchus mykiss	1.04
		Oryzias latipes	7.3
		Pimephales promelas	5.56[f]
		Poecilia reticulata	6.25

[a] Toxic threshold concentration (3% reduction in cell density).
[b] Preferred endpoint (growth rate).
[c] Preferred endpoint (growth rate) and exposure time.
[d] Geometric mean of 227, 189, and 156 mg/L, parameter population growth (density).
[e] Most relevant exposure time, parameters immobilisation and mortality (geometric mean of 14, 0.13, 0.46, 1.8, and 2.0 mg/L).
[f] Geometric mean of 5.13, 5.65, 5.81, and 5.68 mg/L, parameter mortality.

Table 13. 2-Chloroaniline: selected marine data for ERL derivation (in mg/L).

Acute Taxonomic group	NOEC/EC10	Chronic Taxonomic group	L(E)C50
		Bacteria	
		Vibrio fischeri	14.0[a]

[a] Geometric mean of 15 and 13 mg/L, preferred exposure duration (15 min), parameter bioluminescence.

5.1.1.2 $MPC_{eco, water}$ and $MPC_{eco, marine}$

Freshwater

The base set is complete with respect to short-term data. Long-term NOECs are available for bacteria, algae, and crustacea, but not for fish. As the trophic levels of the NOECs do not include the trophic level of the lowest acute L/EC50 (*i.e.* fish), an assessment factor of 100 is applied to the lowest of the available NOECs. The lowest NOEC is 32 µg.L^{-1} for *Daphnia magna*. This results in an $MPC_{eco, water}$ of 32 / 100 = 0.32 µg/L.

Marine

Because there are no toxicity data for specifically marine taxa (only for bacteria), an assessment factor of 1000 is applied, resulting in an $MPC_{eco, marine}$ of 32 / 1000 = 0.032 µg/L.

5.1.1.3 $MPC_{sp, water}$ and $MPC_{sp, marine}$

The derivation of an $MPC_{sp, water}$ and $MPC_{sp, marine}$ is not applicable because BCF < 100 L/kg (see section 4.1).

5.1.1.4 $MPC_{hh food, water}$ and $MPC_{hh food, marine}$

An $MPC_{hh food, water}$ is calculated using the TL_{hh} of 9 ng/kg_{bw}/d as derived in section 3.1.5 and assuming that fish consumption contributes for 10% to this threshold level, daily consumption of fish is 115 g, and body weight is 70 kg. This results in an $MPC_{hh food}$ of 0.1 × 9 × 70 / 0.115 = 0.548 µg/kg_{fish}. Using a BCF_{fish} of 2.72 L/kg and a BMF of 1 kg/kg, the resulting $MPC_{hh food, water}$ becomes 0.548 / (2.72 × 1) = 0.20 µg/L. For the $MPC_{hh food, marine}$, an extra biomagnification factor has to be applied. But since this BMF_2 is 1, the $MPC_{hh food, marine}$ equals the $MPC_{hh food, water}$ and is 0.20 µg/L

5.1.1.5 Selection of the MPC_{water} and MPC_{marine}

Freshwater

The following $MPCs_{water}$ are derived for 2-chloroaniline:
$MPC_{eco, water}$ = 0.32 µg/L
$MPC_{hh food, water}$ = 0.20 µg/L

The MPC_{water} is the lowest value of the available MPC_{water} values, which is $MPC_{hh food, water}$. Thus, the MPC_{water} for 2-chloroaniline is 0.20 µg/L.

Marine

The following $MPCs_{marine}$ are derived for 2-chloroaniline:
The $MPC_{eco, marine}$ = 0.032 µg/L.
$MPC_{hh food, marine}$ = 0.20 µg/L

The MPC_{marine} is equal to the lowest of the available $MPCs_{marine}$, which is $MPC_{eco, marine}$ of 0.032 µg/L. Thus, the MPC_{marine} for 2-chloroaniline is 0.032 µg/L.

5.1.1.6 $MPC_{dw, water}$

For the calculation of $MPC_{dw, water}$, it is assumed that consumption of drinking water contributes for 10% to the TL_{hh} of 9 ng/kg_{bw}/d (as derived in section 3.1.5), daily consumption of drinking water is 2 L, and body weight is 70 kg. The $MPC_{dw, water}$ is then (0.1 × 9 × 70) / 2 = 32 ng/L = 0.032 µg/L. Because of the low log K_{ow} of 2-chloroaniline, it is assumed that the substance is hardly, if at all, removed from water with simple treatment (coagulation, rapid filtration, or desinfection) (personal communication Susanne Wuijts, drinking water expert at RIVM). Therefore, the fraction not removable with simple treatment is set to 1, resulting in a final $MPC_{dw, water}$ of 0.032 µg/L.

5.1.1.7 MPC_{gw}

For the selection of the MPC_{gw}, the following MPC_{water} values have to be considered:
$MPC_{eco,gw}$ = $MPC_{eco, water}$ = 0.32 µg/L
$MPC_{human, gw}$ = $MPC_{dw, water}$ = 0.032 µg/L

The MPC_{gw} is the lowest value of these values and thus, the MPC_{gw} for 2-chloroaniline is 0.032 µg/L.

5.1.1.8 $MAC_{eco, water}$ and $MAC_{eco, marine}$

Freshwater
For the derivation of the Maximum Acceptable Concentration for ecosystems ($MAC_{eco, water}$), an assessment factor of 100 is applied to the lowest L(E)C50, because BCF < 100 L/kg, log K_{ow} < 3, the base set for acute data is complete, and interspecies variation spans a factor of > 100. The lowest LC50 is found for *Oncorhynchus mykiss* and equals 1.04 mg/L. The resulting $MAC_{eco, water}$ is 10 µg/L.

Marine
Because there are no toxicity data for specifically marine taxa (only for bacteria), an additional assessment factor of 10 is used to derive the $MAC_{eco, marine}$, resulting in a $MAC_{eco, marine}$ of 1.0 µg/L.

5.1.1.9 $SRC_{eco, water}$

Since more than two NOECs are available for base set-species and the geometric mean of the short-term data (13 mg/L) divided by 10 is smaller than the geometric mean of the long-term data (6.1 mg/L), an assessment factor of 10 is applied to the geometric mean of the short-term data. The $SRC_{eco, water}$ is therefore 13 /10 = 1.3 mg/L = 1.3 × 10^3 µg/L.

5.1.1.10 NC

The derived MPCs are divided by a factor of 100 to obtain negligible concentrations (NCs):
NC_{water} = 2.0 × 10^{-3} µg/L
NC_{gw} = 3.2 × 10^{-4} µg/L
NC_{marine} = 3.2 × 10^{-4} µg/L

5.1.2 3-Chloroaniline

5.1.2.1 Toxicity data

The available toxicity data for 3-chloroaniline (both for freshwater and marine organisms) are tabulated in Table A2.5 – Table A2.7 in Appendix 2. The data used in the ERL derivation are summarised in Table 14 for freshwater data and in Table 15 for marine data.
As there is no reason to assume that the toxicity of 3-chloroaniline in freshwater differs from that in salt water, the derivation of risk limits is based on the combined datasets for both compartments.

Table 14. 3-Chloroaniline: selected freshwater ecotoxicity data for ERL derivation (in mg/L).

Acute Taxonomic group	NOEC/EC10	Chronic Taxonomic group	L(E)C50
Bacteria		Protozoa	
Pseudomonas putida	41.4[a]	*Tetrahymena pyriformis*	84.5[f]
Algae		Algae	
Pseudokirchneriella subcapitata	10[b]	*Chlorella pyrenoidosa*	21
Scenedesmus subspicatus	8[c]	*Pseudokirchneriella subcapitata*	19[b]
Crustacea		*Scenedesmus subspicatus*	21[c]
Daphnia magna	0.00645[d]	Crustacea	
Pisces		*Daphnia magna*	0.464[g]
Danio rerio	1[e]	Pisces	
		Carassius auratus	55.7
		Danio rerio	21.2[h]
		Leuciscus idus	14
		Oryzias latipes	8.8
		Poecilia reticulata	13.4

[a] Geometric mean of 19 and 90.2 mg/L, parameter cell density, first value is a toxic threshold concentration (3% reduction in cell density).
[b] Preferred endpoint (growth rate)
[c] Preferred endpoint (growth rate) and exposure time.
[d] Geometric mean of 0.013 and 0.0032 mg/L, parameter reproduction.
[e] Lowest value, parameter growth (length).
[f] Geometric mean of 100, 76.9, 103, and 64.4 mg/L, parameter population growth (density).
[g] Most relevant exposure time, parameters immobilisation and mortality (geometric mean of 0.35, 2.7, 0.1, and 0.49 mg/L).
[h] Geometric mean of 18.8 and 24 mg/L, parameter mortality.

Table 15. 3-Chloroaniline: selected marine data for ERL derivation (in mg/L).

Acute Taxonomic group	NOEC/EC10	Chronic Taxonomic group	L(E)C50
		Bacteria	
		Vibrio fischeri	14.6[a]

[a] Geometric mean of 13.4 and 16 mg/L, preferred exposure duration (15 min), parameter bioluminescence.

5.1.2.2 $MPC_{eco, water}$ and $MPC_{eco, marine}$

Freshwater

The base set is complete with respect to short-term and long-term data. An assessment factor of 10 is applied to the lowest NOEC available, which is 6.45 µg/L for *Daphnia magna*. This results in an $MPC_{eco, water}$ of 6.45 / 10 = 0.65 µg/L.

Marine

Because there are no toxicity data for specifically marine taxa (only for bacteria), an assessment factor of 100 was applied, resulting in an $MPC_{eco, marine}$ of 6.45 / 100 = 0.065 µg/L.

5.1.2.3 $MPC_{sp, water}$ and $MPC_{sp, marine}$

The derivation of $MPC_{sp, water}$ and $MPC_{sp, marine}$ is not applicable because BCF < 100 L/kg (see section 4.2).

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5.1.2.4 $MPC_{hh\ food,\ water}$ and $MPC_{hh\ food,\ marine}$

For the calculation of $MPC_{hh\ food,\ water}$, it is assumed that fish consumption contributes for 10% to the TL_{hh} of 9 ng/kg_{bw}/d (as derived in section 3.2.5), daily consumption of fish is 115 g, and body weight is 70 kg. This results in an $MPC_{hh,\ food}$ of (0.1 × 9 × 70) / 0.115 = 0.548 µg/kg_{fish}/d. Using a BCF of 1.33 L/kg and a BMF of 1 kg/kg (default value because biomagnification is considered to be absent), the resulting $MPC_{hh\ food,\ water}$ is 0.548 / (1.33 × 1) = 0.41 µg/L. For the $MPC_{hh\ food,\ marine}$, an extra biomagnification factor has to be applied. But since this BMF_2 is 1, the $MPC_{hh\ food,\ marine}$ equals the $MPC_{hh\ food,\ water}$ and is 0.41 µg/L.

5.1.2.5 Selection of the MPC_{water} and MPC_{marine}

Freshwater
The following $MPCs_{water}$ are derived for 3-chloroaniline:
$MPC_{eco,\ water}$ = 0.65 µg/L
$MPC_{hh\ food,\ water}$ = 0.41 µg/L

The MPC_{water} is the lowest value of the available MPC_{water} values, which is $MPC_{hh\ food,\ water}$. Thus, the MPC_{water} for 3-chloroaniline is 0.41 µg/L.

Marine
The following $MPCs_{marine,\ ecotox}$ are derived for 3-chloroaniline:
$MPC_{eco,\ marine}$ = 0.065 µg/L.
$MPC_{hh\ food,\ marine}$ = 0.41 µg/L

The MPC_{marine} is the lowest of the $MPCs_{marine}$ determined, which is $MPC_{eco,\ marine}$. The MPC_{marine} is 0.065 µg/L.

5.1.2.6 $MPC_{dw,\ water}$

For the calculation of $MPC_{dw,\ water}$, it is assumed that consumption of drinking water contributes for 10% to the TL_{hh} of 9 ng/kg_{bw}/d (as derived in section 3.2.5), daily consumption of drinking water is 2 L, and body weight is 70 kg. The $MPC_{dw,\ water}$ is then (0.1 × 9 × 70) / 2 = 32 ng/L = 0.032 µg/L. Because of the low log K_{ow} of 3-chloroaniline, it is assumed that the substance is hardly, if at all, removed from water with simple treatment (coagulation, rapid filtration, or desinfection) (personal communication Susanne Wuijts, drinking water expert at RIVM). Therefore, the fraction not removable with simple treatment is set to 1, resulting in a final $MPC_{dw,\ water}$ of 0.032 µg/L.

5.1.2.7 MPC_{gw}

For the selection of the MPC_{gw}, the following MPC_{water} values have to be considered:
$MPC_{eco,gw}$ = $MPC_{eco,\ water}$ = 0.65 µg/L
$MPC_{human,\ gw}$ = $MPC_{dw,\ water}$ = 0.032 µg/L

The MPC_{gw} is the lowest value of these values and thus, the MPC_{gw} for 3-chloroaniline is 0.032 µg/L.

5.1.2.8 $MAC_{eco,\ water}$ and $MAC_{eco,\ marine}$

Freshwater

For the derivation of the $MAC_{eco,\ water}$, an assessment factor of 100 is applied to the lowest EC50, because BCF < 100 L/kg, log K_{ow} < 3, the base set is complete, and interspecies variation spans a factor of > 100. The lowest EC50 is found for *Daphnia magna*: 0.464 mg/L. The resulting $MAC_{eco,\ water}$ is 4.6 µg/L.

Marine

Because there are no toxicity data for specifically marine taxa (only for bacteria), an additional assessment factor of 10 was used to derive the $MAC_{eco,\ marine}$, resulting in a $MAC_{eco,\ marine}$ of 0.46 µg/L.

5.1.2.9 $SRC_{eco,\ water}$

Since the chronic base set is complete, $SRC_{eco,\ water}$ for the aquatic compartment is calculated as the geometric mean of the chronic toxicity data with an assessment factor of 1.
The $SRC_{eco,\ water}$ = 1.8 mg/L = 1.8×10^3 µg/L.

5.1.2.10 NC

The derived MPCs are divided by a factor of 100 to obtain negligible concentrations (NCs):

NC_{water} = 4.1×10^{-3} µg/L
NC_{gw} = 3.2×10^{-4} µg/L
NC_{marine} = 6.5×10^{-4} µg/L

5.1.3 4-Chloroaniline

5.1.3.1 Toxicity data

Toxicity data for 4-chloroaniline (both for freshwater and marine organisms) are tabulated in Table A2.8 – Table A2.10 in Appendix 2. The data selected for ERL derivation are given in Table 16 for freshwater data and in Table 17 for marine data.

As there is no reason to assume that the toxicity of 4-chloroaniline in freshwater differs from that in salt water, the derivation of risk limits is based on the combined datasets for both compartments.

Table 16. 4-Chloroaniline: selected freshwater ecotoxicity data for ERL derivation (in mg/L).

Acute Taxonomic group	NOEC/EC10	Chronic Taxonomic group	L(E)C50
Bacteria		Bacteria	
Pseudomonas putida	72	*Bacillus subtilis*	385
Rotifera		Protozoa	
Brachionus rubens	10.6[a]	*Tetrahymena pyriformis*	15.1[g]
Algae		Rotifera	
Pseudokirchneriella subcapitata	1[b]	*Brachionus rubens*	100
Scenedesmus subspicatus	1[c]	Algae	
Crustacea		*Chlorella pyrenoidosa*	4.1
Daphnia magna	0.00566[d]	*Chlorella vulgaris*	46.9[h]
Pisces		*Pseudokirchneriella subcapitata*	4.7[b]
Danio rerio	0.0133[e]	*Scenedesmus subspicatus*	6.3[b]
Oncorhynchus mykiss	0.2	Crustacea	
Oryzias latipes	0.75[f]	*Daphnia magna*	0.124[i]
		Insecta	
		Chironomus plumosus	43
		Pisces	
		Carassius auratus	54.4
		Danio rerio	41.2[j]
		Ictalurus punctatus	23
		Lepomis macrochirus	2.4
		Leuciscus idus	17.7[k]
		Oncorhynchus mykiss	13.6[l]
		Oryzias latipes	18.3[m]
		Pimephales promelas	22.9[n]
		Poecilia reticulata	26.0

[a] Lowest value, parameter carrying capacity.
[b] Preferred endpoint (growth rate).
[c] Preferred endpoint (growth rate) and exposure time.
[d] Most relevant endpoint, parameter reproduction (geometric mean of 0.01 and 0.0032 mg/L).
[e] The reported LOEC is 0.04 mg/L, parameter number of eggs in the F1 and F2 generation. At this concentration > 20% effect was observed. As this effect parameter was the most sensitive in the study, the LOEC was divided by 3 to derive a NOEC.
[f] The reported LOEC is 2.25 mg/L, parameter weight. The effect percentage was not reported. As this effect parameter was the most sensitive in the study, the LOEC was divided by 3 to derive a NOEC.
[g] Lowest value, parameter cell density (geometric mean of 114, 5.63 and 5.42 mg/L).
[h] Geometric mean of 50.8 and 43.2 mg/L, parameter cell density.
[I] Most relevant exposure time, parameters immobilisation and mortality (geometric mean of 0.05 and 0.31 mg/L).
[j] Geometric mean of 46, 34.5, and 44 mg/L, parameter mortality.
[k] Geometric mean of 26.5, 16.5, 9.8, and 23 mg/L, parameter mortality.
[l] Geometric mean of 11, 14, and 16.3 mg/L, parameter mortality.
[m] Geometric mean of 28, 37.7, and 5.8 mg/L, parameter mortality.
[n] Geometric mean of 32.5, 30.6, and 12 mg/L, parameter mortality.

Table 17. 4-Chloroaniline: selected marine data for ERL derivation (in mg/L).

Acute Taxonomic group	NOEC/EC10	Chronic Taxonomic group	L(E)C50
		Bacteria	
		Vibrio fischeri	9.1[a]

[a] Geometric mean of 3.76, 34.3, and 5.9 mg/L, preferred exposure duration (15 min), parameter bioluminescence.

5.1.3.2 $MPC_{eco,\ water}$ and $MPC_{eco,\ marine}$

Freshwater

The base set is complete for short-term and long-term data. An assessment factor of 10 is applied to the lowest NOEC available, which is 5.66 µg/L for *Daphnia magna*. This results in an $MPC_{eco,\ water}$ of 5.66 / 10 = 0.57 µg/L.

Marine

Because there are no toxicity data for specifically marine taxa (only for bacteria), an assessment factor of 100 is used to derive an $MPC_{eco,\ marine}$ of 5.66 / 100 = 0.057 µg/L.

5.1.3.3 $MPC_{sp,\ water}$ and $MPC_{sp,\ marine}$

The derivation of $MPC_{sp,\ water}$ and $MPC_{sp,\ marine}$ is not applicable because BCF < 100 L/kg (see section 4.3).

5.1.3.4 $MPC_{hh\ food,\ water}$ and $MPC_{hh\ food,\ marine}$

The TL_{hh} of 9 ng/kg_{bw}/d as derived in section 3.3.5 is used to calculate the $MPC_{hh\ food,\ water}$ and $MPC_{hh\ food,\ marine}$. Further, it is assumed that 10% of the TL_{hh} can be attributed to the consumption of fish, fish consumption is 115 g_{fish}/d, and body weight is 70 kg.
This results in an $MPC_{hh,\ food}$ of (0.1 × 9 × 70) / 0.115 = 0.548 µg/kg_{fish}/d.
Using a BCF of 2.48 L/kg and a BMF of 1 kg/kg (default value because biomagnification is considered to be absent), the resulting $MPC_{hh\ food,\ water}$ is 0.548 / (2.48 × 1) = 0.22 µg/L. For the $MPC_{hh\ food,\ marine}$, an extra biomagnification factor has to be applied. But since this BMF_2 is 1, the $MPC_{hh\ food,\ marine}$ equals the $MPC_{hh\ food,\ water}$ and is 0.22 µg/L.

5.1.3.5 Selection of the MPC_{water} and MPC_{marine}

Freshwater

The following $MPCs_{water}$ are derived for 4-chloroaniline:
$MPC_{eco,\ water}$ = 0.57 µg/L
$MPC_{hh\ food,\ water}$ = 0.22 µg/L

The MPC_{water} is the lowest value of the available MPC_{water} values, which is $MPC_{hh\ food,\ water}$. Therefore, the MPC_{water} for 4-chloroaniline is 0.22 µg/L.

Marine

For 4-chloroaniline, the available $MPCs_{marine}$ are:
$MPC_{eco,\ marine}$ = 0.057 µg/L
$MPC_{hh\ food,\ marine}$ = 0.22 µg/L

The lowest MPC, which is used to set the MPC_{marine} is the $MPC_{eco,\ marine}$.
Thus, the MPC_{marine} = 0.057 µg/L.

5.1.3.6 $MPC_{dw, water}$

For 4-chloroaniline a drinking water standard of 0.10 µg/L is available, based on its formation as a metabolite of the pesticide diflubenzuron (Gesellschaft Deutscher Chemiker (1993) and WHO-IPSC (1996). However, 4-chloroaniline also occurs 'on its own' and thus the DWS value can be compared to the value derived using the TL_{hh} based on the carcinogenic properties of the compound, and the lowest value should be chosen as the $MPC_{dw,water}$.

For the calculation of $MPC_{dw, water}$, it is assumed that consumption of drinking water contributes for 10% to the TL_{hh} of 9 ng/kg_{bw}/d (as derived in section 3.3.5), daily consumption of drinking water is 2 L, and body weight is 70 kg. The $MPC_{dw, water}$ is then (0.1 × 9 × 70) / 2 = 32 ng/L = 0.032 µg/L. Because this value is lower than the drinking water standard, the final $MPC_{dw,water}$ is based on this value.

Because of the low log K_{ow} of 4-chloroaniline, it is assumed that the substance is hardly, if at all, removed from water with simple treatment (coagulation, rapid filtration, or desinfection) (personal communication Susanne Wuijts, drinking water expert at RIVM). Therefore, the fraction not removable with simple treatment is set to 1, resulting in a final $MPC_{dw, water}$ of 0.032 µg/L.

5.1.3.7 Selection of the MPC_{gw}

For the selection of the MPC_{gw}, the following MPC_{water} values have to be considered:
$MPC_{eco,gw}$ = $MPC_{eco, water}$ = 0.57 µg/L
$MPC_{human, gw}$ = $MPC_{dw, water}$ = 0.032 µg/L

The MPC_{gw} is the lowest value of these values and thus, the MPC_{gw} for 4-chloroaniline is 0.032 µg/L.

5.1.3.8 $MAC_{eco, water}$ and $MAC_{eco, marine}$

Freshwater
For the derivation of the $MAC_{eco, water}$, an assessment factor of 100 is applied to the lowest EC50, because BCF < 100 L/kg, log K_{ow} < 3, the base set is complete, and interspecies variation spans a factor of > 1000. The lowest EC50 is 0.124 mg/L for *Daphnia magna*. The resulting $MAC_{eco, water}$ is 1.2 µg/L.

Marine
Because there are no toxicity data for specifically marine taxa (only for bacteria), an additional assessment factor of 10 is used to derive the $MAC_{eco, marine}$, resulting in a $MAC_{eco, marine}$ of 0.12 µg/L.

5.1.3.9 $SRC_{eco, water}$

The chronic base set is complete and therefore, the $SRC_{eco, water}$ for the aquatic compartment is calculated as the geometric mean of the chronic toxicity data. However, two of the three NOECs for fish are calculated by dividing a LOEC by a factor of 3. This approach is not supported by the current INS guidance (Van Vlaardingen and Verbruggen, 2007) because the effect percentage either exceeded 20% or was not reported. However, as the LOECs represented the most sensitive effect parameter in the study, it is decided to calculate the $SRC_{eco, water}$ using the NOECs calculated from the LOECs. With an assessment factor of 1 on the geomean of the complete chronic dataset, this results in a $SRC_{eco, water}$ of 0.55 mg/L = 5.5×10^2 µg/L. For comparison, the $SRC_{eco, water}$ calculated in accordance with the INS guidance (without the two NOECs) is 9.8×10^2 µg/L.

5.1.3.10 NC

The derived MPCs were divided by a factor of 100 to obtain negligible concentrations (NCs):

NC_{water} = 2.2×10^{-3} µg/L
NC_{gw} = 3.2×10^{-4} µg/L
NC_{marine} = 5.7×10^{-4} µg/L

5.2 ERLs for sediment

The log $K_{p,\ susp\text{-}water}$ of the three chloroanilines is below the trigger value of 3 (see sections 4.1, 4.2 and 4.3). $MPC_{sediment}$ values are therefore not derived.

6 Preliminary risk analysis

Monitoring data for fresh surface waters in the Netherlands were retrieved from WaterStat (RIZA and RIKZ). Only data for 1990 and 2000 were found. The monitoring data are summarised in Table 18. The average concentrations range from 0.01 to 0.045 µg/L, 0.011 to 0.017 µg/L, and 0.01 to 0.2 µg/L for 2-, 3-, and 4-chloroaniline, respectively. For 0 to 61.5% (2-chloroaniline), 36.4 to 66.7% (3-chloroaniline), and 58.3 to 100% (4-chloroaniline) of the measurements, the concentrations were below the detection limit.

The annual average and maximum concentrations did not exceed MPC_{water} and $MAC_{eco, water}$ for any compound at any location. At one location (Schaar van Ouden Doel), the annual average concentration exceeded the MPC_{dw}. The negligible concentration NC_{water}, is always exceeded when the detection limit is exceeded.

Table 18. Monitoring data for 2-, 3-, and 4-chloroaniline in surface water at several locations in the Netherlands (data retrieved from WaterStat (RIZA and RIKZ)).

Location	Date	Number of data	Number of data < LOQ[1]	Max [µg/L]	90th P [µg/L]	Avg [µg/L]	Med [µg/L]	Min [µg/L]
2-chloroaniline								
Eijsden ponton	1990	12	6	0.02	0.02	0.01	0.01	0.01
IJmuiden (km 2)	1990	13	8	0.08	0.02	0.013	0.01	0.01
Lobith ponton	1990	12	0	0.05	0.04	0.022	0.02	0.01
Schaar van Ouden Doel	1990	13	1	0.1	0.07	0.045	0.04	0.01
Vrouwezand	1990	10	2	0.03	0.02	0.015	0.02	0.01
3-chloroaniline								
Eijsden ponton	1990	11	7	0.04	0.03	0.011	0.01	0.01
IJmuiden (km 2)	1990	11	7	0.04	0.03	0.011	0.01	0.01
Lobith ponton	1990	11	4	0.06	0.03	0.017	0.01	0.01
Schaar van Ouden Doel	1990	12	5	0.03	0.03	0.013	0.01	0.01
Vrouwezand	1990	9	6	0.03	0.02	0.011	0.01	0.01
4-chloroaniline								
Eijsden ponton	1990	12	8	0.03	0.03	0.012	0.01	0.01
IJmuiden (km 2)	1990	13	8	0.07	0.02	0.014	0.01	0.01
Lobith ponton	1990	12	7	0.04	0.03	0.014	0.01	0.01
	2000	13	13	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Schaar van Ouden Doel	1990	13	9	0.03	0.03	0.01	0.01	0.01
Vrouwezand	1990	10	7	0.02	0.02	0.01	0.01	0.01

[1] LOQ = limit of quantification.

7 Conclusions

In this report, the risk limits negligible concentration (NC), maximum permissible concentration (MPC), maximum acceptable concentration for ecosystems ($MAC_{eco, water}$), and serious risk concentration for ecosystems ($SRC_{eco, water}$) are derived for 2-, 3-, and 4-chloroaniline in water and groundwater. No risk limits were derived for the sediment compartment because exposure of sediment is considered negligible. The ERLs that were obtained are summarised in the table below.

Monitoring data mainly from 1990 revealed that average concentrations measured in the field always exceeded the NC_{water} when the detection limit was exceeded. The annual average and maximum concentrations did not exceed MPC_{water} and $MAC_{eco, water}$ for all three compounds at all locations. At one location (Schaar van Ouden Doel), the annual average concentration exceeded the MPC_{dw}.

Table 19. Derived MPC, NC, $MAC_{eco ,water}$ and $SRC_{eco, water}$ values for three chloronanilines (in µg/L).

Environmental risk limit[1]	2-chloroaniline	3-chloroaniline	4-chloroaniline
MPC_{water}	0.20	0.41	0.22
$MPC_{dw, water}$	3.2×10^{-2}	3.2×10^{-2}	3.2×10^{-2}
MPC_{gw}	3.2×10^{-2}	3.2×10^{-2}	3.2×10^{-2}
MPC_{marine}	3.2×10^{-2}	6.5×10^{-2}	5.7×10^{-2}
NC_{water}	2.0×10^{-3}	4.1×10^{-3}	2.2×10^{-3}
NC_{gw}	3.2×10^{-4}	3.2×10^{-4}	3.2×10^{-4}
NC_{marine}	3.2×10^{-4}	6.5×10^{-4}	5.7×10^{-4}
$MAC_{eco, water}$	10	4.6	1.2
$MAC_{eco, marine}$	1.0	0.46	0.12
$SRC_{eco, water}$	1.3×10^{3}	1.8×10^{3}	5.5×10^{2}

[1] subscripts: water = freshwater; dw = drinking water; gw = groundwater; marine = marine waters
$MPC_{dw, water,}$ = MPC based on human consumption of drinking water.

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Appendix 1. Information on bioconcentration

Table A1.1	Bioconcentration data for 2-chloroaniline
Table A1.2	Bioconcentration data for 3-chloroaniline
Table A1.3	Bioconcentration data for 4-chloroaniline

Legend

Species	species used in the test
Species properties	if available, the age, size, weight, or life stage of the species used in the test mo = months ww = wet weight
Substance purity	chemical grade or purity
Analysed	method used for analysing the test substance FTD-GC = flame thermionic detector gas-chromatography LSC = liquid scintillation counting photometry- GC = photometry gas-chromatography RP-HPLC-UV = reversed phase high performance liquid chromatography with UV detection
Test type	S = static R = static with renewal F = flow through CF = continuous flow through
Test water	dtw = dechlorinated tap water tw = tap water nw = natural water Cu^{2+}-free = copper-free water
Exposure time	d = days
Criterion	BCF = bioconcentration factor
Ri	reliability index according to Klimisch et al. (1997)

Table A1.1. Bioconcentration data for 2-chloroaniline

Species	Species properties	Substance purity [%]	Analysed	Test type	Test water	pH	Hardness $CaCO_3$ [mg/L]	Temp. [ºC]	Exposure time	Exposure conc. [mg/L]	BCF [L/kg]	BCF type	Calculation method	Ri	Notes	Reference
Pisces																
Cyprinus carpio L.	8.5 – 9.2 cm, 15.5 – 20.4 g	> 97	FTD-GC	CF	dtw	7.0 - 7.2	35 - 39	25 ± 1	14	0.0104	0.8	whole fish	equilibrium	1	1	Tsuda et al., 1993
Cyprinus carpio L.	8.5 – 9.2 cm, 15.5 – 20.4 g	> 97	FTD-GC	CF	dtw	7.0 - 7.2	35 – 39	25 ± 1	14	0.0003	1.7	whole fish	equilibrium	1	1	Tsuda *et al*., 1993
Danio rerio	adult males and females, 150 - 450 mg		LSC	S	tw	8.1 ± 0.1	230 ± 20 (CaO)	26 ± 1	4.2	0.0242	15.3	whole fish	equilibrium	3	2	Kalsch et al., 1991

Notes
1 BCF is geometric mean of measurements at t = 1, 3, 7, 10, and 14 d. Fish were exposed to a mixture of 2-, 3-, and 4-chloroaniline.
2 Activity was constant (± 10%) during exposure. Total radioactivity was measured: parent compound and metabolites could not be distinguished.

Table A1.2. Bioconcentration data for 3-chloroaniline

Species	Species properties	Substance purity [%]	Analysed	Test type	Test water	pH	Hardness $CaCO_3$ [mg/L]	Temp. [ºC]	Exposure time	Exposure conc. [mg/L]	BCF [L/kg]	BCF type	Calculation method	Ri	Notes	Reference
Pisces																
Cyprinus carpio L.	8.5 - 9.2 cm, 15.5 - 20.4 g	> 97	FTD-GC	CF	dtw	7.0 - 7.2	35 - 39	25 ± 1	14	0.0147	0.8	whole fish	equilibrium	1	1	Tsuda et al., 1993
Cyprinus carpio L.	8.5 - 9.2 cm, 15.5 - 20.4 g	> 97	FTD-GC	CF	dtw	7.0 - 7.2	35 - 39	25 ± 1	14	0.00067	2.2	whole fish	equilibrium	1	1	Tsuda et al., 1993
Danio rerio	adult males and females, 150 - 450 mg		LSC	S	tw	8.1 ± 0.1	230 ± 20 (CaO)	26 ± 1	4.2	0.0217	11.5	whole fish	equilibrium	3	2	Kalsch et al., 1991

Notes
1 BCF is geometric mean of measurements at t = 1, 3, 7, 10, and 14 d. Fish were exposed to a mixture of 2-, 3-, and 4-chloroaniline.
2 Activity was constant (± 10%) during exposure. Total radioactivity was measured: parent compound and metabolites could not be distinguished.

Table A1.3. Bioconcentration data for 4-chloroaniline

Species	Species properties	Substance purity [%]	Analysed	Test type	Test water	pH	Hardness $CaCO_3$ [mg/L]	Temp. [ºC]	Exposure time	Exposure conc. [mg/L]	BCF [L/kg]	BCF type	Calculation method	Ri	Notes	Reference
Pisces																
Cyprinus carpio L.	8.5 – 9.2 cm, 15.5 – 20.4 g	> 97	FTD-GC	CF	dtw	7.0 - 7.2	35 - 39	25 ± 1	14	0.0104	0.8	whole fish	equilibrium	1	1	Tsuda et al., 1993
Cyprinus carpio L.	8.5 – 9.2 cm, 15.5 – 20.4 g	> 97	FTD-GC	CF	dtw	7.0 - 7.2	35 – 39	25 ± 1	14	0.0003	1.7	whole fish	equilibrium	1	1	Tsuda *et al.,* 1993
Danio rerio	adult ♀♂, 150 – 450 mg		LSC	S	tw	8.1 ± 0.1		26 ± 1	1	0.0255	8.1	whole fish	equilibrium	3	2	Kalsch *et al*., 1991
Danio rerio			photometry & GC	R		7.8 ± 0.2		23 - 25	14	1	7		equilibrium	2	3	Gesellschaft Deutscher Chemiker, 1993
Danio rerio			photometry & GC	R		7.8 ± 0.2		23 - 25	14	5	4		equilibrium	2	3	Gesellschaft Deutscher Chemiker, 1993
Leuciscus idus melanotus	5 - 6 cm, ca. 1.5 g	98, radiochem. pur. 99	LSC	S	tw & dw			20 - 25	3	0.052	< 10	whole fish	Cfish/Cwater	3		Freitag *et al*., 1982
Leuciscus idus melanotus	2 - 5 g		LSC	S	tw & dw	7		23 ± 3	3	0.052	< 20	whole fish	Cfish/Cwater	3	4	Korte *et al*., 1978
Leuciscus idus melanotus	5 - 6 cm, ca. 1.5 g	> 98	LSC	S	tw & dw			20 - 25	3	0.05	13	whole fish	Cfish/Cwater	3	5	Freitag *et al*., 1984
Oryzias latipes	sexually in-active adults, 200 - 500 mg	≥ 98	LSC	S	nw			20 - 21	0.222	0.00761	11	whole fish	Cfish/Cwater	3	6	Bradbury *et al*., 1993
Poecilia reticulata	males, ca. 5 mo, 725 mg (ww males and females)	> 98	RP-HPLC-UV	F	tw, Cu^{2+}-free	7 - 8	200 - 215	23 ± 1	1.63	25.2589	13.4	whole fish	equilibrium	3	7	De Wolf *et al*., 1994

Notes
1 BCF is geometric mean of measurements at t = 1, 3, 7, 10, and 14 d. Fish were exposed to a mixture of 2-, 3-, and 4-chloroaniline.
2 Activity was constant (± 10%) during exposure. Total radioactivity was measured: parent compound and metabolites could not be distinguished.
3 Based on OECD 305B, exposure concentration given as nominal concentration.
4 100% a.r. recovered.
5 Two different values for BCF are given in different tables.
6 No equilibrium was reached.
7 Exposure concentration is close to 14-d LC50 of 26.0 mg/L. Effects on behaviour (swimming behaviour less rapid, less fright/flight reactions) were observed after 30 min.

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Appendix 2. Detailed aquatic toxicity data

Table A2.1	Acute toxicity of 2-chloroaniline to freshwater organisms
Table A2.2	Acute toxicity of 2-chloroaniline to marine organisms
Table A2.3	Chronic toxicity of 2-chloroaniline to freshwater organisms
Table A2.4	Chronic toxicity of 2-chloroaniline to marine organisms
Table A2.5	Acute toxicity of 3-chloroaniline to freshwater organisms
Table A2.6	Acute toxicity of 3-chloroaniline to marine organisms
Table A2.7	Chronic toxicity of 3-chloroaniline to freshwater organisms
Table A2.8	Acute toxicity of 4-chloroaniline to freshwater organisms
Table A2.9	Acute toxicity of 4-chloroaniline to marine organisms
Table A2.10	Chronic toxicity of 4-chloroaniline to freshwater organisms

Legend

Species	species used in the test
Species properties	if available, the age (h = hour, d = day, mo = month), size, weight, or life stage of the species used in the test h = hours d = days w = weeks mo = months y = years
A	analysed Y = test substance analysed in test solution N = test substance not analysed in test solution or no data
Test type	S = static R = static with renewal F = flow through CF = continuous flow through IF = intermittent flow through
Substance purity	chemical grade or purity 'high' = highest purity available ag = analyitical grade pa = pro analyse
Test water	am = artificial medium rw = reconstituted water (water with additional salts) dtw = dechlorinated tap water tw = tap water nw = natural water
Exp. time	exposure time h = hours d = days min = minutes CLC = complete life cycle
Criterion	L(E)Cx = test result showing x% mortality (LCx) or effect (Ecx); L(E)C50s are usually determined for acute effects, EC10s for chronic effects NOEC = no observed effect concentration, statistically determined LOEC = lowest observed effect concentration, statistically determined
Test endpoint	AUC = area under the (growth) curve
Ri	reliability index according to Klimisch et al. (1997)

Table A2.1. Acute toxicity of 2-chloroaniline to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference	Original reference
Bacteria																
Escherichia coli	1E+04 cells.mL^{-1}	N	S	'high'	am		37			EC50	growth rate	281	3		Nendza and Seydel, 1988, 1990	
Escherichia coli	1E+04 cells.mL^{-1}, in log. phase	N	S	'high'	am		37			LOEC	cell density	727	3	1	Nendza and Seydel, 1990	
Mycobacterium smegmatis	1E+04 cells.mL^{-1}, in log. phase	N	S	'high'	am		37			LOEC	cell density	523	3	1	Nendza and Seydel, 1990	
Protozoa																
Tetrahymena pyriformis		N	S	ag	am		30		24 h	EC50	cell number	200	3		Yoshioka et al., 1985	
Tetrahymena pyriformis	strain GL-C	N	S		am	7.35	27 ± 1	75	40 h	EC50	population growth (density)	227	2		Schultz, 1997	
Tetrahymena pyriformis	strain GL-C	N	S	> 95	am	7.35	27 ± 1	75	40 h	EC50	population growth (density)	189	2		Schultz, 1999	
Tetrahymena pyriformis	strain GL-C	Y	S	> 95	am	7.3	28		48 h	EC50	population growth (density)	156	2	2	Schultz et al., 1989	
Algae																
Chlorella pyrenoidosa		N		≥ 99					96 h	EC50	cell density	32	2	3	Maas-Diepeveen and Van Leeuwen, 1986	
Pseudokirchneriella subcapitata									48 h	EC50	growth rate	57	2		NITE, 2002	Ministry of Environment, Japan, 2000
Pseudokirchneriella subcapitata									72 h	EC50	biomass (AUC)	13	2		NITE, 2002	Ministry of Environment, Japan, 2000
Scenedesmus pannonicus		Y	S	> 99.9						EC50	growth	32	3		Canton et al., 1985	
Scenedesmus subspicatus		N	S		am	8.0 - 9.3	24 ± 1		72 h	EC50	biomass (AUC)	40	2		Kühn and Pattard, 1990	
Scenedesmus subspicatus		N	S		am	8.0 - 9.3	24 ± 1		72 h	EC50	growth rate	150	2		Kühn and Pattard, 1990	
Scenedesmus subspicatus	cell wall removed									LOEC	O_2 production	0.00957	3	4	Schmidt and Schnabl, 1988	
Scenedesmus subspicatus								27	168 h	EC50	cell density	58	3		Gesellschaft Deutscher Chemiker, 1991	Schmidt, 1989
Crustacea																
Daphnia magna	6 - 24 h old		S		am		20 ± 2	250	24 h	EC50	immobilisation	33	1	5	Gesellschaft Deutscher Chemiker, 1991	Kühn, 1989
Daphnia magna									24 h	EC50	immobilisation	11.5	1	5	Gesellschaft Deutscher Chemiker. 1991	Bayer AG, 1988
Daphnia magna	6 - 24 h old	N	S	ag	rw	6.0 ± 0.1	22 ± 2		24 h	EC50	immobilisation	9.03	1		Cronin et al., 2000	
Daphnia magna	6 - 24 h old	N	S	ag	rw	7.8 ± 0.1	22 ± 2		24 h	EC50	immobilisation	6.54	1		Cronin et al., 2000	
Daphnia magna	6 - 24 h old	N	S	ag	rw	9.0 ± 0.1	22 ± 2		24 h	EC50	immobilisation	4.53	1		Cronin et al., 2000	
Daphnia magna	≤ 24 h old	Y	R		am	8.0 ± 0.2	25 ± 1	250	24 h	EC50		6	2	6	Kühn et al., 1989b	
Daphnia magna	6 - 24 h old		S		am		20 ± 2	250	48 h	EC50	immobilisation	14	1	5	Gesellschaft Deutscher Chemiker, 1991	Kühn, 1989
Daphnia magna		N		≥ 99					48 h	LC50	mortality	0.13	1	7	Maas-Diepeveen and Van Leeuwen, 1986	
Daphnia magna	≤ 24 h old	Y		> 99.9			19		48 h	EC50	immobilisation	0.46	2		Canton et al., 1985	
Daphnia magna	6 - 24 h old	N	S		am	8.0 ± 0.2	20	240	48 h	EC50	immobilisation	1.8	2		Kühn et al., 1989a	
Daphnia magna									48 h	EC50	immobilisation	2.0	2		NITE, 2002	Ministry of Environment, Japan, 2000
Daphnia magna	≤ 24 h old	Y		> 99.9			19		48 h	LC50	mortality	5.6	3		Canton et al., 1985	

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference	Original reference
Gammarus fasciatus	21.9 mg, 10.7 mm (control weight at test end)	Y	IF	> 99.0	dtw	6.8	18 ± 1	16	96 h	LC50	mortality	5.4	1	8	EI DuPont Denemours & Co. Inc., 1989	
Pisces																
Carassias auratus	45 d old, ca. 3.5 g, ca. 4.0 cm		R	> 95	am	7.5	20 ± 1	110	48 h	LC50	mortality	65.4	1		Liu et al., 1996	
Danio rerio	ca. 3 mo old, 200 - 350 mg, males and females	Y	R		tw	8.6 ± 0.3	26.5 ± 1		96 h	LC50	mortality	5.23	2	9	Zok et al., 1991	
Leuciscus idus									48 h	LC50	mortality	3.1	3		Gesellschaft Deutscher Chemiker, 1991	Handbuch der Gefährlichen Güter, 1987
Oncorhynchus mykiss	2 y old	N	R		nw		16 - 21.5 (within single tests ± 1 °C)		24 h	LC50	mortality	42	3	10	Lysak and Marcinek, 1972	
Oncorhynchus mykiss	2.7 cm, 0.329 g ww	Y	IF	99.60%	nw	7.3 - 7.4	11.7 - 12.8	72 - 79	96 h	LC50	mortality	1.04	1	6	Haskell Laboratory, 1992	
Oryzias latipes			R						48 h	LC50	mortality	48.98	3	11	Yoshioka et al., 1986	
Oryzias latipes									96 h	LC50	mortality	7.3	2		NITE, 2002	Ministry of Environment, Japan, 2000
Pimephales promelas	26 - 34 d old (juveniles)	Y	CF	> 95	nw	7.8	25	45	96 h	LC50	mortality	5.13	1	12	Broderius et al., 1995	
Pimephales promelas	26 - 34 d old (juveniles)	Y	CF	> 95	nw	7.8	25	45	96 h	LC50	mortality	5.65	1	12	Broderius et al., 1995	
Pimephales promelas	36 d, 25.3 mm, 0.235 g	Y	F	≥ 98%	dtw or nw	7.64	25.7	41.4	96 h	LC50	mortality	5.81	1		Brooke et al., 1984	
Pimephales promelas	29 d, 20.0 mm, 0.105 g	Y	F	≥ 98%	dtw or nw	7.6	24.9	44.9	96 h	LC50	mortality	5.68	1		Geiger et al., 1986	
Pimephales promelas	30 - 35 d old		F		nw		25	43.3 - 48.5		LC50	mortality	5.83	3	13	Hall et al., 1989	
Poecilia reticulata	2 - 3 mo	N	R		am		22 ± 1	25	14 d	LC50	mortality	6.25	2		Hermens et al., 1984	
Poecilia reticulata	3 - 4 w	Y	R	> 99.9			23 ± 2			LC50	mortality	32	3	13	Canton et al., 1985	
Poecilia reticulata	3 - 4 w	Y	R	> 99.9			23 ± 2			EC50	behaviour	0.32	3	13	Canton et al., 1985	

Notes:
1 Reported as Minimal Inhibition Concentration (MIC).
2 Unclear if the EC50 is based on nominal or measured concentrations. Recovery of the test substance was > 80% of nominal in an abiotic control containing a concentration equal to the EC50.
3 In accordance with OECD 201 (1984) with slight modifications.
4 Reported as an IC10, which was defined as the lowest concentration that differs statistically from the control.
5 In accordance with DIN 38 412 Part 11.
6 Test result based on nominal concentrations, which were > 80% of nominal.
7 In accordance with NEN 6501 (1980) with slight modifications.
8 In accordance with ASTM and US EPA 1986 guidelines.
9 In accordance with OECD guideline (1984); guideline no. not reported.
10 LC50 calculated as geometric mean of the reported 48-h LC0 (14.5 $mg.L^{-1}$) and 24-h LC100 (121.5 $mg.L^{-1}$).
11 In accordance with OECD 203 (1982); unit LC50 not reported.
12 Unclear if the LC50 is based on nominal or mean measured concentrations. Recovery of the test substance was > 90% of nominal.
13 Exposure time is not reported.

Table A2.2. Acute toxicity of 2-chloroaniline to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference	Original reference
Bacteria																
Vibrio fischeri							15		5 min	EC50	bioluminescence	16.1	1	1	Gesellschaft Deutscher Chemiker, 1991; Kaiser and Palabrica, 1991	King and Painter, 1981
Vibrio fischeri		N	S				15		5 min	EC50	bioluminescence	14.3	2	1	Ribo and Kaiser, 1984	
Vibrio fischeri		N	S				15		15 min	EC50	bioluminescence	15.0	2	1	Ribo and Kaiser, 1984	
Vibrio fischeri		N		≥ 99					15 min	EC50	bioluminescence	13	2	1	Maas-Diepeveen and Van Leeuwen, 1986	
Vibrio fischeri							15		30 min	EC50	bioluminescence	9.34	1	1	Gesellschaft Deutscher Chemiker, 1991	Hessisches Ministerium für Umwelt und Reaktorsicherheit (Hrsg.)
Vibrio fischeri		N	S				15		30 min	EC50	bioluminescence	15.7	2	1	Ribo and Kaiser, 1984	
Vibrio fischeri		N	S	pa						EC50	bioluminescence	18.8	2	1	Reynolds et al., 1987	
Vibrio fischeri							15		30 min	EC10	bioluminescence	0.67	2	1	Gesellschaft Deutscher Chemiker, 1991	Hessisches Ministerium für Umwelt und Reaktorsicherheit (Hrsg.)

Notes:
1 Microtox test.

Table A2.3. Chronic toxicity of 2-chloroaniline to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference	Original reference
Bacteria																
Pseudomonas putida					am	7	25	85	16 h	NOEC	growth	55	1	1	Gesellschaft Deutscher Chemiker, 1991	Bayer AG, 1978, 1979,1986
Algae																
Pseudokirchneriella subcapitata									48 h	NOEC	growth rate	32	2		NITE, 2002	Ministry of Environment, Japan, 2000
Pseudokirchneriella subcapitata									72 h	NOEC	biomass (AUC)	3.2	2		NITE, 2002	Ministry of Environment, Japan, 2000
Scenedesmus subspicatus		N	S		am	8.0 - 9.3	24 ± 1		72 h	EC10	growth rate	25	2		Kühn and Pattard, 1990	
Scenedesmus subspicatus		N	S		am	8.0 - 9.3	24 ± 1		72 h	EC10	biomass (AUC)	6	2		Kühn and Pattard, 1990	
Scenedesmus subspicatus		N	S		am	7	27	550	8 d	LOEC	growth	3.90	2	2	Schmidt and Schnabl, 1988	
Crustacea																
Daphnia magna	≤ 24 h old	Y	R		am	8.0 ± 0.2	25 ± 1	250	21 d	NOEC	survival, reproduction rate, time to 1st reproduction	0.032	2	3	Kühn et al., 1989b	
Daphnia magna									21 d	EC50	reproduction	0.043	3		NITE, 2002	Ministry of Environment, Japan, 2000

Notes:
1 Reported as Toxic Threshold Concentration (TTC, 3% reduction in cell density).
2 Reported as IC10, which was defined as the lowest concentration that differs statistically from the control.
3 Test result based on nominal concentrations, which were > 80% of nominal.

Table A2.4. Chronic toxicity of 2-chloroaniline to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri		N	S		am	7	20	21.9	6 h	EC50	growth	300	2	1	Gellert and Stommel, 1999
Vibrio fischeri		N	S		am	7	20	21.9	6 h	EC50	growth	500	3	2	Gellert and Stommel, 1999

Notes:
1 Test performed in quartz glass plates.
2 Test performed in polystyrene plates. Adsorption of the test compound to the microplates cannot be excluded.

Table A2.5. Acute toxicity of 3-chloroaniline to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference	Original reference
Bacteria																
Escherichia coli	1E+04 cells.mL^{-1}	N	S	'high'	am		37			EC50	growth rate	345	3		Nendza and Seydel, 1988, 1990	
Escherichia coli	1E+04 cells.mL^{-1}	N	S	'high'	am		37			LOEC	cell density	523	3	1	Nendza and Seydel, 1990	
Mycobacterium smegmatis	1E+04 cells.mL^{-1}	N	S	'high'	am		37			LOEC	cell density	255	3	1	Nendza and Seydel, 1990	
Protozoa																
Tetrahymena pyriformis		N	S	ag	am		30		24 h	EC50	cell number	100	2		Yoshioka et al., 1985	
Tetrahymena pyriformis	strain GL-C	N	S	> 95	am	7.35	27 ± 1	75	40 h	EC50	population growth (cell density)	76.9	2		Schultz, 1999	
Tetrahymena pyriformis	strain GL-C	Y	S	> 95	am	7.3	28		48 h	EC50	population growth (cell density)	103	2	2	Arnold *et al*., 1990	
Tetrahymena pyriformis	strain GL-C	Y	S	> 95	am	7.3	28		48 h	EC50	population growth (cell density)	64.4	2	2	Schultz *et al*., 1989	
Algae																
Chlorella pyrenoidosa		N		≥ 99					96 h	EC50	cell density	21	2	3	Maas-Diepeveen and Van Leeuwen, 1986	
Pseudokirchneriella subcapitata									48 h	EC50	growth rate	19	2		NITE, 2002	Ministry of Environment, Japan, 2000
Pseudokirchneriella subcapitata									72 h	EC50	biomass (AUC)	10	2		NITE, 2002	Ministry of Environment, Japan, 2000
Scenedesmus subspicatus								27	168 h	EC50	cell density	31.8	3		Gesellschaft Deutscher Chemiker, 1991	Schmidt 1989
Scenedesmus subspicatus		N	S		am	8.0 - 8.8		24 ± 1	48 h	EC50	growth rate	53	2		Kühn and Pattard, 1990	
Scenedesmus subspicatus									72 h	EC50	growth rate	21	2		Gesellschaft Deutscher Chemiker, 1991	Hessisches Ministerium für Umwelt und Reaktor-sicherheit (Hrsg.)
Scenedesmus subspicatus		N	S		am	8.0 - 8.8		24 ± 1	48 h	EC50	biomass (AUC)	26	2		Kühn and Pattard, 1990	
Scenedesmus subspicatus	cell wall removed									LOEC	O_2 production	0.255	3	4	Schmidt and Schnabl, 1988	
Crustacea																
Ceriodaphnia dubia	< 24 h old	Y	S				23 ± 1		48 h	EC50	immobilisation	0.103	4		Warne and Westbury, 1999	Mulhall, 1997
Daphnia magna	≤ 24 h old	Y	R		am	8.0 ± 0.2	25 ± 1	250	24 h	EC50		1.9	2	5	Kühn *et al*., 1989b	
Daphnia magna	6 - 24 h old		S		am		20	240	24 h	EC50	immobilisation	14	2	6	Gesellschaft Deutscher Chemiker, 1991	Kühn, 1989
Daphnia magna	6 - 24 h old	N	S	ag	rw	6.0 ± 0.1	22 ± 2		24 h	EC50	immobilisation	8.05	1		Cronin *et al*., 2000	
Daphnia magna	6 - 24 h old	N	S	ag	rw	7.8 ± 0.1	22 ± 2		24 h	EC50	immobilisation	4.53	1		Cronin *et al*., 2000	
Daphnia magna	6 - 24 h old	N	S	ag	rw	9.0 ± 0.1	22 ± 2		24 h	EC50	immobilisation	3.21	1		Cronin *et al*., 2000	
Daphnia magna	6 - 24 h old	N	S		am	8.0 ± 0.2	20	240	48 h	EC50	immobilisation	0.35	2		Kühn *et al*., 1989a	
Daphnia magna	6 - 24 h old		S		am		20	240	48 h	EC50	immobilisation	2.7	2	6	Gesellschaft Deutscher Chemiker, 1991	Kühn, 1989
Daphnia magna		N		≥ 99					48 h	LC50	mortality	0.1	1	7	Maas-Diepeveen and Van Leeuwen, 1986	
Daphnia magna									48 h	EC50	immobilisation	0.49	2		NITE, 2002	Ministry of Environment, Japan, 2000
Daphnia magna									24 h	EC50	immobilisation	0.26 - 15	3		Gesellschaft Deutscher Chemiker, 1991	Hessisches Ministerium für Umwelt und Reaktor-sicherheit (Hrsg.)
Pisces																
Carassias auratus	45 d old, ca. 3.5 g, ca. 4.0 cm length		R	> 95	am	7.5	20 ± 1	110	48 h	LC50	mortality	55.7	2		Liu et al., 1996	

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference	Original reference
Danio rerio	ca. 3 mo old, 200 - 350 mg, males and females	Y	R		tw	8.6 ± 0.3	26.5 ± 1		96 h	LC50	mortality	18.8	2	8	Zok et al., 1991	
Danio rerio	3 - 12 mo old, 3 ± 0.5 cm		S		am	7	22 ± 2	250	96 h	LC50	mortality	24	1		Gesellschaft Deutscher Chemiker, 1991	Bayer AG, 1979 - 1984
Leuciscus idus	3 - 12 mo old, 6 ± 2 cm		S		am	7	20	270	96 h	LC50	mortality	14	1	9	Gesellschaft Deutscher Chemiker, 1991	Bayer AG, 1979 - 1984
Leuciscus idus										LC50	mortality	12 - 25	4		Atri, 1986	OECD, 1982
Oryzias latipes									96 h	LC50	mortality	8.8	2		NITE, 2002	Ministry of Environment, Japan, 2000
Poecilia reticulata	2 - 3 mo old	N	R		am		22 ± 1	25	14 d	LC50	mortality	13.4	2		Hermens *et al*., 1984	

Notes:
1 Reported as Minimal Inhibition Concentration (MIC).
2 Unclear if the EC50 is based on nominal or mean measured concentrations. Recovery of the test substance was > 80% of nominal in an abiotic control containing a concentration equal to the EC50.
3 In accordance with OECD 201 (1984) with slight modifications.
4 Reported as IC10, which was defined as the lowest concentration that differs statistically from the control.
5 Test result based on nominal concentrations, which were > 80% of nominal.
6 In accordance with DIN 38 412 Part 11.
7 In accordance with NEN 6501 (1980) with slight modifications.
8 In accordance with OECD guideline (1984). Guideline no. not reported.
9 In accordance with DIN 38 412 Part 20.

Table A2.6. Acute toxicity of 3-chloroaniline to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference	Original reference
Bacteria																
Vibrio fischeri		N	S				15		5 min	EC50	bioluminescence	12.5	2	1	Ribo and Kaiser, 1984	
Vibrio fischeri		N	S				15		15 min	EC50	bioluminescence	13.4	2	1	Ribo and Kaiser, 1984	
Vibrio fischeri		N		≥ 99					15 min	EC50	bioluminescence	16	2	1	Maas-Diepeveen and Van Leeuwen, 1986	
Vibrio fischeri							15		30 min	EC50	bioluminescence	23.1	1	1	Gesellschaft Deutscher Chemiker, 1991	Hessisches Ministerium für Umwelt und Reaktorsicherheit (Hrsg.)
Vibrio fischeri		N	S				15		30 min	EC50	bioluminescence	14.0	2	1	Ribo and Kaiser, 1984	
Vibrio fischeri							15		30 min	EC10	bioluminescence	2.69	2	1	Gesellschaft Deutscher Chemiker, 1991	Hessisches Ministerium für Umwelt und Reaktorsicherheit (Hrsg.)
Vibrio fischeri		N	S				15		4.8 min	EC50	bioluminescence	20.2	4		Warne and Westbury, 1999	Mulhall, 1997
Vibrio fischeri		N	S				15		15 min	EC50	bioluminescence	24.6	4		Warne and Westbury, 1999	Mulhall, 1997
Vibrio fischeri		N	S				15		30 min	EC50	bioluminescence	40.6	4		Warne and Westbury, 1999	Mulhall, 1997

Notes:
1 Microtox test.

Table A2.7. Chronic toxicity of 3-chloroaniline to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference	Original reference
Bacteria																
Pseudomonas putida					am	7	25	85	16 h	NOEC	growth	19	2	1	Gesellschaft Deutscher Chemiker, 1991	Bayer AG, 1979 - 1984
Pseudomonas putida							25		16 - 18 h	EC10	growth	90.2	2		Gesellschaft Deutscher Chemiker, 1991	Hessisches Ministerium für Umwelt und Reaktorsicher-heit (Hrsg.)
Pseudomonas putida							25		16 - 18 h	EC50	growth	178.7	2		Gesellschaft Deutscher Chemiker, 1991	Hessisches Ministerium für Umwelt und Reaktorsicher-heit (Hrsg.)
Algae																
Pseudokirchneriella subcapitata									48 h	NOEC	growth rate	10	2		NITE, 2002	Ministry of Environment, Japan, 2000
Pseudokirchneriella subcapitata									72 h	NOEC	biomass (AUC)	1.0	2		NITE, 2002	Ministry of Environment, Japan, 2000
Scenedesmus subspicatus		N	S		am	8.0 - 8.8		24 ± 1	48 h	EC10	growth rate	9.8	2		Kühn and Pattard, 1990	
Scenedesmus subspicatus									72 h	EC10	growth rate	8	2		Gesellschaft Deutscher Chemiker, 1991	Hessisches Ministerium für Umwelt und Reaktorsicher-heit (Hrsg.)
Scenedesmus subspicatus		N	S		am	8.0 - 8.8		24 ± 1	48 h	EC10	biomass (AUC)	6.8	2		Kühn and Pattard, 1990	
Scenedesmus subspicatus		N	S		am	7	27	550	8 d	LOEC	growth	4.10	3	2	Schmidt and Schnabl 1988	
Crustacea																
Daphnia magna	≤ 24 h	Y	R		am	8.0 ± 0.2	25 ± 1	250	21 d	NOEC	reproduction rate, appearance of first offspring	0.013	2	3	Kühn *et al*., 1989b	
Daphnia magna									21 d	NOEC	reproduction	0.0032	2		NITE, 2002	Ministry of Environment, Japan, 2000
Daphnia magna									21 d	EC50	reproduction	0.012	3		NITE, 2002	Ministry of Environment, Japan, 2000
Daphnia magna		N		≥ 99					21 d	LC50	mortality	0.26	3	4	Maas-Diepeveen and Van Leeuwen, 1986	
Daphnia magna	≤ 24 h	N	R	≥ 99	am or nw	8.4 ± 0.1	20 ± 0.5	200	21 d	LOEC	intrinsic rate of increase (r_m)	0.032	3	5	Maas-Diepeveen and Van Leeuwen, 1986	
Daphnia magna		N		≥ 99					21 d	LOEC	mean size	0.32	3	5	Maas-Diepeveen and Van Leeuwen, 1986	
Pisces																
Danio rerio	fertilised eggs	Y	R	98	rw	7.4 - 8.4	24 ± 2	210	28 d	NOEC	survival	5.6	1	3	Van Leeuwen et al., 1990	
Danio rerio	fertilised eggs	Y	R	98	rw	7.4 - 8.4	24 ± 2	210	28 d	NOEC	growth (length)	1	1	3	Van Leeuwen et al., 1990	
Danio rerio	fertilised eggs	Y	R	98	rw	7.4 - 8.4	24 ± 2	210	28 d	LC50	mortality	6.8	3	3	Van Leeuwen *et al*., 1990	

Notes:
1 Toxic Threshold Concentration (TTC, 3% reduction in cell density).
2 Reported as IC10, which was defined as the lowest concentration that differs statistically from control.
3 Test result based on nominal concentrations, which were > 80% of nominal.
4 In accordance with NEN 6502 (1980).
5 In accordance with NEN 6502 (1980). Reported as Lowest Rejected Concentration Tested (LRCT).

Table A2.8. Acute toxicity of 4-chloroaniline to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference	Original reference
Bacteria																
Bacillus subtilis		N	S		am		37	0.17	log. growth phase	EC50	growth	385	2		Ogawa *et al*., 1991	
Escherichia coli	1E+04 cells.mL^{-1}, in log. phase	N	S	'high'	am		37			LOEC	cell density	357	3	1	Nendza and Seydel, 1990	
Escherichia coli	1E+04 cells.mL^{-1}	N	S	'high'	am		37			EC50	growth rate	383	3		Nendza and Seydel, 1988, 1990	
Mycobacterium smegmatis	1E+04 cells.mL^{-1}, in log. phase	N	S	'high'	am		37			LOEC	cell density	65.1	3	1	Nendza and Seydel, 1990	
Protozoa																
Tetrahymena pyriformis	strain GL-C	N	S	> 95	am	7.35	27 ± 1	75	40 h	EC50	population growth (cell density)	114	2		Schultz, 1999	
Tetrahymena pyriformis	strain GL-C	Y	S	> 95	am	7.3	28		48 h	EC50	population growth (cell density)	5.63	2	2	Arnold et al., 1990	
Tetrahymena pyriformis	strain GL-C	Y	S	> 95	am	7.3	28		48 h	EC50	population growth (cell density)	5.42	2	2	Schultz et al., 1989	
Tetrahymena pyriformis		N	S	ag	am		30		24 h	EC50	cell number	10	3		Yoshioka et al., 1985	
Uronema parduczi									22 h	LOEC		2.3	4	3	Atri, 1986	Janicke and Hilge, 1980
Rotifera																
Brachionus rubens		Y	S		am		25 ± 1	106	24 h	LC50	mortality	100	2	4	Halbach *et al*., 1983	
Algae																
Chlorella pyrenoidosa		N		> 99					96 h	EC50	cell density	4.1	2	5	Maas-Diepeveen and Van Leeuwen, 1986	
Chlorella vulgaris	ca. 7.5E+06 cells.mL^{-1}	N	S		am		36.5		6 h	EC50	cell density	50.8	2	6	Kramer and Trümper, 1986	
Chlorella vulgaris	ca. 7.5E+06 cells.mL^{-1}	N	S		am		36.5		6 h	EC50	cell density	43.2	2	7	Kramer and Trümper, 1986	
Pseudokirchneriella subcapitata									48 h	EC50	growth rate	4.7	2		NITE, 2002	Ministry of Environment, Japan, 2000
Pseudokirchneriella subcapitata									72 h	EC50	biomass (AUC)	1.5	2		NITE, 2002	Ministry of Environment, Japan, 2000
Scenedesmus subspicatus		N	S		am	8.0 – 9.3	24 ± 1		72 h	EC50	biomass (AUC)	2.2	2		Kühn and Pattard, 1990	
Scenedesmus subspicatus	ca. 1E+04 cells.mL^{-1}	N	S	98	am	7	22 ± 2	550	96 h	EC50	biomass (AUC)	2.4	2		Geyer *et al*., 1985	
Scenedesmus subspicatus		N	S		am	8.0 – 9.3	24 ± 1		72 h	EC50	growth rate	6.3	2		Kühn and Pattard, 1990	
Scenedesmus subspicatus						7		27	168 h	EC50	cell density	2.1	3		Gesellschaft Deutscher Chemiker, 1993	Schmidt, 1989
Scenedesmus subspicatus	cell wall removed									LOEC	O_2 production	9.57E-05	3	8	Schmidt and Schnabl, 1988	
Ascomycota																
Pichia sp.	from act. sludge (municipal STP)	N	S	'high'	am		22			EC50	growth	78.7	3		Kwasniewska and Kaiser, 1984	
Rhodotorula rubra	from shore of Lake Ontario	N	S	'high'	am		22			EC50	growth	109	3		Kwasniewska and Kaiser, 1984	
Rhodotorula sp.	from act. sludge (municipal STP)	N	S	'high'	am		22			EC50	growth	ca. 128	3		Kwasniewska and Kaiser, 1984	
Saccharomyces cerevisiae		N		'high'	am	3.2	28		16 - 18 h	EC20	fermentation	17.9	3	9	Weber et al., 2000	

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference	Original reference
Crustacea																
Daphnia magna					am				24 h	EC50	immobilisation	0.06	1	10	Gesellschaft Deutscher Chemiker, 1993	Rott, 1981
Daphnia magna	6 - 24 h old	N	S	> 95	am		22 ± 1		24 h	EC50	immobilisation	18.0	2		Zhao *et al*., 1995	
Daphnia magna	< 24 h old	N	S		am	8.0 ± 0.2	20	250	24 h	EC50	immobilisation	3.2	2		Bringmann and Kühn, 1982	
Daphnia magna		N		> 99					48 h	LC50	mortality	0.05	1	11	Maas-Diepeveen and Van Leeuwen, 1986	
Daphnia magna	6 - 24 h old	N	S		am	8.0 ± 0.2	20	240	48 h	EC50	immobilisation	0.31	2		Kühn *et al*., 1989a	
Daphnia magna	< 24 h old	N	S	98			20 ± 1		48 h	EC50	immobilisation	0.104	3	12	Steinberg *et al*., 1992	
Daphnia magna	< 24 h old	N	S	98			20 ± 1		48 h	EC50	immobilisation	0.167	3	13	Steinberg *et al*., 1992	
Daphnia magna	< 24 h old	N	S	98			20 ± 1		48 h	EC50	immobilisation	0.197	3	14	Steinberg *et al*., 1992	
Daphnia magna	< 24 h old	N	S	98			20 ± 1		48 h	EC50	immobilisation	0.153	3	15	Steinberg *et al*., 1992	
Daphnia magna	< 24 h old		S	98	am		20 ± 1		48 h, 2 h contact	EC50		0.105	3	12	Lee *et al*., 1993	
Daphnia magna	< 24 h old		S	98	am		20 ± 1		48 h, 2 h contact	EC50		0.172	3	13	Lee *et al*., 1993	
Daphnia magna	< 24 h old		S	98	am		20 ± 1		48 h, 2 h contact	EC50		0.204	3	14	Lee *et al*., 1993	
Daphnia magna	< 24 h old		S	98	am		20 ± 1		48 h, 2 h contact	EC50		0.162	3	15	Lee *et al*., 1993	
Daphnia magna									24 h	EC50		0.06	4		Atri, 1986	OECD, 1982; Anonymous, 1981
Insecta																
Chironomus plumosus	early 4th instar		S	95	am	7.2	22	40	48 h	EC50	immobilisation	43	2		Julin and Sanders, 1978	
Pisces																
Carassias auratus	45 d old, ca. 3.5 g, ca. 4.0 cm		R	> 95	am	7.5	20 ± 1	110	48 h	LC50	mortality	54.4	2		Liu *et al*., 1996	
Danio rerio						7.8 ± 0.1	23 ± 1	200	48 h	LC50	mortality	46	1	16	Gesellschaft Deutscher Chemiker, 1993; Atri, 1986	Spieser, 1981
Danio rerio	ca. 3 mo old, 200 - 350 mg, ♂♀	Y	R		tw	8.6 ± 0.3	26.5 ± 1		96 h	LC50	mortality	34.5	2	17	Zok et al. 1991	
Danio rerio	embryos (eggs)	N	R	99	tw	7.2	27.5	427	96 h	LC50	mortality	44	2		Burkhardt-Holm et al., 1999	
Danio rerio	ca. 2 mo old, 2 - 3 cm		S	98	tw		21 ± 1		96 h, 2 h contact	LC50	mortality	30.7	3	12	Lee et al., 1993	
Danio rerio	ca. 2 mo old, 2 - 3 cm		S	98	tw		21 ± 1		96 h, 2 h contact	LC50	mortality	31.0	3	13	Lee *et al*., 1993	
Danio rerio	ca. 2 mo old, 2 - 3 cm		S	98	tw		21 ± 1		96 h, 2 h contact	LC50	mortality	30.9	3	14	Lee *et al*., 1993	
Danio rerio	ca. 2 mo old, 2 - 3 cm		S	98	tw		21 ± 1		96 h, 2 h contact	LC50	mortality	31.6	3	15	Lee *et al*., 1993	
Ichtalurus punctatus		N	S	95	rw	7.2	22	40	96 h	LC50	mortality	23	2		Julin and Sanders, 1978	
Lepomis macrochirus		N	S	95	rw	7.2	22	40	96 h	LC50	mortality	2.4	2		Julin and Sanders, 1978	
Leuciscus idus	1.85 g (initial), 6.11 cm (initial)	N	R	98	nw or tw	7.6 ± 0.1	20	325	48 h	LC50	mortality	26.5	2	18	Braunbeck and Segner, 1992	
Leuciscus idus	1.85 g (initial), 6.11 cm (initial)	N	R	98	nw or tw	7.6 ± 0.1	20	325	48 h	LC50	mortality	16.5	2	19	Braunbeck and Segner, 1992	
Leuciscus idus	3.70 g (initial), 7.28 cm (initial)	N	R	98	nw or tw	7.6 ± 0.1	14	325	48 h	LC50	mortality	9.8	2	20	Braunbeck and Segner, 1992	

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference	Original reference
Leuciscus idus		N					10 - 20		48 h	LC50	mortality	23	2	21	Knie et al., 1983	
Oncorhynchus mykiss	63.8 ± 7.1 g (control)	Y	F	98	nw	7.17	10.5	46.2	96 h	LC50	mortality	11	2	22	Hermens et al., 1990	
Oncorhynchus mykiss		N	S	95	rw	7.2	12	40	96 h	LC50	mortality	14	2		Julin and Sanders, 1978	
Oncorhynchus mykiss	1 - 5 g	Y	F	> 99	nw	7.8	15	135	96 h	LC50	mortality	16.3	2		Hodson, 1985	
Oncorhynchus mykiss	2 y old	N	R		nw		16 - 21.5 (within single tests ± 1 °C)		24 h	LC50	mortality	19	3	23	Lysak and Marcinek, 1972	
Oryzias latipes	ca. 2 cm, 0.2 g	N		ag	dw	neutralised	25		48 h	LC50	mortality	28	2	24	Tonogai et al., 1982	
Oryzias latipes	juveniles, 28 - 43 d old, 18 -71 mg	Y	CF	99.9	nw	7.88	25 ± 1	45.8	96 h	LC50	mortality	37.7	1		Holcombe et al., 1995	
Oryzias latipes									96 h	LC50	mortality	5.8	2		NITE, 2002	Ministry of Environment, Japan, 2000
Pimephales promelas	juveniles, 26 - 34 d old, lab. cultured	Y	CF	> 95	nw	7.8	25	45	96 h	LC50	mortality	32.5	1	25	Veith and Broderius, 1987; Broderius et al., 1995	
Pimephales promelas	34 d	Y	F	≥ 98	dtw or nw	7.7	24.5	44.3	96 h	LC50	mortality	30.6	1		Geiger et al., 1988	
Pimephales promelas		N	S	95	rw	7.2	22	40	96 h	LC50	mortality	12	2		Julin and Sanders, 1978	
Poecilia reticulata	2 - 3 mo old	N	R		am		22 ± 1	25	14 d	LC50	mortality	26.0	2		Hermens *et al*., 1984	

Notes:

1 Reported as Minimal Inhibition Concentration (MIC).
2 Unclear if the EC50 is based on nominal or mean measured concentrations. Recovery of the test substance was > 80% of nominal in an abiotic control containing a concentration equal to the EC50.
3 Reported as Toxische Grenz-Konzentration.
4 LC50 is based on nominal concentrations. Recovery of the test substance was not reported.
5 In accordance with OECD 201 (1984) with slight modifications.
6 Obtained from extinction measurements at 680 nm.
7 Obtained from extinction measurements at 750 nm.
8 Reported as an IC10, which was defined as the lowest concentration that differs statistically from the control.
9 The test was performed in minimal medium in order to increase the sensitivity of the yeast cells.
10 In accordance with OECD 202.
11 In accordance with NEN 6501 (1980) with slight modifications.
12 No dissolved humic material (DHM).
13 0.5 $mg.L^{-1}$ DHM.
14 5 $mg.L^{-1}$ DHM.
15 50 $mg.L^{-1}$ DHM.
16 In accordance with OECD 203.
17 In accordance with OECD guideline. Guideline no. not reported.
18 Diet 1 of two different diets and 20 °C (in accordance with DIN 38 412).
19 Diet 2 of two different diets and 20 °C (in accordance with DIN 38 412).
20 Diet 2 of two different diets and 14 °C.
21 In accordance with DIN 38412 Teil 15.
22 Unclear if the LC50 is based on nominal or mean measured concentrations. Spike recoveries were 98.2 and 103.7%.
23 LC50 calculated as the geometric mean of the reported 48-h LC0 (11 $mg.L^{-1}$) and 24-h LC100 (33 $mg.L^{-1}$).
24 Reported as Median Tolerance Limit (TLm).
25 In accordance with ASTM 1980. Unclear if the LC50 is based on nominal or mean measured concentrations. Recovery of the test substance was > 90% of nominal.

Table A2.9. Acute toxicity of 4-chloroaniline to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri		N	S				15		5 min	EC50	bioluminescence	3.20	2	1	Ribo and Kaiser, 1984
Vibrio fischeri		N	S				15		15 min	EC50	bioluminescence	3.76	2	1	Ribo and Kaiser, 1984
Vibrio fischeri		N	S	> 95	am		20	32.9	15 min	EC50	bioluminescence	34.3	2	1	Zhao *et al*., 1993, 1995
Vibrio fischeri		N		> 99					15 min	EC50	bioluminescence	5.9	2	1	Maas-Diepeveen and Van Leeuwen, 1986
Vibrio fischeri		N	S	'high'			15		30 min	EC50	bioluminescence	5.08	2	1	Ribo and Kaiser, 1984
Mollusca															
Mya arenaria	ca. 5 cm, 20 g	Y	R		nw		10	30	29 h	LC50	mortality	15.1	3	2	McLeese et al., 1979
Mya arenaria	ca. 5 cm, 20 g	Y	R		nw		10	30	96 h	LC50	mortality	< 49	3	2, 3	McLeese et al., 1979
Crustacea															
Crangon septemspinosa	6.4 - 8.3 cm, 2.4 - 4.5 g	Y	R		nw		10	30	10 h	LC50	mortality	12.5	3	2	McLeese *et al*., 1979
Crangon septemspinosa	6.4 - 8.3 cm, 2.4 - 4.5 g	Y	R		nw		10	30	96 h	LC50	mortality	< 46	3	2, 3	McLeese *et al*., 1979

Notes
1 Microtox test.
2 Exposure time not fixed (time to lethality experiment). Unclear if the LC50 is based on nominal or measured concentrations, but concentrations remained practically constant (percentage recovery was not reported).
3 Only one concentration was tested.

Table A2.10. Chronic toxicity of 4-chloroaniline to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference	Original reference
Bacteria																
Pseudomonas putida		N				7	25		16 - 18 h	EC10	growth	72	2		Knie *et al*., 1983	
Pseudomonas putida									18 h	LOEC		31	4	1	Atri, 1986	Janicke and Hilge, 1980
Rotifera																
Brachionus rubens		Y	R		am		25 ± 1	106	10 d	EC10	intrinsic rate of natural increase (r_m)	13.0	2	2	Halbach et al., 1983	
Brachionus rubens		Y	R		am		25 ± 1	106	10 d	EC10	carrying capacity (K)	10.6	2	2	Halbach et al., 1983	
Brachionus rubens		Y	R		am		25 ± 1	106	10 d	EC10	frequency of the density oscilations	2.36	3	2	Halbach et al., 1983	
Brachionus rubens		Y	R		am		25 ± 1	106	10 d	EC10	"pregnancy" of the density oscilations	4.51	3	2	Halbach et al., 1983	
Algae																
Pseudokirchneriella subcapitata									48 h	NOEC	growth rate	1.0	2		NITE, 2002	Ministry of Environment, Japan, 2000
Pseudokirchneriella subcapitata									72 h	NOEC	biomass (AUC)	0.32	2		NITE, 2002	Ministry of Environment, Japan, 2000
Scenedesmus subspicatus		N	S		am	8.0 – 9.3	24 ± 1		72 h	EC10	growth rate	1	2		Kühn and Pattard, 1990	
Scenedesmus subspicatus		N	S		am	8.0 – 9.3	24 ± 1		72 h	EC10	biomass (AUC)	0.4	2		Kühn and Pattard, 1990	
Scenedesmus subspicatus	ca. 1E+04 cells.mL^{-1}	N	S	98	am	7	22 ± 2	550	96 h	EC10	biomass (AUC)	0.4	2		Geyer et al., 1985	
Scenedesmus subspicatus		N	S		am	7	27	550	8 d	LOEC	growth	0.0255	3	3	Schmidt and Schnabl, 1988	
Scenedesmus subspicatus									7 d	LOEC		1.3	3	1	Atri, 1986	Janicke and Hilge, 1980
Scenedesmus subspicatus		N	S		am	8.0 – 8.8	24 ± 1		96 h	EC10	biomass (AUC)	1.4	3		Kühn and Pattard, 1990	
Crustacea																
Daphnia magna	≤ 24 h old	Y	R		am	8.0 ± 0.2	25 ± 1	250	21 d	NOEC	reproduction rate, appearance 1st offspring	0.01	2	4	Kühn et al., 1989b	
Daphnia magna									21 d	NOEC	reproduction	0.0032	2		NITE, 2002	Ministry of Environment, Japan, 2000
Daphnia magna						7.8 ± 0.4	20 ± 0.5	250	21 d	NOEC	reproduction rate young animals	0.00006	4		Gesellschaft Deutscher Chemiker, 1993	Rott, 1984
Daphnia magna						7.8 ± 0.4	20 ± 0.5	250	21 d	NOEC	mortality rate adults	0.00001	4		Gesellschaft Deutscher Chemiker, 1993	Rott, 1984
Pisces																
Danio rerio			F						21 d	NOEC	lethal and other effects	1.8	2	5	Gesellschaft Deutscher Chemiker, 1993	Adolphi et al., 1984
Danio rerio	6 mo	Y	CF	> 99	tw	7.2 – 7.4	25.8 - 26.4	360	CLC (3 gen.)	NOEC	fertilisation rate in F1 and F2	0.2	1		Bresch et al., 1990	
Danio rerio	6 mo	Y	CF	> 99	tw	7.2 – 7.4	25.8 - 26.5	360	CLC (3 gen.)	LOEC	number of eggs in F1 and F2	0.04	1	6	Bresch et al., 1990	
Danio rerio	6 mo	Y	CF	> 99	tw	7.2 – 7.4	25.8 - 26.5	360	CLC (3 gen.)	NOEC	development (presence of anomalies)	0.2	1		Bresch et al., 1990	
Oncorhynchus mykiss	juveniles, ca. 4 - 5 g	Y	CF	> 99	tw	7.4	15 - 17	360	56 d	NOEC	growth (weight)	0.2	1	4	Bresch et al., 1991	
Oryzias latipes	larvae, 0 - 3 d old		CF		nw				28 d	NOEC	survival	8.23	2		Holcombe et al., 1995	
Oryzias latipes	larvae, 0 - 3 d old		CF		nw				28 d	LOEC	weight	2.25	2	7	Holcombe et al., 1995	

Notes
1 Reported as Toxische Grenz-Konzentration.
2 The EC10 was recalculated from the data using a log-logistic dose-response relationship. The test result is based on nominal concentrations. Recovery of the test substance was not reported.
3 Reported as an IC10, which was defined as the lowest concentration that differs statistically from the control.
4 Test result based on nominal concentrations, which were > 80% of nominal.
5 In accordance with the guideline Umweltbundesamt I 4.5 - 97 125/2/6.
6 At this concentration > 20% effect was observed.
7 Effect percentage was not reported.

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