2019

oekotoxzentrum
centre ecotox
Schweizerisches Zentrum für angewandte Ökotoxikologie
Centre Suisse d'écotoxicologie appliquée

SQC (EQS_{sed}) – Proposal by the Ecotox Centre for: *4-nonylphenol, branched and linear*

First proposal: 14.05.2019 (last bibliographic research)
27.09.2019 (implementation of the expertise)

Imprint

Publisher

Swiss Centre for Applied Ecotoxicology, 1015 Lausanne

Commissioned by

FOEN, Federal Office of the Environment, Water Quality Section, 3003 Bern

Authors

Alexandra Kroll, Carmen Casado-Martinez, Swiss Centre for Applied Ecotoxicology

Scientific Support

Dr Karen Duis, ECT Oekotoxikologie GmbH, Böttgerstr. 2-14, D-65439 Flörsheim/Main, Germany. External reviewer.

Please note that the suggested EQS and contents of this dossier do not necessarily reflect the opinion of the external reviewer.

Contact

Alexandra Kroll: Alexandra.Kroll@oekotoxzentrum.ch
Carmen Casado-Martinez: Carmen.Casado@centreecotox.ch

Citation Proposal

Alexandra Kroll, Carmen Casado-Martinez. 2019. SQC (EQS_{sed}) – Proposal by the Ecotox Centre for: 4-nonylphenol, branched and linear. Lausanne (CH): Swiss Centre for Applied Ecotoxicology; 38 pp.

Summary

SQC (EQS_{sed}): 131 µg/kg d.w.

In the framework of the Module Sediment, which is intended to help cantons in sediment quality assessment, the Ecotox Centre develops proposals for Environmental Quality Criteria for sediment (SQC). SQC are derived applying the methodology described in the EU-Technical Guidance (TGD) for Deriving Environmental Quality Standards (EQS). In order to ensure that the dossiers are internationally comparable, the English terminology of the TGD will be used in the remainder of the dossier. These criteria provide a first screening tool to evaluate sediment chemical quality and the potential risk for the aquatic ecosystem. Based on the scientific literature available at present a generic SQC for 4-nonylphenol of 131 µg/kg d.w. is proposed for standard sediments with 1 % OC.

Zusammenfassung

SQK (EQS_{sed}): 131 µg/kg TS

Im Rahmen des Sedimentmoduls, das den Kantonen bei der Bewertung der Sedimentqualität helfen soll, entwickelt das Oekotoxzentrum Vorschläge für Umweltqualitätskriterien für Sedimente (SQK). Diese Kriterien dienen als Methode für ein erstes Screening zur Bewertung der chemischen Sedimentqualität und des potenziellen Risikos für aquatische Ökosysteme. Auf der Basis von Literaturdaten für die Wirkung von 4-Nonylphenol und unter Verwendung der Methode, die in der Technischen Richtlinie der EU zur Ableitung von Umweltqualitätsnormen beschriebenen wird, schlägt das Oekotoxzentrum einen allgemeines SQK für 4-Nonylphenol von 131 µg/kg TS für Standardsedimente mit 1 % OC vor.

Résumé

CQS (EQS_{sed}): 131 µg/kg p.s.

Dans le cadre du module Sédiments qui devrait aider les cantons à évaluer la qualité des sédiments, le Centre Ecotox élabore des propositions de critères de qualité environnementale pour les sédiments (CQS). Les CQS sont dérivés en appliquant la méthodologie décrite dans le Guide Technique de l'UE (TGD) pour la Dérivation des Normes de Qualité Environnementale (EQS). Afin que les dossiers soient comparables au niveau international, la terminologie anglaise du TGD est utilisée ci-dessous. Ces critères fournissent un premier outil de dépistage pour évaluer la qualité chimique des sédiments et le risque potentiel pour l'écosystème aquatique. Sur la base des données sur les effets existants dans la littérature un CQS générique pour le 4-nonylphénole de 131 µg/kg p.s. est proposé pour les sédiments standards avec 1 % CO.

Sommario

CQS: 131 µg/kg p.s.

Nell'ambito del modulo Sedimenti, che è finalizzato ad aiutare i Cantoni nella valutazione della qualità dei sedimenti, il Centro Ecotox sviluppa proposte per i criteri di qualità ambientale per i sedimenti (CQS). I CQS sono derivati applicando la metodologia descritta nella Guida Tecnica dell'UE (TGD) per la Derivazione degli Standard di Qualità Ambientale (EQS). Per garantire che i dossier siano comparabili a livello internazionale, viene utilizzata la terminologia inglese del TGD. Questi criteri forniscono un primo strumento di screening per valutare la qualità chimica dei sedimenti e il potenziale rischio per l'ecosistema acquatico. Sulla base della letteratura scientifica disponibile allo stato attuale un CQS generico per il 4-nonilfenolo di 131 µg/kg p.s. è proposto per sedimenti standard con 1% CO.

Table of content

1 General Information

Extended general information on the alkylphenol 4-nonylphenol is provided in the Ecotox Centre EQS Dossier for 4-nonylphenol in water (Ecotox Centre 2016)[1]. Selected information from the EQS water Dossier and additional information relevant for sediment is presented in this chapter. Registration information, EQS dossiers and other reports referred to are:

- EC nonylphenol EQS dossier (2005)
- ECHA Information on Registered Substances CAS 104-40-5 (2011a)
- ECHA Information on Registered Substances CAS 84852-15-3 (2011b)
- European Union Risk Assessment Report 4-nonylphenol (branched) and nonylphenol (2002a)
- ECHA support document for identification of 4-nonylphenol, branched and linear, as substances of very high concern (2012)

1.1 Identity and physico-chemical properties

Nonylphenols vary in the substitution position of the nonyl group on the phenol molecule; and the degree of branching of the nonyl group. The nonyl moiety is formed by polymerizing propylene resulting in a varied degree of branching, with many of the individual branched isomers having specific CAS numbers.

Like the Ecotox Centre EQS Dossier for 4-nonylphenol in water (Ecotox Centre 2016), the EU EQS substance data sheet and the EU risk assessment for 4-nonylphenol, this assessment covers two substances identified on the second ESR (Existing Substances Regulation, Council Regulation (EEC) No 793/93) priority list: linear nonylphenol (EINECS Number: 246-672-0, CAS Number: 25154-52-3) and branched 4-nonylphenol (EINECS Number: 284-325-5, CAS Number: 84852-15-3). Nonylphenol as originally defined by CAS (Chemical Abstract Service, CAS Number: 25154-52-3) covered all nonylphenols, however, numbering was subsequently revised. REACH information on registered substances is available for CAS 84852-15-3 and CAS 104-40-5 (EC name "p-nonylphenol"; IUPAC name "4-nonylphenol"). According to the ECHA Support document for the identification of 4-nonylphenol, branched and linear, as substances of very high concern linear nonylphenol is only likely to be present at very low levels in commercial mixtures (ECHA 2012). These are predominantly 4-nonylphenol with a varied and undefined degree of branching in the alkyl group. A non-exhaustive list of substances covered by the group entry is provided in the same document (Table 5, ECHA (2012)). As opposed to the EU EQS substance data sheet and the EU risk assessment for 4-nonylphenol (EC 2005, European Commission 2002a), the document is not restricted to a set of CAS numbers.

In the following, 4-nonylphenol (NP) is used as the generic name referring to these substances. In case the source of information cited uses a different terminology, the respective CAS number is given if possible.

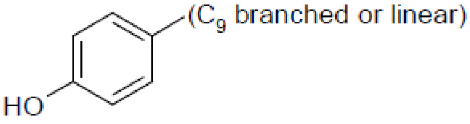
The log K_{oc} and log K_{ow} reported for 4-nonylphenol are in the range of 3.73-5.69 and 4.48-5.76 (Table 1) triggering an assessment for sediments according to the EC TGD EQS (EC 2018).

Table 1 summarizes identity and physico-chemical parameters for 4-nonylphenol required for EQS derivation according to the TGD (EC 2018). Where available, experimentally collected data is identified as (exp.) and estimated data as (est.). When not identified, no indication is available in the cited literature.

---

[1] The dossier can be requested to info@oekotoxzentrum.ch

Table 1 Information required for EQS derivation according to the TGD (EC 2018). Where available, CAS numbers are provided.

Characteristics	**Values**	**References**
Common name	4-Nonylphenol, branched and linear	ECHA (2012)
IUPAC name	4-Nonylphenol, branched and linear [substances with a linear and/or branched alkyl chain with a carbon number of 9 covalently bound in position 4 to phenol, covering also UVCB[2]- and well-defined substances which include any of the individual isomers or a combination thereof]	ECHA (2012)
Chemical group	phenol	
Structural formula		ECHA (2012)
Molecular formula	$C_{15}H_{24}O$	ECHA (2012)
CAS	84852-15-3 (branched isomers) 25154-52-3 (linear isomers)	Strub (2010), EC (2005)
EINECS	284-325-5 (branched isomers) 246-672-0 (linear isomers)	
Code SMILES	CC(C)CCCCCCC1=CC=C(C=C1)O CCCCCCCCCC1=CC=C(C=C1)O	PubChem (2019a,b)
Molecular weight [g/mol]	220.34	
Melting point [°C]	< -7 °C (CAS 84852-15-3) 42 °C (CAS 104-40-5)	
Boiling point [°C]	302 °C (CAS 84852-15-3) 293 - 297 °C (CAS 104-40-5)	
Vapor pressure [Pa]	0.3 Pa at 25 °C	
Henry's law constant $[Pa\cdot m^3/mol]$	11.02 at 20 °C (calculated based on information available for CAS 84852-15-3)	ECHA (2012)
Water solubility [mg/L]	5.7 at 25 °C, pH 6 – 7 (CAS 84852-15-3) 7 at 25 °C, pH unknown (CAS 104-40-5)	
Dissociation constant (pK_a)	pK_a ca. 10 (value could be higher than this), at this pK_a value nonylphenol would be non-dissociated at environmental pHs	ECHA (2012)
Octanol-water partition coefficient (log K_{ow})[a]	[1] 5.4 at 23 °C, pH 5.7 (CAS 84852-15-3, HPLC) [2] 4.48 (CAS 84852-15-3, no information on method) [3] ~5 at 40 °C (CAS 84852-15-3, HPLC) [4] 5.76 (CAS 104-40-5, no information on method) [5] 5.14	[1] ECHA (2011b, 2012) [2] European Commission (2002b) [3] ECHA (2011b) [4] ECHA (2011a)

---

[2] Substance of Unknown or Variable composition, Complex reaction products or Biological materials

Characteristics	Values	References
	[6] 5.92 (CAS 84852-15-3, est.) [7] 5.99 (CAS 104-40-5, est.)	[5] geometric mean of 1-4, used for K_{oc} derivation [6] KOWWIN™ v1.68 [7] KOWWIN™ v1.68
Sediment-water adsorption coefficient (log K_{OC} or K_p)	[1] 3.73 (est.) [2] 4.58 (K_{oc} at 20 °C 38260; CAS 104-40-5, est.) [3] 4.04 (K_{oc} 11060; CAS 84852-15-3, exp.) [4] 4.35-5.69 (CAS 84852-15-3, exp., three soils) [5] 4.71 (CAS 84852-15-3, exp., sediment) [6] 3.97 (radiolabeled, branched 4-NP, soil) [7] 4.9 (radiolabeled, linear 4-NP, soil) [8] 4.59 (4-n-nonylphenol, K_{oc} 38900 sediment and groundwater from an aquifer in Bolivar, South Australia) [9] 4.89 (4-n-nonylphenol, K_{oc} 78035 in a loam soil associated with wastewater reuse) [10] 5.05 (4-nonylphenol [mixture of compounds with branched side chain], river water) [11] 4.7–5.6 (4-nonylphenol, sewage treatment plant) [12] 4.14 (est.)	[1] KRW Fact Sheet cited in Hansler et al. (2006) [2] ECHA (2011a) [3] Milinovic et al. (2015) cited in ECHA (2011b) [4] Roy et al. (1998) cited in European Commission (2002a) [5] Burgess et al. (2005) [6, 7] Düring et al. (2002) [8] Ying et al. (2003) [9] Ying & Kookana (2005) [10] Gong et al. (2012) [11] Sekela et al. (1999) [12] estimated using K_{oc} [5], see Appendix I
Sediment (or soil) adsorption coefficient (K_d [mL/g])	[1] 24 - 1059 (4-nonylphenol, five different soils)	[1] Milinovic et al. (2015), also cited in ECHA (2011b)
Adsorption coefficient for high molecular weight humic substances $\log_{KHMHS}$	4.57–5.09 (nonylphenol)	Yeh et al. (2014)
Aqueous hydrolysis DT_{50}	[1] 2.483 h at 25 °C (CAS 104-40-5, est.) [2] Hydrolysis testing for 4-nonylphenol is not scientifically necessary (CAS 84852-15-3)	[1] ECHA (2011a) [2] ECHA (2011b)
Aqueous photolysis DT_{50}	[1] 10-15 hours (continuous clear sky, noon, summer sunlight, surface layer of natural waters) [2] 2.3 h (4-n-nonylphenol, humic acids and Fe (III) as sensitizers)	Ahel et al. (1994a), also cited in ECHA (2011b) [2] Martínez-Zapata et al. (2013), also cited in ECHA (2011b)
Biodegradation in aqueous environment DT_{50} [d]	[1] 2.5 (freshwater, nonylphenol [mixture of monoalkyl phenols predominantly para-substituted], dissipation, 16°C) [2] ~ 56 (seawater, [4-nonylphenol	[1] Sundaram & Szeto (1981), also cited in ECHA (2012)

Characteristics	Values	References
	[mixture of different branched isomers], degradation, 11±2 °C)	[2] Ekelund et al. (1993), also cited in ECHA (2012)
Biodegradation in water-sediment systems DT_{50} [d]	[1] 28 (30 µg/L nominal water concentration, dissipation, 20±1.8 °C) [2] 104 (300 µg/L nominal water concentration, dissipation, 20±1.8 °C) [3] Nonylphenol, primary degradation, aerobic DegT50 = 13.6 – 99.0 days (30 °C) DegT50 = 40.8 days (20 °C) [4] Nonylphenol, primary degradation, anaerobic DegT50 = 46.2 – 69.3 days (30 °C) DegT50 = 99 days (20 °C) [5] 4-n-nonylphenol, anaerobic Degradation > 90% after 32 days [6] 4-n-nonylphenol, aerobic DegT50 > 154 days [7] Nonylphenol, anaerobic, original Sediment: dissipation 80-85% after 6 months Spiked Sediment (100 ppm nonylphenol): dissipation 50% after 6 months [8] Nonylphenol, aerobic, 25-30 % increase after 6 months [9] Nonylphenol technical mixture, anaerobic (methanogenic, sulphate reducing and nitrate reducing), 0 % dissipation within 703 days [10] 4-n-NP, anaerobic (nitrate reducing) 100 % dissipation after 91-104 days [11] 4-n-NP, anaerobic (methanogenic, sulphate reducing reducing), 0 % dissipation within 703 days [12] Nonylphenol dissipated from water to sediment (0 % nonylphenol in water after 10 days) Sediment: 80 % dissipation after 71 days [13] 4-n-Nonylphenol, aerobic (CAS 104-40-5), DisT50 = 5.8 days [14] 4-n-Nonylphenol, methanogenic, DisT50 > 70 days [15] 4-Nonylphenol (mixture of different branched isomers), aerobic/anaerobic, DegT50 > 56 days	[1, 2] Heinis et al. (1999) [3] Yuan et al. (2004) [4] Chang et al. (2004) [5,6] Bradley et al. (2008) [7, 8] Dutka et al. (1998) [9-11] De Weert et al. (2011) [12] European Commission (2002a); Sundaram & Szeto (1981) [13,14] Ying & Kookana (2003) [15] European Commission (2002a); Ekelund et al. (1993)

Characteristics	Values	References
Biodegradation in soil DT_{50} [d]	[1] 4.5 – 16.7 (soil, degradation, 30 °C) [2] 31 – 51 (soil & sludge, dissipation, 20/16 ± 1°C in a 16:8 h cycle)	[1] Topp & Starratt (2000), also cited in ECHA (2012) [2] Dettenmaier & Doucette (2007), also cited in ECHA (2012)

[a] data obtained from HPLC-based or unknown methods are in grey font and were not used for EQS derivation.

1.2 Regulatory context and environmental limits

Table 2 summarizes existing regulation and environmental limits in Switzerland, Europe and elsewhere for 4-nonylphenol.

Table 2 Existing regulation and environmental limits for 4-nonylphenol in Switzerland, Europe and elsewhere.

Europe	
Directive 2003/53/EC on the 26th amendment of Directive 76/769/EEC	Decision to restrict marketing and use of “nonylphenol”
ANNEX XVII to REACH	Details on the manufacture, placing on the market and use of “nonylphenol”
Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000	Classified as a "priority hazardous substance"
Commission Regulation (EC) No 2268/95	“Nonylphenol” included in the second priority list identifying substances requiring Attention
Prior Informed Consent Regulation (PIC) Regulation (EU) 649/2012	Inclusion of “nonylphenol” in Annex I
EQS – Water Framework Directive (inland water)[3], 31 October 2005	AA-EQS: 0.3 µg/L MAC-EQS: 2 µg/L $QS_{freshwater, sed}$: 180 µg/kg dry weight
Netherlands	Freshwater JG-MKN: 0.3 µg/L MAC-MKN: 2 µg/L
Germany	Watercourses and lakes, Transitional and coastal waters: AA-EQS: 0.3 µg/L MAC-EQS: 2 µg/L
Others	
Canadian Environmental Protection Act, 1999 (CEPA) Second Priority Substances List (PSL2)	Inclusion of “nonylphenol” in PSL2
Canadian Water Quality Guidelines for the Protection of Aquatic Life	Aquatic life guideline values, expressed on a TEQ basis using 4-nonylphenol toxic equivalency factors: Freshwater 1.0 µg/L (91-d LOEC of 10.3 µg/L (rainbow trout), safety factor of 0.1 (CCME 1991)

---

[3] EQS refers to CAS no 84852-15-3

	Marine 0.7 µg/L (interim guideline; 28-d LOEC of 6.7 µg/L (mysid *A. bahia*), safety factor of 0.1 (CCME 1991))
U.S. EPA proposed significant new use rule (SNUR) under the Toxic Substances Control Act (TSCA)	For 13 nonylphenols and nonylphenol ethoxylates, EPA is proposing to designate any use as a "significant new use," and for 2 additional NPs, EPA is proposing that any use other than use as an intermediate or use as an epoxy cure catalyst would constitute a "significant new use." This would require notifying EPA at least 90 days before manufacturing (including import) or processing.
U.S. EPA Ambient Aquatic Life Water Quality Criteria Nonylphenol	Freshwater 28 µg/L (one-hour average once in 3 years) 6.6 µg/L (four-day average once in 3 years) Saltwater 7 µg/L (one-hour average once in 3 years) 1.7 µg/L (four-day average once in 3 years)
Switzerland	
EQS- Ecotox Centre (17.10.2016)	AA-EQS: 0.043 µg/L MAC-EQS: 3.8 µg/L
Chemical Risk Reduction Ordinance (ORRChem), Annex 1.8	Prohibitions on placing on the market of products containing "nonylphenol"
Water protection ordinance (WPO) (01.06.18)	Annex 22, Additional requirements for groundwater which is used for drinking water or is intended as such: 0.1 µg/L per individual substance.

According to the high partitioning, limit values have been also derived for sediments. Table 3 summarizes available sediment quality guidelines (SQGs), each of which have been derived with a different purpose and therefore a different methodology.

Limit values available from European countries range from 36 to 250 µg/kg d.w. when expressed for 1 % OC for inland and freshwater. The EC QS_{sed} was calculated based on the EqP method because no experimental data with sediment dwelling organisms was available when the substance data sheet was completed (EC 2005). INERIS (2003) also derived a QS_{sed} for CAS 25154-52-3 using the EqP method. RIVM published an indicative sediment MTR (RIVM 2019 (accessed)), however, only for CAS 104-40-5. The derivation method is not reported. The Danish EQS was likely derived according to the EC TGD and is the highest value among those reported in Europe.

An Interim sediment quality guideline (ISQG) is also available from the Canadian Council of Ministers of the Environment (Canadian Council of Ministers of the Environment (CCME) 2002) for CAS 84852153 based on the "Protocol for the Derivation of Canadian Sediment Quality Guidelines for the Protection of Aquatic Life" (Canadian Council of Ministers of the Environment (CCME) 1995). ISQGs are proposed if information for the derivation of the limit value is only available for one of the two recommended derivation approaches (either a modification of the National Status and Trends Program (modified NSTP) approach or the spiked-sediment toxicity test (SSTT) approach).

Table 3 Sediment quality guidelines reported in the literature.

SQG description	Value [µg/kg d.w.]	Development method	Reference
QS_{sed}	36 (1 % TOC) 180 (5 % TOC)	EC TGD, tentative values derived by EqP method	CAS 84852153 and 25154-52-3, EC (2005)
PNEC / QS_{sed}	39[a]	Derived by EqP method	CAS 25154-52-3, France, INERIS (2003)
ISQG marine ISQG freshwater	1000 (1 % TOC) 5000 (5 % TOC) 1400 (1 % TOC) 7000 (5 % TOC)	Based on Protocol for the Derivation of Canadian Sediment Quality Guidelines for the Protection of Aquatic Life	CAS 84852153, Environment Canada (2002)
MTR	106[a]	Method not reported	CAS 104-40-5, Netherlands, RIVM (2019 (accessed))
EQS Inland water EQS other surface waters	25000 × f_{oc} 2500 × f_{oc}	Method not reported	25154-52-3, Denmark, Leth-Petersen & Westengaard Guldagger (2017)

f_{oc} = mass fraction of organic carbon for the sediment. MTR = Maximaal Toelaatbaar Risiconiveau.

[a] Standard sediment OC not available. Most probably 5 to 10 % according to information for other substances.

1.3 Use and emissions

As summarized in the UN draft fact sheet on 4-nonylphenol (International Panel on Chemical Pollution (IPCP) 2017), 4-nonylphenol was first produced in 1940 followed by strong increase in production and use. Annual production levels (reported and estimated) were up to 154 200 t in the United States, 16 500 t in Japan in the year 2000, up to 16 000 t in China, and almost 73 500 t in the European Union in 1997. The use of 4-nonylphenol was restricted in the EU in 2005 (Directive 2003/53/EC on the 26th amendment of Directive 76/769/EEC), which is expected to have decreased production by 50 %. The latest application date for authorization for 4-nonylphenol ethoxylates is July 4, 2019. Use of these compounds must stop January 4, 2021 („sunset date“). As of 1.8.2006, Switzerland has restricted the use of 4-nonylphenol in the same way as implemented at EU level (Chemical Risk Reduction Ordinance (ORRChem), Annex 1.8). At the same time, 4-nonylphenol is produced in developing countries and economies in transition including China, India, and across South America with annual production estimated to be increasing at least partially. Nonylphenols are not produced naturally.

Direct release of 4-nonylphenol from production seems possible as reported in Canada (Canadian Council of Ministers of the Environment (CCME) 2002). Diffuse emission of 4-nonylphenol is expected during use of 4-nonylphenol-containing products. Elevated concentrations have been reported in closer proximity to urban or industrialized areas and storm water releases. The degradation of nonylphenol ethoxylates (especially from wastewater treatment plants), are a source of release of NPs into the environment, one study reporting 60 – 65 % of incoming nonylphenolic compounds entering a WWTP being released into the environment (European Commission 2002a). Further, nonylphenol is the major transformation product (80 %) of alkylphenol polyethoxylates (reviewed in Olaniyan et al. (2020)). Consequently, treated wastewaters and contaminated sludge applied to open lands are key sources of 4-nonylphenol.

1.4 Mode of action and relative sensitivity of taxonomic groups

As summarized in ECHA (2012), *in vitro* studies have demonstrated that 4-nonylphenol bind to estrogen receptors (ER) and can displace estradiol from the receptor. Results indicate that the ER-mediated pathway is activated. Thus, 4-nonylphenols has the potential to exert estrogen-like effects and disrupt endocrine homeostasis *in vivo*. Nevertheless, for test organisms for which only very few adverse outcome pathways have been reported, it may be difficult or impossible to identify the underlying mode of action. *In vitro* data show no significant difference between linear and branched isomers, thus all 4-nonylphenols are considered to exert estrogen mediated effects (ECHA 2012).

Due to its endocrine effects to fish, 4-nonylphenol (branched and linear) was included in the REACH Candidate List of substances of very high concern for Authorization in December 2012 (ECHA 2019). According to Article 57(f) REACH regulation (EC 2006), 4-nonylphenol needs to be classified as SVHC (Substances of Very High Concern).

Effects of 4-nonylphenol to other taxa are potentially also due to endocrine action. *In vitro* induction of vitellogenin expression in amphibian cell cultures exposed to 4-nonylphenol has been reported ((Kloas et al. 1999) also cited in ECHA (2012)). The *in vivo* relevance of these findings cannot be comprehensively evaluated as understanding of vertebrate steroid hormones and function in non-mammalians is scarce (as summarized in (ECHA 2012)). An example is estradiol and 17 α-ethinylestradiol having been shown to act on larval gonadal sex differentiation and sex -ratio of several frog and toad species (summarized in Kortenkamp et al. (2011)).

A specific effect to crustaceans might exist but has not been sufficiently documented (European Commission 2002a). There is only limited information available about endocrine disrupting effects of 4-nonylphenol on (aquatic) invertebrates. An example of effects to molluscs is the sensitivity of the mudsnail *Potamopyrgus antipodarum* to endocrine disruption by “4-n-nonylphenol” in a whole-sediment biotest (Duft et al. 2003). A clear dose-response relationship was not observed in this study; the LOEC for increase in unshelled embryos was 10 µg/kg d.w. of sediment. In general, due to the lack of knowledge on hormonal systems of most invertebrates biochemical endpoints are not available. ECHA thus concluded that “no specific mode of action can be ascertained and no conclusion can be drawn if a substance is an actual endocrine disruptor on invertebrate species alone” (ECHA 2012).

2 Environmental fate

2.1 Stability and degradation products

The EU risk assessment report concluded that abiotic degradation of 4-nonylphenol in water is expected to be negligible (European Commission 2002b). The ECHA information on registered substances for 4-nonylphenol (CAS 84852-15-3) states that due to the same observation, **hydrolysis** testing for 4-nonylphenol is not scientifically necessary (ECHA 2011b). The hydrolysis half-life of p-nonylphenol (CAS 104-40-5) is estimated to be 2.483 h indicating that p-nonylphenol is moderately hydrolysable (ECHA 2011a).

Photostability of 4-nonylphenol (CAS 84852-15-3) and “4-n-nonylphenol” was studied e.g. in natural waters by exposing the solutions in filtered lake water (dissolved organic carbon = 4 mg/L) to sunlight, artificial water and reservoir water, or artificial water only (Ahel et al. (1994a), Martínez-Zapata et al. (2013), respectively, also cited in ECHA (2011b)). Photodegradation was judged as likely transformation route for 4-nonylphenol in water.

In general, 4-nonylphenol undergoes **biodegradation** in water, sediment and soil systems suggesting a categorization as inherently biodegradable for these systems (European Commission 2002b). 4-nonylphenol biodegradation is affected by the mixture of isomers with differing degrees of branching in the nonyl chain. In general, increased branching in alkyl chains reduces biodegradability resulting in linear 4-nonylphenol isomers probably degrading faster than branched isomers (ECHA 2011b).

A test for ready biodegradability of 4-nonylphenol (CAS No. 84852-15-3) is available (Gledhill et al., 1999 cited in (ECHA 2011b)). 4-nonylphenol did not meet criteria for ready biodegradability, but degradation (48 %) occurred (as measured by CO_2 evolution). Specific analyses of 4-nonylphenol in the water phase in a different study confirmed degradation (Staples et al., 2001 cited in ECHA (2011b)).

“P-nonylphenol” (CAS 104-40-5) was found to be 50 % degraded in 58 days in water (as measured by labeled CO_2 evolution; ECHA (2011a)). According to laboratory and field studies assessed for the registration of 4-nonylphenol (CAS No. 84852-15-3), 4-nonylphenol will biodegrade with half-lives ranging from 7 to 95 days (normalized for environmental temperature) in water, suggesting it is non-persistent under the majority of environmental conditions (ECHA 2011b). Mixing, adsorption, abiotic processes and the presence of particular algal and fungal species among others have been demonstrated to influence removal of 4-nonylphenol in water bodies.

Likewise, it is suggested that 4-nonylphenol is biodegradable in oxic sediments (marine and freshwater) and thus non-persistent (ECHA 2011b). 4-nonylphenol may biodegrade more slowly under low temperature and anoxic conditions. Under anoxic conditions, pre-exposure to 4-nonylphenol or nitrate reducing conditions may enhance the degradation of 4-nonylphenol. Overall, degradation in anoxic sediments was reported to be higher in nitrate reducing conditions, followed by sulfate-reducing and methanogenic conditions.

Dutka et al. (1998) reported that after heavily polluted harbour sediments had been additionally spiked with 4-nonylphenol, measured 4-nonylphenol concentrations increased under anaerobic conditions over six months. The formation of nonylphenol through biodegradation of e.g. nonylphenol ethoxylates may have contributed to the maintenance of increased nonylphenol levels under anaerobic conditions. Further, 4-nonylphenol concentrations were found to be heterogeneous throughout the sediment samples despite sediment homogenization. The authors concluded that processes other than biodegradation impact the availability of 4-nonylphenol to detection.

In soils, 4-nonylphenol has been reported to be biodegradable and would be rapidly dissipated in well-aerated soils following application of sewage sludge. Reported half-lives for 4-nonylphenol degradation in soil were between 4.5 and 51 d (ECHA 2011b). 4-nonylphenol degradation in soils is dependent on soil temperature and soil moisture conditions as well as on oxygen conditions (Topp et al. (2000) cited in ECHA (2011b)).

Irrespective of the compartment tested, studies on the biodegradation of 4-nonylphenol show a wide variation in test results. The reasons for this include possible toxicity of 4-nonylphenol to microorganisms, adaptation of the microorganisms to 4-nonylphenol and varying 4-nonylphenol isomer composition. The half-life of 4-nonylphenol in the environment could be different than the estimated values depending on local conditions (European Commission 2002b). Tests with differentially labelled [^{14}C]nonylphenol demonstrate that both, the alkyl chain and the aromatic ring are biodegraded (ECHA 2011b).

Degradation pathways of 4-nonylphenol (linear and branched) and thus degradation products depend on the branching, the length, and the position on the ring of the alkyl chain, and on the microorganisms present (reviewed by Corvini et al. (2006)). Linear 4-nonlyphenol is often used as model compound but is not best suited for metabolic studies as most of the degradation pathways reported proceed via the oxidation of the linear alkyl chain and are not compatible with the quaternary α-carbon structure of branched 4-nonylphenols. An efficient removal of branched 4-nonylphenol could be expected upon the cooperation of bacteria and fungi based on the combination of decomposition of the aromatic ring and the attack the nonyl chain.

When branched 4-nonylphenol was applied in a bioreactor inoculated with culture enrichments (*Pseudomonas spp*. and a *Stenotrophomonas sp*.) from 4-nonylphenol-contaminated soil, carboxylic acids, branched alkanes, and short-chain alkylphenols (three and four carbons) were detected in the effluent (Soares et al. 2003). In *Sphingomonadaceae* (a family of alphaproteobacteria that are characterized by sphingolipids in their outer cell wall), for example, branched 4-nonylphenols are degraded to nonanol congeners with high volatility and high degree of branching, making them dead-end products that are volatilized, and only the ring moiety of 4-nonylphenol is assimilated (reviewed by Corvini et al. (2006)).

Degradation products of 4-nonylphenol have not been discussed in the registration dossiers and EU risk assessment report (ECHA 2011a, 2011b, European Commission 2002a) and were not considered in the Ecotox Centre EQS Dossier for 4-nonylphenol in water (Ecotox Centre 2016).

Due to the dependency of degradation pathways relevant to sediment on local conditions and microorganisms present, this dossier will likewise not assess the potential toxicity of 4-nonylphenol degradation products.

2.2 Sorption/desorption processes

Experimental data and calculated partition coefficients suggest that 4-nonylphenol will be strongly absorbed to soils, sludges and sediments (European Commission 2002b). 4-nonylphenol adsorption is controlled by two major interactions: hydrophilic interaction with mineral components and hydrophobic interaction with organic matter (John et al. 2000). Adsorption of 4-nonylphenol to sediments contributes markedly to the loss of 4-nonylphenol from the water column (Toyama et al. (2011) cited in ECHA (2011b)).

The key study in the ECHA information on registered substances for CAS 84852-15-3 by Milinovic et al. (2015, assessed as highly reliable) using five field-collected soils reported that K_d (Log K_d) for 4-nonylphenol at 20 °C ranged from 24 to 1059 mL/g (1.4 to 3.0) and a K_{oc} value of 11060 (type of mean not reported; Log K_{oc} 4.04). A strong relationship between the soil organic carbon and adsorption was suggested. Desorption experiments showed 4-nonylphenol sorption was irreversible, i.e. desorption rates were < 5 % (ECHA 2011b, Milinovic et al. 2015).

Düring et al. (2002) investigated sorption and desorption behavior of 4-nonyl[^{14}C]phenol in 51 soils using the batch equilibrium approach. Linear 4-nonylphenol behaves differently from the branched isomers of 4-nonylphenol. Branching of the isomers of 4-nonylphenol probably hinders diffusion within aggregates and organic matter and limits specific interaction with the soil matrix. This will result in lower partition coefficients of branched isomers when compared to those of linear 4-nonylphenol. Overall, K_P (sorption partition coefficient) values correlated with organic carbon content of the soils yielding a Log K_{OC} of 3.97.

Yeh et al. (2014) tested the specific sorption of 4-nonylphenol to humic substances (HS) extracted from sediment and separated into high molecular weight HS (HMHS, 0.45 µm-1 kDa) and low molecular weight HS (LMHS < 1 kDa). HMHS had a higher humification degree than LMHS. No absorption to LMHS was detected, while a Log K_{HMHS} of 4.57–5.09 for HMHS was determined.

2.3 Bioavailability

Bioavailability is a complex process which depends on many factors including the sorption capacity of the sediment considered (e.g. OC content), the hydrophobicity of the compound, and the physiology, feeding behavior and burrowing activity of the benthic organism considered (Warren et al. 2003).

The scientific opinion of the EFSA on the effect assessment for pesticides on sediment organisms recognizes that "*the most appropriate metric for bioavailability in soils and sediments appears to be the 'freely dissolved pore water concentration' rather than the total sediment concentration, particularly for compounds with a log $K_{OW} < 5$*" (EFSA 2015).

The adsorption of a specific 4-nonylphenol isomer (4(3′,5′-dimethyl-3′-heptyl)-phenol, p353NP) to commercial humic acid and extracted fulvic acids (from peat) and resulting bioavailability to a "nonylphenol" degrading *Sphingomonas* strain was tested (Vinken et al. 2004). In equilibrium dialysis, p353NP-humic acid associates were formed in high amounts, whereas no adducts with fulvic acids occurred. No effects of dissolved humic substances on the bioavailability of p353NP for biodegradation by *Sphingomonas* were observed. The authors conclude that the association between "nonylphenol" and humic acids occurs rapidly and is reversible.

To investigate the influence of organic matter on the availability of "nonylphenol" ("a mixture of various isomers") for uptake by tomato seedlings, earthworm casts were added to soil under laboratory microcosm conditions (Jiang et al. 2018). The application of earthworm casts increased the sorption capacity of soils for "nonylphenol" and in turn decreased the desorption from soil. The uptake and translocation of "nonylphenol" in tomato seedlings was reduced and thus growth was promoted during the first 3 weeks.

Likewise, bioavailability of "p-nonylphenol" (CAS 84852–15–3) from sediment to a mysid (*Americamysis bahia*) and an amphipod (*Ampelisca abdita*) has been reported to depend on organic carbon concentration and the type of organic carbon present (Burgess et al. 2005). Cellulose (42 % OC), chitin (42 % OC), lignin (65 % OC), humic acid (31 % OC, extracted from several uncontaminated sediments from the temperate estuary Narragansett Bay (RI, USA), insoluble in seawater at pH less than 8.5), and uncontaminated sediment from North Jamestown, USA (1.6 % OC) were used as organic carbon source. In all cases, the dose-response curve for the amphipod *A. abdita* was deflected to the right, reflecting a decrease in toxicity. Hydrophobicity of the organic carbon material increased the effect: in the presence of lignin, humic acid, and sediment, LC_{50} values increased by factors greater than two to six, while in the presence of cellulose, an increase of approximately two, chitin by less than a factor of two was observed. The presence of organic carbon did not lower toxicity to mysids as effectively, potentially due to the greater sensitivity of *A. bahia* (about three fold in this study) to nonylphenol. Thus, the organic carbon concentration was sufficient to substantially reduce bioavailability to *A. abdita* but not to *A. bahia*.

Overall, bioavailability in soil and sediment is influenced by OC content and type, but is expected to be likewise influenced by mineral components due to the physico-chemical properties of 4-nonylphenol (see section 1.6).

2.4 Bioaccumulation and biomagnification

The EU risk assessment report on 4-nonylphenol states that "Experimental data indicate that nonylphenol bioconcentrates to a significant extent in aquatic species." (European Commission 2002a). It does not classify as PBT/vPvB substance (persistent, bioaccumulative and toxic/very persistent, very bioaccumulative; PBT Working Group (2008)).

In the frame of the risk assessment of 4-nonylphenol for REACH registration, the BCF (bioconcentration factor) of 896 (lipid normalized based on lipid concentrations provided in the same study) determined by Ekelund et al. (1990, cited in ECHA (2011b)) in the fish *Gasterosteus aculeatus* was used. A second test yielded a BCF of 833. Values are based on whole body tissue wet weight measurements.

The risk assessment of 4-nonylphenol for REACH registration lists a BCF for earthworms calculated based on Log K_{ow} data as there is no experimental data available. The reported Log K_{ow} of 5.4 results in a calculated BCF of 3015 (ECHA 2011b), exceeding the threshold for characterization as "bioaccumulative" (≥2000, EC (2006).

Ademollo et al. (2017) analyzed the accumulation of 4-nonylphenol by clams (*Ruditapes philippinarum*) from contaminated sediments. The BSAFs (biota-sediment accumulation factors) calculated based on 4-nonylphenol concentrations in clams and sediments, lipid fraction of clams and OC content of sediments ranged from 5.78 to 0.39 (calculated by assessor based on the following values: site Poveglia/April, clam NP 181 ± 63.8 µg/kg fresh weight, 0.86 % lipids, sediment NP 28 ± 12.6 µg/kg d.w., 1.3 % OC; site Marghera/June, clam NP 72 ± 53.1 µg/kg f.w., 0.96 % lipids, sediment NP 225 ± 63.7 µg/kg d.w., 0.84 % OC).

To derive 10-d BSAF of 4-nonylphenol in the marine gammarid *Ampelisca abdita,* Fay et al. (2000) used reference sediment (central Long Island Sound, USA, reference site) equilibrated with 4-nonylphenol ("technical mix of isomers") in seawater for seven days. The resulting mean 10-d BSAF was 0.933 (standard deviation 0.451), with lipid-normalized body burdens being positively correlated with organic carbon-normalized sediment contaminant concentrations (r^2, 0.66–0.98), but not with sediment 4-nonylphenol concentrations. The estimated lethal body burden LR_{50} for NP was 1.1 mmol/g wet tissue (95 % confidence interval, 0.8–1.4).

BSAFs were also determined for *Lumbriculus variegatus* exposed to [^{14}C] labeled 4-nonylphenol in three different spiked freshwater lake sediments. Lipid-normalized and OC content-normalized BSAFs were 55.4 (standard error 1.2), 14.2 (standard error 1.2), and 34.8 (standard error 2.3) (Mäenpää & Kukkonen 2006). The authors noted that no clear steady state was achieved for 4-nonylphenol tissue residue after 264 h (11 d) exposure.

The reported BCFs (fish) are above the trigger for derivation of QS for the protection from secondary poisoning for top predators (BCF ≥100, EC (2018)). To account for protection of top predators, a QS_{water} based on EQS_{biota} has been derived by the Ecotox Centre with a value of 294 ng/L, which is above the AA-EQS of 43 ng/L.

Concerning the risk of benthic invertebrates to transfer toxic and bioaccumulative substances to higher trophic levels, the EFSA scientific opinion for sediment risk assessment proposes to perform spiked sediment bioaccumulation tests with benthic invertebrates for substances that show significant bioaccumulation in fish (BCF ≥ 2000) when the substance is (1) persistent in sediment (DT_{50} >120 d in water-sediment fate studies) and log K_{ow} >3; or (2) non-persistent in sediment, log K_{ow} >3 and >10 % of the substance found in the sediment in a water-sediment fate study (EFSA 2015). While the BCF for nonylphenol is above the EFSA threshold for some fish species (Lee et al. 2015), it does neither fulfil all criteria (1) with the log K_{ow} >3 but DT_{50} <120, nor can all criteria (2) be assessed, with nonylphenol being non-persistent at most environmental conditions (among others depending on sediment physico-chemical parameters), log K_{ow} >3 but no data of a true water-sediment fate study being available.

Thus, it is concluded that benthic invertebrates might contribute to the risk to higher organisms through trophic transfer depending on the physico-chemical properties of the respective sediment.

3 Analysis

3.1 Methods for analysis and quantification limit

Different methods to analyze 4-nonylphenol in sediment exist, each with different detection limits (Table 4). Detection limits of approx. 0.5 µg/kg d.w. are achieved by solid-phase extraction followed by liquid chromatography-tandem mass spectrometry (LC-MS/MS; Government of British Columbia 2017) and gas chromatography-mass spectrometry (de Voogt et al. 1997). Analytical capacities in routine analysis laboratories may reach LOQ of 5 µg/kg d.w. (Laberca) while analytical methods implemented at research laboratories may reach LOQ as low as 0.180 µg/kg d.w. by in-cell clean-up pressurized liquid extraction and gas chromatography-tandem mass spectrometry (PLE – GC-MS/MS; Pintado-Herrera et al. 2016).

Table 4 Methods for 4-nonylphenol analysis in sediments and corresponding limits of detection (LOD) and limits of quantification (LOQ) (µg/kg d.w.). n. a. means not reported.

LOD	LOQ	Analytical method	Reference
0.5	n. a.	SPE extraction – LC-MS/MS	Government of British Columbia (2017)
0.5	n. a.	GC-MS, quadrupole MSD system	de Voogt *et al.* (1997)
0.054	0.180	PLE – GC-MS/MS[a]	Pintado-Herrera et al. 2016
n.a.	5[b]	GC-MS/MS	Laberca, laboratoire d'étude des résidus et contaminants dans les aliments

[a] 4-nonylphenol isomers, pressurized liquid extraction and gas chromatography – tandem mass spectrometry determination.

[b] LOQ derived at 5 for nonylphenols (4-nonylphenol) and also at 5 for 4-n-nonylphenol.

3.2 Environmental concentrations

Measured environmental concentrations (MEC) in sediments for Switzerland are available for sediments and suspended matter in small streams from monitoring campaigns implemented in 2017 and 2018 (Table 5). The MEC_{sed} measured at 5 small streams between spring and autumn in 2017 ranged from < 0.054 µg/kg d.w. to 256.0 µg/kg d.w. in sediments and from < 0.054 to 580.3 µg/kg d.w. in suspended matter. The concentrations measured in August 2018 at 18 small streams ranged from < 5 to 106.6 µg/kg d.w. for nonylphenols (4-nonylphenol), being < 5 µg/kg d.w. for 4-n-nonylphenol linear. Concentrations found at the Glatt River in the 80s as reported by Ahel et al. (1994b) ranged from 510 to 13100 µg/kg d.w.

The same range of concentrations are reported in neighboring countries, with maximum concentrations of 110 µg/kg d.w. measured at the Schwechat River in Austria (Umweltbundesamt Östereich 2005) and 37300 µg/kg d.w. at the Luppel River in Germany (Müller et al. 2019). Overall, higher concentrations are measured close to wastewater treatment plants and in urbanized and industrialized areas whereas concentrations in marine and coastal sediments are lower compared to freshwater sediments.

Table 5 Measured environmental concentrations in sediments (MEC) of 4-nonylphenol in Switzerland and elsewhere. All concentrations expressed as µg/kg d.w.

Country	MEC (min-max)	No. of sites	Comments	Reference
Switzerland	<0.054 – 256.0 (sediments) <0.054 – 580.3 (suspended matter)	5	4-nonylphenol isomers, small streams sampled every five weeks in 2017, analysis of the < 2 mm sediment fraction	Ecotox Centre, unpublished data
Switzerland	<5 – 106.6 (nonylphenols - 4-nonylphenol) <5 (4-n-nonylphenol linear) (river sediments)	18	Nonylphenols (4-nonylphenol), small streams sampled once in August 2018, analysis of the < 2 mm sediment fraction	Ecotox Centre, unpublished data
Switzerland	510-13100 (river sediments)		"nonylphenol", River Glatt, sampled from 1983 to 1986	Ahel et al. (1994b) cited in European Commission (2002a)
Germany	Max 37300	5	"nonylphenol",River Luppel	Müller et al. (2019)
Austria	Max 110		"4-Nonylphenol techn.", River Schwechat	Umweltbundesamt Östereich (2005)
U.S.	<2.9 to 2960 (river sediments)	30	"nonylphenol", average 162 µg/kg, below detection limit at 6 sites	Naylor et al. (1992) cited in European Commission (2002a)
Canada	290-1280 (downstream pulp mill) 1290-41100 (downstream near STP) 0.29-6.73 (river sediments)		"4-nonylphenol" was acetylated, acetyl derivative was measured	Lee and Peart (1995) also cited in European Commission (2002a)
Canada	170-720 (river and lake sediments)	9	"4-nonylphenol", heavily industrialized sites from the Great Lakes and St. Lawrence River sites	Bennie et al. (1997)
Japan	500–13000 (river sediments)		"nonylphenol" (10 isomer peaks in GC-MS analysis), concentration in water was higher during summer	Isobe et al. (2001)
Korea	25.4–932 (river sediments)		"nonylphenol", occurrence was related with urbanized areas	Li et al. (2004)
China	3500–32400 (lake sediments)		"nonylphenol" (mixture of isomers), occurrence correlated with STW discharges	Wu et al. (2007)
Finland	180-890 (lake sediments 1 km downstream STP)		"nonylphenol", background concentration in the lake 0.43 µg/kg	Suoanttila, 1996 cited in European Commission (2002a)
Germany	10–153 (marina sediments) < 10–55 (marine sediments)		"nonylphenol" (technical mixture of isomers), transported several hundred km into the sea	Bester et al. (2001)

Country	MEC (min-max)	No. of sites	Comments	Reference
Spain	364-604 (coastal sediments)	2	"4-n-nonylphenol, nonylphenol", only branched isomers detected in sediment samples	Salgueiro-González et al. (2019)
Italy	5-42 (marine sediments)		"standard nonylphenol", Lagoon of Venice, mean 14 µg/kg	Marcomini et al. (1990) cited in European Commission (2002a)

4 Effect data (spiked sediment toxicity tests)

A non-filtered bibliographic search was performed for 4-nonylphenol in the US Ecotox Data Base (U.S. EPA 2016) which did not yield data on sediment organisms. Likewise, a search in the German Environmental Office database ETOX did not yield any relevant results. A key word search was performed on Scopus (nonylphenol + sediment + toxicity, no restriction regarding publication date) resulted in 101 publications, 23 of which were considered for review, only 6 were based on spiked sediment tests. Potentially unpublished data was searched for in registration dossiers, risk assessment dossiers and EQS dossiers (EC 2005, ECHA 2011a, 2011b, European Commission 2002a, INERIS 2003). The EU risk assessment report does not include studies on benthic organisms exposed via spiked sediment, only exposure via water phase is considered (European Commission 2002a).

Relevance ("C" score in the table below) and reliability ("R" score in the table below) of studies are evaluated according to the CRED-criteria (Moermond et al. 2016) adapted for sediments by Casado-Martinez et al. (2017).

According to the EU TGD (EC 2018) "*What is considered chronic or acute is very much dependent on 1) the species considered and 2) the studied endpoint and reported criterion*". According to EFSA, true chronic tests should cover a range of 28-65 d when half-life of a pesticide in sediment is >10 d (EFSA, 2015). Therefore, effect data from 10 d tests with *Hyalela azteca, Chironomus riparius, Leptocheirus plumulosus* and *Ampelisca abdita* were considered as acute effect data.

Previously, the only true long-term endpoints based on spiked sediment exposure have been reported by Bettinetti & Provini (2002) for *Chironomus riparius* and *Tubifex tubifex*. These endpoints are considered relevant without restrictions and reliable with restrictions after assessment against CRED-relevant information (see Table 5). This study was selected as key study in the ECHA information for registered substances for CAS 84852-15-3 (ECHA 2011b). Despite organic carbon content of sediments strongly influencing 4-nonylphenol sorption to sediment constituents, only organic matter content was quantified in this study. Normalization to organic carbon content is thus only possible through extrapolation (OM=1.7*OC).

The long-term study on the marine invertebrate *Leptocheirus plumulosus* by Zulkosky et al. (2002) indicates that this species may be more sensitive than *Chironomus riparius* and *Tubifex tubifex*, however, as the highest concentration tested did not induce a statistically significant effect, the resulting LOEC is unbounded and cannot be used for EQS derivation. In the REACH registration process for CAS 84852-15-3, this study was chosen as a supporting study due to lack of some information on experimental conditions (ECHA 2011b).

In a joined effort by the Italian National Research Council and Danish Environmental Protection Agency, three additional studies on *Lumbriculus variegatus* (number, biomass, reproduction, growth, mortality) *Chironomus riparius* (emergence) and *Hyalella azteca* (survival, growth, reproduction) were conducted (Kamper 2015, Seierø 2015, Valsecchi 2015). The reported endpoints are considered relevant without restrictions and reliable without/with restrictions (see Table 6). The resulting effect data are 1-2 orders of magnitude below previously published results for *Chironomus riparius* and *Tubifex tubifex.*

The 6 acute effect data considered reliable and relevant cannot be used directly to derive EQS_{sed} but they are retained as they can be used as supporting information for example when choosing the assessment factor (AF).

Table 6 Sediment effect data collection for 4-nonylphenol in µg/kg d.w. Data were evaluated for relevance and reliability according to the CRED criteria for sediments (Casado-Martinez et al. 2017) adapted based on Moermond et al. (2016). Data assessed as not relevant and not reliable is in grey font. Data used for QS development is underlined. Abbreviations: n. a. = not available.

Group	Species	Test compound	Exposure	Equilibration time	Endpoint	Test duration	Effect concentration	Value (µg /kg d.w.)	Sediment type	Normalized value (µg /kg d.w., 1 % OC)	Normalized value (µg /kg d.w., 5 % OC)	Chem. analytics	Notes	Validity	References
Acute toxicity data in freshwater															
Insecta	*Chironomus riparius*	4-nonylphenol CAS n.a.	static	20 h stirring, 72 h settling	Mortality	10 d	LC50	350000	Natural sediment, > 250 µm, 2.3 % OM[a]	259259	1296296	measured		R2, C1	Bettinetti et al. (2002)
Insecta	*Chironomus riparius*	4-nonylphenol CAS n.a.	static	20 h stirring, 72 h settling	Mortality	10 d	LC50	314000	Natural sediment, > 250 µm, 2.3 % OM[a]	232593	1162963	measured		R2, C1	Bettinetti et al. (2002)
Insecta	*Chironomus riparius*	4-nonylphenol CAS n.a.	static	20 h stirring, 72 h settling	Mortality	10 d	LC50	465000	Natural sediment, > 250 µm, 2.3 % OM[a]	344444	1722222	measured		R2, C1	Bettinetti et al. (2002)
Insecta	*Chironomus riparius*	4-nonylphenol CAS n.a.	static	20 h stirring, 72 h settling	Mortality	10 d	LC50	315000	Natural sediment, > 250 µm, 2.3 % OM[a]	233333	1166667	measured		R2, C1	Bettinetti et al. (2002)
					Mortality, geometric mean			371094							
Insecta	*Chironomus riparius*	4-nonylphenol CAS 84852-15-3	static	72 h at test conditions	Survival	10 d	LC50	25000	Artificial sediment (OECD), 1.6 % OC	15625	78125	measured	Effect concentrations based on measured start concentration	R3, C1	Seierø (2015)
Insecta	*Chironomus riparius*	4-nonylphenol CAS 84852-15-3	static	72 h at test conditions	Growth	10 d	EC50	> 29000	Artificial sediment (OECD), 1.6 % OC	> 18125	> 90625	measured	Effect concentrations based on measured start concentration	R3, C2	Seierø (2015)
Insecta	*Chironomus riparius*	Nonylphenol CAS n.a.			Mortality	14 d	MATC[a]	26100						R4, C4	Naylor (1995)
Insecta	*Chironomus riparius*	4-nonylphenol CAS n.a.	static		Survival	10 d			Natural sediment ("S2"), 24.3 % OC, 49 % < 20 µm, 5.6 % 20-37 µm, 9.7 % 37 - 63 µm, 11.1 % 63-125 µm, 12.1 % 125-200 µm, 10.1 % 200-400 µm, 2.5 % 400-2000 µm			measured	60 % survival at highest concentration tested, LC50 cannot be derived	R3, C2	Mäenpää & Kukkonen (2006)
Insecta	*Chironomus dilutus (formerly C. tentans)*	Nonylphenol CAS n.a.	n.a.	n.a.	Mortality	14 d	LC50	> 34200	26.4 % sand, 52 % silt, 21.6 % clay, 1.27 % OC	> 26929	> 134646	n.a	Report not available for assessment	R4, C4	England and Bussard (1993) cited in Environment Canada (2002)
Crustacea (Amphipoda)	*Hyalella azteca*	Nonylphenol CAS n.a.	static	7 d	Mortality	10 d	LC50	<535000	Natural sediment, 61 % sand, 39 % fines, OC 0.75 %	<304348	<1521739	measured		R2, C2	Phillips et al. (2009)

Group	Species	Test compound	Exposure	Equilibration time	Endpoint	Test duration	Effect concentration	Value (µg /kg d.w.)	Sediment type	Normalized value (µg /kg d.w., 1 % OC)	Normalized value (µg /kg d.w., 5 % OC)	Chem. analytics	Notes	Validity	References
Acute toxicity data in marine water															
Crustacea (Amphipoda)	*Leptocheirus plumulosus*	Technical nonylphenol CAS n.a.	static	7 d shaking	Survival	10 d	LC50*	94400*	Natural sediment (standard US EPA site CLIS) ^{a}			measured and nominal	*calculated by assessor	R2, C2	Zulkosky et al. (2002)
Crustacea (Amphipoda)	*Ampelisca abdita*	4-nonylphenol CAS n.a.	static	7 d shaking	Survival	10 d	100 % mortality	347000	Natural sediment (standard US EPA site CLIS) ^{a}			nominal	LR50 1.1 µmol/g wet tissue	R4, C2	Fay et al. (2000)
Chronic toxicity data in freshwater															
Insecta	*Chironomus riparius*	4-nonylphenol CAS n.a.	static	20 h stirring, 72 h settling	Emergence	28 d	EC10	258900	Natural sediment, > 250 µm, 2.3 % OM^a	191778	958889	measured		R2, C1	Bettinetti & Provini (2002)
Insecta	*Chironomus riparius*	4-nonylphenol CAS n.a.	static	20 h stirring, 72 h settling	Emergence	28 d	EC10	203000	Natural sediment, > 250 µm, 2.3 % OM^a	150370	751852	measured		R2, C1	Bettinetti & Provini (2002)
					Emergence, geometric mean			229253							
Insecta	*Chironomus riparius*	4-nonylphenol CAS 84852-15-3	static	72 h at test conditions	Emergence ratio	27 d	NOEC	9000	Artificial sediment (OECD), 1.6 % OC	5625	28125	measured	Effect concentrations based on measured start concentration; emergence of controls < 70 % (59 %)	R3, C1	Seierø (2015)
Insecta	*Chironomus riparius*	4-nonylphenol CAS 84852-15-3	static	72 h at test conditions	Developmental rate	27 d	NOEC	≥ 29000	Artificial sediment (OECD), 1.6 % OC	≥ 18125	≥ 90625	measured	Effect concentrations based on measured start concentration; emergence of controls < 70 % (59 %)	R3, C2	Seierø (2015)
Crustacea (Amphipoda)	*Hyalella azteca*	4-nonylphenol CAS 84852-15-3	renewal	72 h at test conditions	Survival	28 d	NOEC	11000	Artificial sediment (OECD), 2.1 % OC	5238	26190	measured	Effect concentrations based on measured start concentration	R2, C1	Kamper (2015)
Crustacea (Amphipoda)	*Hyalella azteca*	4-nonylphenol CAS 84852-15-3	renewal	72 h at test conditions	Survival	35 d	NOEC	11000	Artificial sediment (OECD), 2.1 % OC	5238	26190	measured	Effect concentrations based on measured start concentration	R2, C1	Kamper (2015)
Crustacea (Amphipoda)	*Hyalella azteca*	4-nonylphenol	renewal	72 h at test conditions	Survival	42 d	NOEC	11000	Artificial sediment (OECD), 2.1 % OC	5238	26190	measured	Effect concentrations	R2, C1	Kamper (2015)

Group	Species	Test compound	Exposure	Equilibration time	Endpoint	Test duration	Effect concentration	Value (µg /kg d.w.)	Sediment type	Normalized value (µg /kg d.w., 1 % OC)	Normalized value (µg /kg d.w., 5 % OC)	Chem. analytics	Notes	Validity	References
		CAS 84852-15-3											based on measured start concentration		
Crustacea (Amphipoda)	*Hyalella azteca*	4-nonylphenol CAS 84852-15-3	renewal	72 h at test conditions	Growth	42 d	NOEC	≥ 17000	Artificial sediment (OECD), 2.1 % OC	≥ 8095	≥ 40476	measured	Effect concentrations based on measured start concentration	R2, C2	Kamper (2015)
Crustacea (Amphipoda)	*Hyalella azteca*	4-nonylphenol CAS 84852-15-3	renewal	72 h at test conditions	Reproduction	42 d	NOEC	≥ 17000	Artificial sediment (OECD), 2.1 % OC	≥ 8095	≥ 40476	measured	Effect concentrations based on measured start concentration	R2, C2	Kamper (2015)
Oligochaeta	*Tubifex tubifex*	4-nonylphenol CAS n.a.	static	20 h stirring, 72 h settling	Cocoons	28 d	EC10	336700	Natural sediment, > 250 µm, 2.3 % OM^a	249407	1247037	measured		R2, C1	Bettinetti & Provini (2002)
Oligochaeta	*Tubifex tubifex*	4-nonylphenol CAS n.a.	static	20 h stirring, 72 h settling	Cocoons	28 d	EC10	382700	Natural sediment, > 250 µm, 2.3 % OM^a	283481	1417407	measured		R2, C1	Bettinetti & Provini (2002)
					Cocoons, geometric mean			358964							
Oligochaeta	*Tubifex tubifex*	4-nonylphenol CAS n.a.	static	20 h stirring, 72 h settling	Young worms	28 d	EC10	335000	Natural sediment, > 250 µm, 2.3 % OM^a	248148	1240741	measured		R2, C1	Bettinetti & Provini (2002)
Oligochaeta	*Tubifex tubifex*	4-nonylphenol CAS n.a.	static	20 h stirring, 72 h settling	Young worms	28 d	EC10	382800	Natural sediment, > 250 µm, 2.3 % OM^a	283481	1417407	measured		R2, C1	Bettinetti & Provini (2002)
					Young worms, geometric mean			358103							
Oligochaeta	*Lumbriculus variegatus*	4-nonylphenol CAS 84852-15-3	static	14 d at test conditions	Number of worms	28 d	EC10	5500	Artificial sediment (OECD), 2.1 (±0.06) % OC	2619	13095	measured	EC10 below lowest test concentration (measured: 17 µg/kg d.w.)	R1, C1	Valsecchi (2015)
Oligochaeta	*Lumbriculus variegatus*	4-nonylphenol CAS 84852-15-3	static	14 d at test conditions	Biomass	28 d	EC10	10000	Artificial sediment (OECD), 2.1 (±0.06) % OC	4762	23810	measured	EC10 below lowest test concentration (measured: 17 mg/kg d.w.)	R1, C1	Valsecchi (2015)
Oligochaeta	*Lumbriculus variegatus*	4-nonylphenol CAS 84852-15-3	static	14 d at test conditions	Reproduction	28 d	EC10	6900	Artificial sediment (OECD), 2.1 (±0.06) % OC	3286	16429	measured	EC10 below lowest test concentration (measured: 17 mg/kg d.w.)	R1, C1	Valsecchi (2015)

Group	Species	Test compound	Exposure	Equilibration time	Endpoint	Test duration	Effect concentration	Value (µg /kg d.w.)	Sediment type	Normalized value (µg /kg d.w., 1 % OC)	Normalized value (µg /kg d.w., 5 % OC)	Chem. analytics	Notes	Validity	References
Oligochaeta	*Lumbriculus variegatus*	4-nonylphenol CAS 84852-15-3	static	14 d at test conditions	Growth	28 d	EC10	10000	Artificial sediment (OECD), 2.1 (±0.06) % OC	4762	23810	measured	EC10 below lowest test concentration (measured: 17 mg/kg d.w.)	R1, C1	Valsecchi (2015)
Oligochaeta	*Lumbriculus variegatus*	4-nonylphenol CAS 84852-15-3	static	14 d at test conditions	Mortality	28 d	EC10	129000	Artificial sediment (OECD), 2.1 (±0.06) % OC	61429	307143	measured		R1, C1	Valsecchi (2015)
Polychaeta	*Capitella sp. I*	4-n-Nonylphenol CAS n.a.	Renewal (water, sed)	24 h shaking/rotating (dark), heated to 50°C, re-shaken 5 h	Mortality	78 d	n.a.*	> 174000	Natural sediment collected at Isefjord (Zealand, Denmark), sieved < 250 µm, 3.85 ± 0.11 % OC	> 45195	> 225974		*only 3 concentrations tested	R3, C3	Hansen et al. (1999)
Polychaeta	*Capitella sp. I*	4-n-Nonylphenol CAS n.a.	Renewal (water, sed)	24 h shaking/rotating (dark), heated to 50°C, re-shaken 5 h	Growth, growth rate	78 d	n.a.*	Significant effect at 174000	Natural sediment collected at Isefjord (Zealand, Denmark), sieved < 250 µm, 3.85 ± 0.11 % OC	Significant effect at 45195	Significant effect at 225974		*only 3 concentrations tested	R3, C3	Hansen et al. (1999)
Polychaeta	*Capitella sp. I*	4-n-Nonylphenol CAS n.a.	Renewal (water, sed)	24 h shaking/rotating (dark), heated to 50°C, re-shaken 5 h	Reproduction (number of eggs, time between broods)	78 d	n.a.*	Significant effect at 174000	Natural sediment collected at Isefjord (Zealand, Denmark), sieved < 250 µm, 3.85 ± 0.11 % OC	Significant effect at 45195	Significant effect at 225974		*only 3 concentrations tested	R3, C3	Hansen et al. (1999)
Amphibia	*Rana catesbiana*	Nonylphenol CAS n.a.	n.a.	n.a.	Mortality	30 d	50 % mortality	260000	99.4 % Sand, <0.7 % silt, <0.7 % clay, 0.05 % OC	5200000	26000000	n.a.	Report not available for assessment	n.a.	Ward and Boeri (1992) cited in Environment Canada (2002)
Chronic toxicity data in marine water															
Crustacea	*Leptocheirus plumulosus*	Nonylphenol CAS n.a.	static	7 d shaking	Survival	28 d	NOEC	≥61500	Natural sediment (Flax Pond), OC 2.6%	≥23654	≥118269	measured and nominal	no statistically significant effect at highest test concentration	R2, C2	Zulkosky et al. (2002)
Crustacea	*Leptocheirus plumulosus*	Nonylphenol CAS n.a.	static	7 d shaking	Mean young per female	28 d	NOEC	≥61500	Natural sediment (Flax Pond), OC 2.6%	≥23654	≥118269	measured and nominal	no statistically significant effect at highest test concentration	R2, C2	Zulkosky et al. (2002)

[a] OC content not reported.

4.1 Graphic representation of effect data

All available data for chronic and acute data listed in Table 6 have been plotted independently of their relevance and reliability before and after normalization to OC content of the sediment (Figures 1a and 1b). Data by Hansen et al. (1999) are not included as these cannot be used for dose-response-modelling.

Without OC-normalization, the only acute unbounded reliable and relevant LC_{50} derived for Crustacea (marine *Leptocheirus plumulosus* 94400 µg/kg d.w.) is lower than the LC_{50} (geometric mean) derived for Insecta (represented by *C. riparius* only, 215691 µg/kg d.w.), but within the range of values reported for Insecta. Likewise, the geometric mean of chronic EC_{10} of Crustacea (14055 µg/kg d.w.) is lower than that derived for Oligochaeta (47920 µg/kg d.w.) and Insecta (229253 µg/kg d.w.). Amphibia are only represented by one data point which cannot be assessed regarding reliability and relevance.

Where OC content was reported, normalization of data was performed (Figure 2b). A comparison for acute data cannot be performed due to lack of relevant and reliable OC-normalized data. The OC content normalized EC_{10} of Crustacea (geometric mean: 669298 µg/kg-OC d.w.) is lower than the EC_{10} (geometric mean: 944530 µg/kg-OC d.w.) of oligochaetes.

Irrespective of normalization, a substantially larger range of valid effect concentrations has been reported for crustaceans (5500 – 382800 µg/kg d.w.; *Leptocheirus plumulosus*, *Hyalela azteca,* chronic exposure) than for oligochaetes (11000 – 65100 µg/kg d.w., *T. tubifex, L. variegatus*, chronic exposure).

The ratio of relevant acute to chronic data for insects (*C. riparius*) is 0.7.

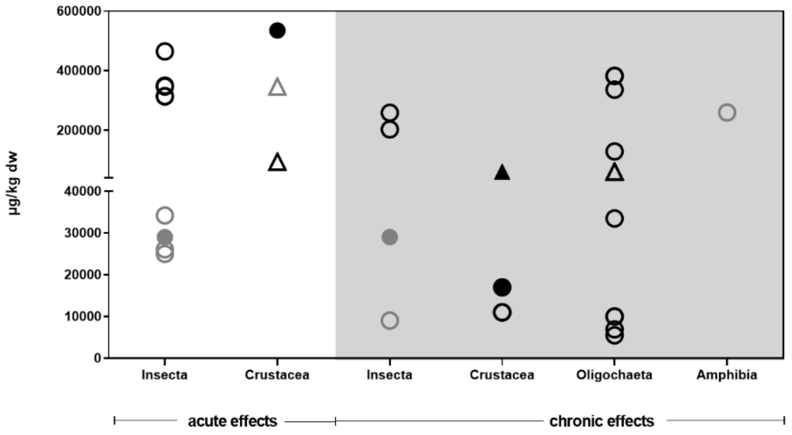


Figure 1a Graphical representation of acute and chronic single effect data from spiked sediment toxicity tests with 4-nonylphenol and nonylphenol as indicated in Table 5. Data are not normalized for OC. Geometric means are not displayed. Δ marine species, ○ freshwater species. Filled symbols: unbounded data. Grey symbols: Non-relevant/non-reliable data.

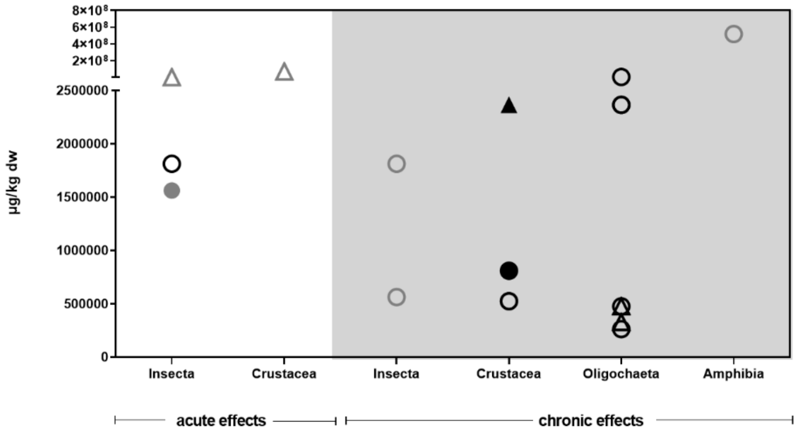


Figure 1b Graphical representation of acute and chronic single effect data from spiked sediment toxicity tests with 4-nonylphenol and nonylphenol as indicated in Table 5, normalized to OC content of the sediment used. Geometric means are not displayed. Δ marine species, ○ freshwater species. Filled symbols: unbounded data. Grey symbols: Non-relevant/non-reliable data.

4.2 Comparison between marine and freshwater species

Regarding effect concentrations for pelagic organisms, the Ecotox Centre aquatic EQS dossier reports that no statistically significant difference was found between marine and freshwater acute data, for chronic exposure, not enough data were available (Ecotox Centre 2016). In the EC EQS dossier it is stated that (no)-effect concentrations do not obviously differ from those obtained for freshwater, thus, the $QS_{saltwater}$ was derived from the same data set as the $QS_{freshwater}$ (EC 2005).

Regarding marine benthic organisms, only one relevant and reliable data point is available for acute effects, and two data points for chronic effects (Table 5, all studies performed on *Leptocheirus plumulosus*). Therefore, the number of effect data on benthic organism group is too scarce to perform a statistical test to evaluate if the sensitivity of marine vs. freshwater species is significantly different.

Consequently, marine and freshwater data were considered jointly for EQS_{sed} derivation.

4.3 Overview of reliable and relevant long-term studies

According to the EC EQS TGD (EC (2018) p. 25): "*All available data for any taxonomic group or species should be considered, provided the data meet quality requirements for relevance and reliability*". The chronic effect data for *Lumbriculus variegatus* (number, biomass, reproduction, growth, mortality) have been evaluated as R1/C1 and as R2/C1 for *Chironomus riparius* (emergence), *Hyalella azteca* (survival, growth, reproduction) and *Tubifex tubifex* (cocoons, young worms). In the following, the study on *Lumbriculus variegatus* (number, biomass, reproduction, growth, mortality) assessed as R1/C1 is summarized.

Valsecchi (2015): Sediment-water toxicity test on *Lumbriculus variegatus* using sediment spiked with 4- nonylphenol.

- Protocol: OECD Guideline for Testing of Chemicals No. 225 "Sediment-Water *Lumbriculus* Toxicity Test Using Spiked Sediment".
- Species: *Lumbriculus variegatus.*
- Origin: in house culture, originally obtained from Dr. Matti Leppänen, Department of Biology, University of Eastern Finland, Joensuu (FIN). Worms were synchronized 17 days before the test, and were adapted to test conditions 14 d before the test.

- Experimental sediment: artificial sediment according to OECD 225, containing 0.4-0.5 % of Urtica powder.
- Spiking and equilibration: 0.14 g nonylphenol was manually dissolved in 10 g (wet weight) of artificial sediment which was then homogenized with 90 g (wet weight) of artificial sediment yielding the stock sediment (1.4 mg/g wet weight, nominal). Stock sediment was mechanically homogenized by mixing overnight (at 300 rpm) and was then diluted in artificial sediment to obtain 7 final test concentrations. Each test sediment was mechanically mixed (300 rpm) for 1 hour and divided into the required number of replicates.
- Overlying water: reconstituted water according to OECD Guideline 225 (set to pH 7.6, total water hardness 275 mg/L as $CaCO_3$). Over time, pH ranged from 8.0 to 8.5, O_2 concentrations ranged from 64 to 95 %, temperature ranged from 20.0 to 20.4 °C, N-NH_4 concentrations ranged from 0.04 to 4.23 mg/L, and total hardness ranged from 289 to 432 mg/L as $CaCO_3$. The validation requirements for the OECD 225 test were met (pH of overlying water between 6 and 9 throughout the test; O_2 concentration in overlying water not below 30% of air saturation value at test temperature during the test).
- Bioassays: the 28 d toxicity test was performed following OECD Guideline for Testing of Chemicals No. 225 “Sediment-Water *Lumbriculus* Toxicity Test Using Spiked Sediment”. The test was performed in 250-mL glass bottles (inner diameter: 6 cm) with 55 mL sediment (75 g; 2 cm depth) and 220 mL water (8 cm depth). Ten individuals were tested per vessel with 3 replicates per treatment and control. Six control replicates are recommended in the guideline, but the minimum of 3 is considered sufficient. Separate vessels (control, the highest and lowest concentration) were prepared to verify test substance concentration in the sediment and partitioning of the tested chemical in the water-sediment system. Overlying water was not changed, evaporation compensated with deionized water if necessary. Overlying water was aerated with a Pasteur pipette (one bubble a second). Light/dark cycle was 16 h light, 8 h dark. Organisms were not additionally fed. All relevant water parameters were measured. Number of worms and ash free dry weight were reported after 28 d.
- Test endpoints: total number of worms, biomass, increase in number (reproduction), and increase in biomass (growth) after 28 d are considered relevant and reliable, the endpoint mortality was only presented based on estimates for interpreting the other effect concentrations and is not part of the OECD 225 test.
- Measured 4-nonylphenol concentrations: 4-nonylphenol concentrations were determined by liquid chromatography tandem mass spectrometry (UHPLC-MS/MS) coupled to a turbulent flow chromatography (TFC) for the on-line purification of the extracts. Test sediment samples (pore water, overlaying water and sediment) were collected after mixing at the start and at the end of the tests. In pore water and in overlaying water, concentrations were always below the limit of detection (0.25 mg/L). The 4-nonylphenol sediment concentration of the test control was always below 0.25 µg/g sediment dry weight. NP sediment concentrations after mixing ranged between 106 and 139 % of the nominal concentration. 4-Nonylphenol sediment concentrations during the test (Start and Day 28) ranged between 84 and 95 % of the mixing concentrations. All the measured concentrations were interpolated to calculate a linear regression relationship between nominal and measured concentrations.
- Statistics: effect concentrations (E(L)Cx) were determined by using the Toxicity Relationship Analysis Program (TRAP) Version 1.22 (US EPA 2013).
- Results: except mortality, effect concentrations (EC_{10}) are below the lowest tested concentration (measured: 17 mg/kg d.w.). An estimate of the dry weight of the worms at start of exposure was obtained as ash-free dry weight of 3 representative sub-samples (N=10) of the batch of synchronised worms used for the test (mean of 4.3 ± 0.2 mg d.w.).

5 Derivation of QS$_{sed}$

According to the EC TGD for EQS, sediment toxicity tests, aquatic toxicity tests in conjunction with equilibrium partitioning (EqP) and field/mesocosm studies are used as several lines of evidence to derive QS$_{sed}$ (EC 2018). Thus, in the following, the appropriateness of the deterministic approach (AF-Method), the probabilistic approach (SSD method) and the EqP approach were examined.

5.1 Derivation of QS$_{sed, AF}$ using the Assessment Factor (AF) method

The derivation of QS$_{sed, AF}$ is determined using assessment factors (AFs) applied to the lowest credible datum from long-term toxicity tests.

The lowest long-term effect datum available for nonylphenol is the EC$_{10}$ of 5500 µg/kg or 261905 µg/kg-OC (2.1 % OC, Table 7) for the number of individuals in *Lumbriculus variegatus*. The effect concentration is below the lowest measured test concentration (14000 µg/kg) but is deemed suitable for EQS derivation.

Table 7 Most sensitive relevant and reliable chronic data summarized from Table 6.

Species	**Exposure duration [d]**	**Endpoint**	**NOEC [µg/kg d.w.]**	**OC [%]**
Chironomus riparius	28 d	Emergence, geometric mean	229253	n.a. (2.3 % OM)
Hyalella azteca	42 d	Survival	11000	2.1
Tubifex tubifex	28 d	Young worms, geometric mean	358103	n.a. (2.3 % OM)
Lumbriculus variegatus	28 d	Number of worms	5500	2.1 (±0.06)

In case of long term tests (NOEC or EC$_{10}$) being available for three species representing different living and feeding conditions, the TGD recommends the application of an assessment factor of 10 on the lowest credible datum (Table 11 in EC (2018)). NOEC/EC$_{10}$ data are available for *Chironomus riparius*, *Hyalella azteca*, *Tubifex tubifex* and *Lumbriculus variegatus*, the suggested assessment factor would thus be 10. The critical datum used in QS$_{sed,AF}$ derivation is for the oligochaete *Lumbriculus variegatus.* No acute effect data on this group of organisms is available for comparison and thus for evaluation of the assessment factor.

Next to unspecific effects of 4-nonylphenol, it acts as endocrine disruptor in various species (see section 1.4). Endocrine disruption by 4-nonylphenol is best documented in fish, having triggered its listing as substance of very high concern for Authorization in December 2012 due to its endocrine effects to fish (ECHA 2019). There are indications that amphibians and potentially crustaceans are susceptible to endocrine disruption by 4-nonylphenol (see section 1.4). The chemically related endocrine disrupter octylphenol has been shown to act on mollusks (Duft et al. 2003, Jobling et al. 2003).

Here, the most sensitive datum (EC$_{10}$) considers the total number of individuals; the EC$_{10}$ for increase in number of worms accounts for reproductive effects and is less sensitive than the endpoint number of individuals (Table 6). Reliable and relevant chronic exposure data are not available for amphibians, which may be specifically susceptible to endocrine effects by 4-nonylphenol. For crustaceans, data for one species (*H. azteca*) is available, but with an unbounded NOEC for reproduction above the lowest critical datum used for EQS derivation.

The protection of species particularly sensitive to endocrine disruption by 4-nonylphenol is considered imperative (also discussed in section 9.1), thus, in view of the identified data gaps, the suggested assessment factor is thus 20:

$$QS_{sed,AF} = \frac{lowest\ EC10\ or\ NOEC}{AF}$$

$$QS_{sed,AF} = \frac{261905\left(\frac{\mu g}{kg - OC}\right)}{20} = 13095\ \left(\frac{\mu g}{kg - OC}\right)$$

The application of an AF of 20 to the lowest credible chronic datum results in a $QS_{sed,AF}$ = 13095 µg/kg-OC d.w., which corresponds to 655 µg/kg d.w. for a sediment with 5 % OC or 131 µg/kg d.w. for a sediment with 1 % OC representing a worst case scenario in Switzerland.

5.2 Derivation of $QS_{sed,SSD}$ using the species sensitivity distribution (SSD) method

The minimum data requirements recommended for the application of the SSD approach for EQS water derivation is preferably more than 15, but at least 10 NOECs/EC_{10}s, from different species covering at least eight taxonomic groups (EC (2018), p. 43). In this case, not enough data from spiked sediment toxicity tests are available for applying the SSD approach.

6 Derivation of $QS_{sed,EqP}$ using the Equilibrium Partitioning approach

If no reliable sediment toxicity data are available, the Equilibrium Partitioning (EqP) can be used to estimate the $EQS_{sed,EqP}$. This approach, developed for non-ionic substances, is used here for comparison purposes given the small data base of sediment toxicity studies.

6.1 Selection of QS for water

An Annual Average Quality Standard (AA-QS) has been proposed by the European Commission which sets a value of 0.3 µg/L for the protection of pelagic species based on the deterministic approach and "traditional toxicity" (not endocrine) effects (EC 2005).

In 2016, the Ecotox Centre revised the quality criteria according to the availability of new effect data collected in the scientific literature for the years 2011-2016 (Ecotox Centre 2016).

Here, the AA-EQS proposed by the Ecotox Centre (0.043 µg/L) in 2016 is used in the application of the EqP since it takes into consideration the most recent published data.

6.2 Selection of partition coefficient

One of the main factors influencing the application of the EqP model is the choice of the partition coefficient. It is stipulated in the ECHA 2017 guideline (p. 143, ECHA (2017)) that “To increase the reliability of PNEC sediment screen derived using the EqP, it is imperative that a conservative but realistic partitioning coefficient (e.g. K_d, K_{oc}, K_{ow}) is chosen. A clear justification must be given for the chosen coefficient and any uncertainty should be described in a transparent way.”

The EC EQS TGD requires deriving a geometric mean of all available K_{oc} values including one derived from a log K_{ow} value (EC 2018).

The key study in the REACH registration of CAS 84852-15-3 by Milinovic et al. (2015, assessed as highly reliable) using five field-collected soils reported a K_{oc} value of 11060 (log K_{oc} 4.04), with a strong relationship indicated between the soil organic carbon and adsorption. Further K_{oc} values were collected from the literature (Table 1). The geometric mean of these as well as of one K_{oc} derived from the geometric mean of available K_{ow} 5.14 (list of K_{oc} is provided in Appendix I) of 62268 was used as basis for $QS_{sed,EqP}$ derivation (6.4, Table 8).

6.3 Selection of OC content for a reference sediment

To account for the influence of OC content on $QS_{sed,EqP}$ development, calculations have been performed for a standard sediment according to the EU TGD with 5 % OC (EC 2018). As 5 % OC might not be representative for sediment in Switzerland, calculation was made as well for a worst-case scenario considering measurement on total sediment with 1 % OC (approx. 10th percentile of OC content in Swiss Rivers).

6.4 Derivation of $QS_{sed,EqP}$

For the derivation of $QS_{sed,EqP}$, the partition coefficient between water and sediment has been estimated as the fraction of organic carbon multiplied by organic carbon partition coefficient ($Kp=f_{OC}*K_{OC}$) as proposed by Di Toro et al. (1991) for non-ionic organic chemicals. The authors considered that, for sediment with an organic fraction higher than 0.2 %, organic carbon is the main driver for chemical sorption.

The derived $QS_{sed,EqP}$ ranges between 26.9 µg/kg for the worst case scenario (sediment with 1 % OC) to 134 µg/kg for the standard sediment in the TGD (with 5 % OC).

An additional AF of 10 should be applied to the resulting $QS_{sed,EqP}$ for substances with log K_{ow} >5. Reported log K_{ow} for 4-nonylphenol and isomeric mixtures range from 4.48-5.76, with a geometric mean of 5.14 (Table 1). The additional AF of 10 is therefore warranted (Table 8).

Table 8 Derived $QS_{sed,EqP}$ for a geometric mean of K_{OC} reported for 4-nonylphenol (Appendix I) and the AA-EQS for water derived by the Ecotox Centre of 0.043 µg/L (Ecotox Centre 2016). The partition coefficient solid-water sediment (Kp_{sed}) is estimated for a sediment with 5 % OC (standard EC TGD sediment) and 1 % TOC (worst case scenario in Switzerland).

	K_{oc} [l/kg]	**Kp_{sed} [l/kg]**	**$K_{sed-water}$ [m^3/m^3]**	**$QS_{sed,EqP}$ [µg/kg w. w.]**	**$QS_{sed,EqP}$ [µg/kg d. w.]**	**Included AF**
1 % OC	62268	622.7	622.7	10.3	**2.7**	10
5 % OC	62268	3113.4	1557.5	51.5	**13.4**	10

7 Derivation of QS_{sed} according to mesocosm/field data

Schmude et al. (1999) exposed benthic, freshwater macroinvertebrates in littoral enclosures to 4-nonylphenol (NP) and evaluated effects over 2-year period. The paper was published in a series of reports on the fate and effects of nonylphenol in an experimental littoral ecosystem (Liber et al. 1999). Nominal concentrations of 3, 30, 100, and 300 mg/L were applied 11 times every 48 h. Maximum nonlyphenol concentrations in sediments and pore water after application of 11x 300 mg/L were 27.4 mg/kg and 29.9 mg/L, respectively. Chironomidae, Oligochaeta, and Mollusca decreased in abundance after application of the highest concentration, with Mollusca staying reduced of throughout most of the study, while oligochaete (Naididae, Tubificidae) and chironomid (Tanytarsini, Chironomini) populations recovered within 6 weeks. The authors concluded that the observed effects on the benthic community were most likely due to exposure from the water, potentially also by more persistent macrophyte-associated residues having contributed to effects on Gastropoda, Naididae, and Tanytarsini. The NOECs for the benthic community ranged from 23 ± 11 (Naididae, Bivalvia) to 243 ± 41 mg/L (Tubificidae, Chironomini) nonylphenol in relation to water concentration. NOECs based on sediment concentrations were not provided. The peak sediment concentrations corresponding to the listed NOECs were 2.7 mg/kg d.w. and 27.4 mg/kg d.w.

As sediment exposure was not tested in the above study, the peak sediment concentrations corresponding to the derived NOECs for aquatic exposure may only be used as supportive information, not for EQS derivation.

Höss et al. (2004) presented a freshwater microcosm study to assess the effect of 4-nonylphenol on nematode communities in the sediment (natural lake sediment, littoral of the oligomesotrophic Lake Ammersee, Germany; fine grained sediment, 0.7 % OC). Seven different NP treatments were dosed over six weeks (controlled-release) resulting in maximum sediment concentrations of 0.29–3.37 mg/kg d.w.), four control microcosms were not exposed to nonylphenol. Within the 15-weeks analysis period, total nematode abundance and species diversity were not affected in any of the NP-treated microcosms (highest dosed treatment resulted in NP concentrations in sediment of 3.4 mg/kg d.w., or 485.7 mg/kg-OC; and in overlying water of 120 mg/L). However, the composition of nematode communities was changed. In particular, species and feeding types composition, as well as the maturity index, were affected in the post-application period, with species composition being altered most clearly. In the highest dosed treatment, deposit-feeding species, classified as colonizers (Eumonhystera), increased in dominance, whereas epistrate feeders and chewers (Prodesmodora and Tobrilus) decreased in relative abundance compared to the control.

Based on the available data, a NOEC cannot be derived. However, the highest dosed NP concentration is in the same order of magnitude as EC_{10} reported for single species exposures (Table 6). However, the highest dosed NP concentration may only be used as supportive information, not for EQS derivation.

8 Toxicity of degradation products

The EU risk assessment report on 4-nonylphenol (EU 2002) and the ECHA support document for the identification of 4-nonylphenol (ECHA 2012) do not cover the potential toxic effects of degradation products.

As detailed in section 2.1, suggested degradation pathways are heterogeneous, depending on the microorganism tested and test conditions, including the type of 4-nonylphenol isomers. The degradation products of 4-nonylphenol have not been unambiguously identified.

Against this background, a risk assessment for sediment is not conducted.

9 Proposed EQS_{sed}

The different QS values for each derivation method included in the EC EQS TGD 2018 are summarized in Table 9. According to the TGD, the most reliable extrapolation method for each substance should be used (EC 2018). In all cases, data from spiked sediment toxicity tests are preferred over the EqP approach.

An EQS_{sed} of 131 µg/kg d.w. (1 % OC) for 4-nonylphenol including the application of an AF of 20 is suggested.

The proposed EQS_{sed} is several orders of magnitude above reported limits of detection and quantification for 4-nonylphenol. Therefore the implementation of the derived EQS_{sed} should not be limited by methodological issues.

Table 9 QS_{sed} derived according to the three methodologies stipulated in the EU-TGD and their corresponding AF. All concentrations expressed as µg/kg d.w.

	Sediment 1 % TOC	**Sediment 5 % TOC**	**AF**
$QS_{sed,SSD}$	--		
$QS_{sed,EqP}$	2.7	13.4	10
$QS_{sed,AF}$	131	655	20
Proposed EQS_{sed}	**131**	655	20

9.1 Uncertainty analysis

According to the TGD, an AF of 10 is foreseen for $EQS_{sed,AF}$ in case of long term tests (NOEC or EC10) being available for three species representing different living and feeding conditions. As discussed in section 5.1, data gaps have been identified with respect to groups of organisms potentially susceptible to endocrine disruption by 4-nonylphenol, in particular amphibian species. Further, no suitable field or mesocosm data are available to evaluate the assessment factor although those retained as supportive information may indicate that the EQS_{sed} should be protective for additional invertebrate groups not included in the available effect database. An AF of 20 is thus suggested.

It should be noted that the most sensitive chronic datum available for EQS_{AF} derivation is below the lowest measured 4-nonylphenol concentration in the respective study (Valsecchi 2015).

The $QS_{sed,EqP}$ is ~50x lower than the proposed $EQS_{sed.}$ The proposed EQS_{sed} is based on effects in oligochaetes, the EQS for surface waters used for the derivation of the $QS_{sed,EqP}$ is based on effects in a green microalgae. The underlying mechanism of action is potentially different in these groups of organisms. Additional effect data to potentially sensitive groups of sediment organisms is recommended.

10 References

Ademollo, N., Patrolecco, L., Matozzo, V., Marin, M.G., Valsecchi, S. and Polesello, S. (2017) Clam bioaccumulation of alkylphenols and polycyclic aromatic hydrocarbons in the Venice lagoon under different pressures. Marine Pollution Bulletin 124(1), 121-129.

Ahel, M., Scully, F.E., Hoigné, J. and Giger, W. (1994a) Photochemical degradation of nonylphenol and nonylphenol polyethoxylates in natural waters. Chemosphere 28(7), 1361-1368.

Ahel, M., Giger, W. and Schaffner, C. (1994b) Behaviour of alkylphenol polyethoxylate surfactants in the aquatic environment—II. Occurrence and transformation in rivers. Water Research 28(5), 1143-1152.

Bennie, D.T., Sullivan, C.A., Lee, H.B., Peart, T.E. and Maguire, R.J. (1997) Occurrence of alkylphenols and alkylphenol mono- and diethoxylates in natural waters of the Laurentian Great Lakes basin and the upper St. Lawrence River. Science of The Total Environment 193(3), 263-275.

Bester, K., Theobald, N. and Schröder, H.F. (2001) Nonylphenols, nonylphenol-ethoxylates, linear alkylbenzenesulfonates (LAS) and bis (4-chlorophenyl)-sulfone in the German Bight of the North Sea. Chemosphere 45(6), 817-826.

Bettinetti, R., Cuccato, D., Galassi, S. and Provini, A. (2002) Toxicity of 4-nonylphenol in spiked sediment to three populations of *Chironomus riparius*. Chemosphere 46(2), 201-207.

Bettinetti, R. and Provini, A. (2002) Toxicity of 4-Nonylphenol to *Tubifex tubifex* and *Chironomus riparius* in 28-Day Whole-Sediment Tests. Ecotoxicology and Environmental Safety 53(1), 113-121.

Bradley, P.M., Barber, L.B., Kolpin, D.W., McMahon, P.B. and Chapelle, F.H. (2008) Potential for 4-n-nonylphenol biodegradation in stream sediments. Environmental Toxicology and Chemistry 27(2), 260-265.

Burgess, R.M., Pelletier, M.C., Gundersen, J.L., Perron, M.M. and Ryba, S.A. (2005) Effects of different forms of organic carbon on the partitioning and bioavailability of nonylphenol. Environmental Toxicology and Chemistry 24(7), 1609-1617.

Canadian Council of Ministers of the Environment (CCME) (1995) Protocol for the Derivation of Canadian Sediment Quality Guidelines for the Protection of Aquatic Life.

Canadian Council of Ministers of the Environment (CCME) (2002) Sediment Quality Guidelines for the Protection of Aquatic Life: Nonylphenol CAS 84852153.

Casado-Martinez, M.C., Mendez-Fernandez, L., Wildi, M., Kase, R., Ferrari, B.J.D. and Werner, I. (2017) Incorporation of sediment specific aspects in the CRED evaluation system: recommendations for ecotoxicity data reporting. SETAC Europe 27th Annual Meeting, Brussels.

Chang, B.V., Yu, C.H. and Yuan, S.Y. (2004) Degradation of nonylphenol by anaerobic microorganisms from river sediment. Chemosphere 55(4), 493-500.

Corvini, P.F.X., Schäffer, A. and Schlosser, D. (2006) Microbial degradation of nonylphenol and other alkylphenols—our evolving view. Applied Microbiology and Biotechnology 72(2), 223-243.

de Voogt, P., de Beer, K. and van der Wielen, F. (1997) Determination of alkylphenol ethoxylates in industrial and environmental samples. TrAC Trends in Analytical Chemistry 16(10), 584-595.

Dettenmaier, E. and Doucette, W.J. (2007) Mineralization and plant uptake of 14C-labeled nonylphenol, nonylphenol tetraethoxylate, and nonylphenol nonylethoxylate in biosolids/soil systems planted with crested wheatgrass. Environmental Toxicology and Chemistry 26(2), 193-200.

De Weert, J.P.A., Viñas, M., Grotenhuis, T., Rijnaarts, H.H.M. and Langenhoff, A.A.M. (2011) Degradation of 4-n-nonylphenol under nitrate reducing conditions. Biodegradation 22(1), 175-187.

Di Toro, D.M., Zarba, C.S., Hansen, D.J., Berry, W.J., Swartz, R.C., Cowan, C.E., Pavlou, S.P., Allen, H.E., Thomas, N.A. and Paquin, P.R. (1991) Technical basis for establishing sediment quality criteria for nonionic organic chemicals using equilibrium partitioning. Environmental Toxicology and Chemistry 10(12), 1541-1583.

Duft, M., Schulte-Oehlmann, U., Weltje, L., Tillmann, M. and Oehlmann, J. (2003) Stimulated embryo production as a parameter of estrogenic exposure via sediments in the freshwater mudsnail Potamopyrgus antipodarum. Aquatic Toxicology 64(4), 437-449.

Düring, R.-A., Krahe, S. and Gäth, S. (2002) Sorption behavior of nonylphenol in terrestrial soils. Environmental Science & Technology 36(19), 4052-4057.

Dutka, B.J., Liu, D., Jurkovic, A., McInnis, R., Lee, H.B., Onuska, F. and Rao, S.S. (1998) Observations from a six month study on the effect of biodegradation processes in sediment on the toxicity potential of targeted chemicals. Environmental Toxicology and Water Quality 13(4), 313-322.

EC (2005) 4-Nonylphenol (branched) and Nonylphenol Environmentla Quality Standards (EQS) Substance Data Sheet. available at: http://circa.europa.eu/.

EC (2006) REGULATION (EC) No 1907/2006 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC.

EC (2018) Technical Guidance for Deriving Environmental Quality Standards Environment, Guidance Document No. 27, Updated version 2018, Document endorsed by EU Water Directors at their meeting in Sofia on 11-12 June 2018.

ECHA (2011a) Information on Registered Substances phenol, 4-nonyl-, linear, CAS 104-40-5 https://echa.europa.eu/registration-dossier/-/registered-dossier/17497/1 Last modified:29-Apr-2019.

ECHA (2011b) Information on Registered Substances phenol, 4-nonyl-, branched, CAS 84852-15-3 https://echa.europa.eu/registration-dossier/-/registered-dossier/15896/1 Last modified:29-Apr-2019.

ECHA (2012) Member state committee support document for identification of 4-nonylphenol, branched and linear as substances of very high concern because due to their endocrine disrupting properties they cause probable serious effects to the environment which give rise to an equivalent level of concern to those of CMRs and PBTs/vPvBs; Adopted on 13 December 2012. https://echa.europa.eu/documents/10162/3024c102-20c9-4973-8f4e-7fc1dd361e7d.

ECHA (2017) Guidance on Information Requirements and Chemical Safety Assessment; Chapter R.7b: Endpoint specific guidance.

ECHA (2019) Candidate List of substances of very high concern for Authorisation https://www.echa.europa.eu/candidate-list-table

Ecotox Centre (2016) EQS - Vorschlag des Oekotoxzentrums für: 4-Nonylphenol, verzweigt und linear (Dübendorf: Swiss Centre for Applied Ecotoxicology).

EFSA (2015) Scientific Opinion on the effect assessment for pesticides on sediment organisms in edge-of-field surface water (PPR Panel). EFSA Journal 13(7), 4176.

Ekelund, R., Granmo, Å., Magnusson, K., Berggren, M. and Bergman, Å. (1993) Biodegradation of 4-nonylphenol in seawater and sediment. Environmental Pollution 79(1), 59-61.

Environment Canada (2002) Canadian Evironmental Quality Guidelines for Nonylphenol and its Ethoxylates (Water, Sediement, and Soil), National Guidelines and Standards Office, Environmental Quality Branch, Environment Canada, Ottawa.

European Commission (2002a) European Union Risk Assessment Report 4-NONYLPHENOL (BRANCHED) AND NONYLPHENOL, CAS Nos: 84852-15-3 and 25154-52-3, EINECS Nos: 284-325-5 and 246-672-0, Institute for Health and Consumer Protection.

European Commission (2002b) European Union Summary Risk Assessment Report 4-NONYLPHENOL (BRANCHED) AND NONYLPHENOL, CAS Nos: 84852-15-3 and 25154-52-3, EINECS Nos: 284-325-5 and 246-672-0, Institute for Health and Consumer Protection.

Fay, A.A., Brownawell, B.J., Elskus, A.A. and McElroy, A.E. (2000) Critical body residues in the marine amphipod *Ampelisca abdita*: Sediment exposures with nonionic organic contaminants. Environmental Toxicology and Chemistry 19(4), 1028-1035.

Gong, J., Ran, Y., Chen, D., Yang, Y. and Zeng, E.Y. (2012) Association of endocrine-disrupting chemicals with total organic carbon in riverine water and suspended particulate matter from the Pearl River, China. Environmental Toxicology and Chemistry 31(11), 2456-2464.

Government of British Columbia (2017) Alkylphenol and ethoxylates in soils and sediments by LC-MS/MS.

Hansen, F.T., Forbes, V.E. and Forbes, T.L. (1999) Effects of 4-n-Nonylphenol on life-history traits and population dynamics of a polychaete. Ecological Applications 9(2), 482-495.

Hansler, R.J., Fleuren, R.H.L.J., Heugens, E.H.W., Janssen, P.J.C.M., Posthumus, R. and Smit, C.E. (2006) Indicatieve milieukwaliteitsnormen 2005-2006 - Overzicht van in 2005 en 2006 door het RIVM afgeleide indicatieve milieukwaliteitsnormen voor stoffen.

Heinis, L.J., Knuth, M.L., Liber, K., Sheedy, B.R., Tunell, R.L. and Ankley, G.T. (1999) Persistence and distribution of 4-nonylphenol following repeated application to littoral enclosures. Environmental Toxicology and Chemistry 18(3), 363-375.

Höss, S., Traunspurger, W., Everin, G.F.S., Jüttner, I., Pfister, G. and Schramm, K.-W. (2004) Influence of 4-nonylphenol on the structure of nematode communities in freshwater microcosms. Environmental Toxicology and Chemistry 23(5), 1268-1275.

INERIS (2003) Nonylphénol, CAS : 25154-52-3. Norme de qualité pour la communauté benthique. Mise a jour 2017. https://substances.ineris.fr/fr/substance/cas/25154-52-3/3

International Panel on Chemical Pollution (IPCP) (2017) [Factsheet] - Overview Report II: An Overview of Current Scientific Knowledge on the Life Cycles, Environmental Exposures, and Environmental Effects of Select Endocrine Disrupting Chemicals (EDCs) and Potential EDCs - Draft, United Nations Environment Programme.

Isobe, T., Nishiyama, H., Nakashima, A. and Takada, H. (2001) Distribution and behavior of nonylphenol, octylphenol, and nonylphenol monoethoxylate in Tokyo Metropolitan Area: their association with aquatic particles and sedimentary distributions. Environmental Science & Technology 35(6), 1041-1049.

Jiang, L., Yang, Y., Jia, L.X., Liu, Y., Pan, B. and Lin, Y. (2018) Effects of earthworm casts on sorption-desorption, degradation, and bioavailability of nonylphenol in soil. Environmental Science and Pollution Research 25(8), 7968-7977.

Jobling, S., Casey, D., Rodgers-Gray, T., Oehlmann, J., Schulte-Oehlmann, U., Pawlowski, S., Baunbeck, T., Turner, A.P. and Tyler, C.R. (2003) Comparative responses of molluscs and fish to environmental estrogens and an estrogenic effluent. Aquatic Toxicology 65(2), 205-220.

John, D.M., House, W.A. and White, G.F. (2000) Environmental fate of nonylphenol ethoxylates: Differential adsorption of homologs to components of river sediment. Environmental Toxicology and Chemistry 19(2), 293-300.

Kamper, A. (2015) Sediment-water toxicity test on Hyalella azteca using sediment spiked with branched 4-nonylphenol, Unpublished Report, Danish Environmental Protection Agency, Danish Ministry of Environment.

Kloas, W., Lutz, I. and Einspanier, R. (1999) Amphibians as a model to study endocrine disruptors: II. Estrogenic activity of environmental chemicals in vitro and in vivo. Science of The Total Environment 225(1), 59-68.

Kortenkamp, A., Martin, O., Faust, M., Evans, R., McKinlay, R., Orton, F. and Rosivatz, E. (2011) State of the art assessment of endocrine disruptors, European Commission.

Lee, C.-C., Jiang, L.-Y., Kuo, Y.-L., Chen, C.-Y., Hsieh, C.-Y., Hung, C.-F. and Tien, C.-J. (2015) Characteristics of nonylphenol and bisphenol A accumulation by fish and implications for ecological and human health. Science of The Total Environment 502, 417-425.

Leth-Petersen, M. and Westengaard Guldagger, S. (2017) Bekendtgørelse om fastlæggelse af miljømål for vandløb, søer, overgangsvande, kystvande og grundvand, NST-4200-00050, Miljø- og Fødevareministeriet, Denmark.

Li, D., Kim, M., Shim, W.J., Yim, U.H., Oh, J.-R. and Kwon, Y.-J. (2004) Seasonal flux of nonylphenol in Han River, Korea. Chemosphere 56(1), 1-6.

Liber, K., Knuth, M.L. and Stay, F.S. (1999) An integrated evaluation of the persistence and effects of 4-nonylphenol in an experimental littoral ecosystem. Environmental Toxicology and Chemistry 18(3), 357-362.

Mäenpää, K. and Kukkonen, J.V.K. (2006) Bioaccumulation and toxicity of 4-nonylphenol (4-NP) and 4-(2-dodecyl)-benzene sulfonate (LAS) in Lumbriculus variegatus (Oligochaeta) and Chironomus riparius (Insecta). Aquatic Toxicology 77(3), 329-338.

Marcomini, A., Pavoni, B., Sfriso, A. and Orio, A.A. (1990) Persistent metabolites of alkylphenol polyethoxylates in the marine environment. Marine Chemistry 29, 307-323.

Martínez-Zapata, M., Aristizábal, C. and Peñuela, G. (2013) Photodegradation of the endocrine-disrupting chemicals 4n-nonylphenol and triclosan by simulated solar UV irradiation in aqueous solutions with Fe(III) and in the absence/presence of humic acids. Journal of Photochemistry and Photobiology A: Chemistry 251, 41-49.

Milinovic, J., Lacorte, S., Rigol, A. and Vidal, M. (2015) Sorption behaviour of nonylphenol and nonylphenol monoethoxylate in soils. Chemosphere 138, 952-959.

Moermond, C.T.A., Kase, R., Korkaric, M. and Ågerstrand, M. (2016) CRED: Criteria for reporting and evaluating ecotoxicity data. Environmental Toxicology and Chemistry 35(5), 1297-1309.

Müller, A.-K., Leser, K., Kämpfer, D., Riegraf, C., Crawford, S.E., Smith, K., Vermeirssen, E.L.M., Buchinger, S. and Hollert, H. (2019) Bioavailability of estrogenic compounds from sediment in the context of flood events evaluated by passive sampling. Water Research 161, 540-548.

Naylor, C.G., Mieure, J.P., Adams, W.J., Weeks, J.A., Castaldi, F.J., Ogle, L.D. and Romano, R.R. (1992) Alkylphenol ethoxylates in the environment. Journal of the American Oil Chemists' Society 69(7), 695-703.

Naylor, C.G. (1995) Environmental Fate and Safety of Nonylphenol Ethoxylates. Surfactants and Wastewater.

Olaniyan, L.W.B., Okoh, O.O., Mkwetshana, N.T. and Okoh, A.I. (2020) Reviews of Environmental Contamination and Toxicology Volume 248. de Voogt, P. (ed), pp. 81-109, Springer International Publishing, Cham.

PBT Working Group (2008) Results of the evaluation of the PBT/vPvB properties of: Phenol, 4-nonyl-, branched (NP); Nonylphenol.

Phillips, B.M., Anderson, B.S., Hunt, J.W., Clark, S.L., Voorhees, J.P., Tjeerdema, R.S., Casteline, J. and Stewart, M. (2009) Evaluation of phase II toxicity identification evaluation methods for freshwater whole sediment and interstitial water. Chemosphere 2009 74(5), 648-53.

Pintado-Herrera, M.G., González-Mazo, E. and Lara-Martín, P.A. (2016) In-cell clean-up pressurized liquid extraction and gas chromatography–tandem mass spectrometry determination of hydrophobic persistent and emerging organic pollutants in coastal sediments. Journal of Chromatography A 1429, 107-118.

PubChem (2019a) 4-nonylphenol (branched) Canonical SMILES https://pubchem.ncbi.nlm.nih.gov/compound/338733

PubChem (2019b) 4-nonylphenol (linear) Canonical SMILES https://pubchem.ncbi.nlm.nih.gov/compound/1752

RIVM (2019 (accessed)) P-Nonylfenol, CAS 104-40-5. Index Stoffen. https://rvszoeksysteem.rivm.nl/stof/detail/1096

Roy, D., Colerangle, J.B. and Singh, K.P. (1998) Is exposure to environmental or industrial endocrine disrupting estrogen-like chemicals able to cause genomic instability? Frontiers in bioscience : a journal and virtual library 3, d913-921.

Salgueiro-González, N., Campillo, J.A., Viñas, L., Beiras, R., López-Mahía, P. and Muniategui-Lorenzo, S. (2019) Occurrence of selected endocrine disrupting compounds in Iberian coastal areas and assessment of the environmental risk. Environmental Pollution 249, 767-775.

Schmude, K.L., Liber, K., Corry, T.D. and Stay, F.S. (1999) Effects of 4-nonylphenol on benthic macroinvertebrates and insect emergence in littoral enclosures. Environmental Toxicology and Chemistry 18(3), 386-393.

Seierø, C. (2015) Sediment-water toxicity test on Chironomus riparius using sediment spiked with branched 4-nonylphenol, Unpublished Report, Danish Environmental Protection Agency, Danish Ministry of Environment.

Sekela, M., Brewer, R., Moyle, G. and Tuominen, T. (1999) Occurrence of an environmental estrogen (4-nonylphenol) in sewage treatment plant effluent and the aquatic receiving environment. Water Science and Technology 39(10), 217-220.

Soares, A., Guieysse, B., Delgado, O. and Mattiasson, B. (2003) Aerobic biodegradation of nonylphenol by cold-adapted bacteria. Biotechnology Letters 25(9), 731-738.

Strub, M.-P. (2010) N° CAS DU NONYLPHENOL ET DE L'OCTYLPHÉNOL, ONEMA – INERIS.

Sundaram, K.M.S. and Szeto, S. (1981) The dissipation of nonlyphenol in stream and pond water under simulated field conditions. Journal of Environmental Science and Health, Part B 16(6), 767-776.

Topp, E. and Starratt, A. (2000) Rapid mineralization of the endocrine-disrupting chemical 4-nonylphenol in soil. Environmental Toxicology and Chemistry 19(2), 313-318.

U.S. EPA (2016) AQUATIC TOXICITY INFORMATION RETRIEVAL (AQUIRE) DATABASE.

Umweltbundesamt Östereich (2005) Untersuchung von Donausedimenten und Schwebstoffen auf ausgewählte organische Stoffe.

Valsecchi, S. (2015) Sediment-water toxicity test on Lumbriculus variegatus using sediment spiked with 4-nonylphenol, Unpublished Report, Water Research Institute - Italian National Research Council (IRSA-CNR).

Vinken, R., Höllrigl-Rosta, A., Schmidt, B., Schäffer, A. and Corvini, P.F.X. (2004) Bioavailability of a nonylphenol isomer in dependence on the association to dissolved humic substances. Water Science abd Technology 50(5), 277-283.

Warren, N., Allan, I.J., Carter, J.E., House, W.A. and Parker, A. (2003) Pesticides and other micro-organic contaminants in freshwater sedimentary environments—a review. Applied Geochemistry 18(2), 159-194.

Wu, Z., Zhang, Z., Chen, S., He, F., Fu, G. and Liang, W. (2007) Nonylphenol and octylphenol in urban eutrophic lakes of the subtropical China. Fresenius Environmental Bulletin 16(3), 227-234.

Yeh, Y.-L., Yeh, K.-J., Hsu, L.-F., Yu, W.-C., Lee, M.-H. and Chen, T.-C. (2014) Use of fluorescence quenching method to measure sorption constants of phenolic xenoestrogens onto humic fractions from sediment. Journal of Hazardous Materials 277, 27-33.

Ying, G.-G., Kookana, R.S. and Dillon, P. (2003) Sorption and degradation of selected five endocrine disrupting chemicals in aquifer material. Water Research 37(15), 3785-3791.

Ying, G.-G. and Kookana, R.S. (2003) Degradation of five selected endocrine-disrupting chemicals in seawater and marine sediment. Environmental Science & Technology 37(7), 1256-1260.

Ying, G.-G. and Kookana, R.S. (2005) Sorption and degradation of estrogen-like-endocrine disrupting chemicals in soil. Environmental Toxicology and Chemistry 24(10), 2640-2645.

Yuan, S.Y., Yu, C.H. and Chang, B.V. (2004) Biodegradation of nonylphenol in river sediment. Environmental Pollution 127(3), 425-430.

Zulkosky, A.M., Ferguson, P.L. and McElroy, A.E. (2002) Effects of sewage-impacted sediment on reproduction in the benthic crustacean *Leptocheirus plumulosus*. Marine Environmental Research 54(3), 615-619.

Appendix I. Sediment-water partition coefficients (K_{oc}) used for the derivation of EQS_{EqP}

$logK_{oc}$	K_{oc}	Reference/Source
3.77	5888	Hansler et al. (2006)
4.58	38019	
4.04	10965	Milinovic in ECHA (2011b)
4.35	22387	Roy et al. (1998)
4.71	51286	Burgess et al. (2005)
3.97	9333	Düring et al. (2002)
4.9	79433	Düring et al. (2002)
4.59	38905	Ying et al. (2003)
4.89	77625	Ying & Kookana (2005)
5.05	112202	Gong et al. (2012)
4.7	50119	Sekela et al. (1999)
5.69	489779	Roy et al. (1998)
4.7	50119	Sekela et al. (1999)
5.2	158489	Sekela et al. (1999)
5.6	398107	Sekela et al. (1999)
5.6	398107	Sekela et al. (1999)
4.14	13747	$logK_{OC}=0.63*logK_{OW}+0.90$ Formula : EC (2018)
	62268	**Geometric mean**