ACES REPORT 23

Decamethylcyclopentasiloxane (D5)

EQS data overview

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Preface

The Department of Environmental Science and Analytical Chemistry (ACES) at Stockholm University was commissioned, by the Swedish Agency for Marine and Water Management and the Swedish Environmental Protection Agency, to perform a literature overview and possible EQS derivation for the specific pollutant Decamethylcyclopentasiloxane (D5). The work was performed under the Water Framework Directive (2000/60/EC) using the European Communities's guidance document "Technical Guidance for Deriving Environmental Quality Standards".

The report was prepared by Sara Sahlin and Marlene Ågerstrand. Michael McLachlan provided input on a draft version of the report.

Stockholm, April 23rd, 2018
The Department of Environmental Science and Analytical Chemistry (ACES)
Stockholm University

Förtydligande från Havs- och vattenmyndigheten

Havs- och vattenmyndigheten planerar att ta med dekametylcyklopentasiloxan (D5) bland de ämnen som regleras i Havs- och vattenmyndighetens föreskrifter (HVMFS 2013:19) om klassificering och miljökvalitetsnormer avseende ytvatten[1]. Stockholms Universitet har därför på uppdrag av Havs- och vattenmyndigheten och Naturvårdsverket tagit fram beslutsunderlag för att kunna etablera bedömningsgrunder för D5. Utifrån litteratursökning och granskning av underlag har förslag på värden beräknats utifrån de riktlinjer som ges i CIS 27 (European Communities, 2011). Slutgiltigt val av värden att utgå ifrån vid statusklassificering har föreslagits av Havs- och vattenmyndigheten och efter dialog med deltagare i en arbetsgrupp (representanter från Kemikalieinspektionen, Naturvårdsverket och Läkemedelsverket). Då stor del av underlaget har varit sekundär information (dvs. inte offentligt tillgänglig) har det för Stockholms universitet inte varit möjligt att granska studiernas tillförlitlighet och relevans.

I enlighet med detta föreslås **11 mg/kg torrvikt** respektive **2,2 mg/kg torrvikt** för limnisk respektive marina sediment. Båda värdena avser sediment med 5% TOC. För biota och skydd av topp-predatorer föreslås värdet **830 µg/kg våtvikt**. Vid omräkning av biotavärdet till limnisk vattenfas erhålls värdet 0,13 µg/L. Någon toxicitet för pelagiska organismer har inte kunnat påvisas utan organismer högre upp i näringskedjan bedöms vara mer känsliga än pelagiska organismer. Vid statusklassificering är det därför lämpligt att huvudsakligen utgå från uppmätta halter i biota eller sediment. På grund av begränsat dataunderlag har alla värden tagits fram genom deterministisk beräkning.

Notera att bedömningsgrunder för D5 ännu inte har beslutats.

[1] https://www.havochvatten.se/hav/vagledning--lagar/foreskrifter/register-vattenforvaltning/klassificering-och-miljokvalitetsnormer-avseende-ytvatten-hvmfs-201319.html

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1. METHOD CONSIDERATIONS

Legal frameworks

The work was performed under the Water Framework Directive (2000/60/EC) using the European Communities's (2011) guidance document "Technical Guidance for Deriving Environmental Quality Standards".

Quality Standards (QS) for pelagic communities are derived to cover long-term (Annual Average: AA-QS) and short-term (Maximum Acceptable Concentration: MAC-QS) exposure. Risks for benthic communities, secondary poisoning of predators and human consumption of fishery products are addressed in the derivation of $QS_{sediment}$, $QS_{biota\ sec\ pois}$ and $QS_{biota\ hh}$, respectively. The critical QS compartment (converted to water concentration) is used to set the overall Environmental Quality standard (EQS). This dossier, however, propose QS expressed for specific compartments.

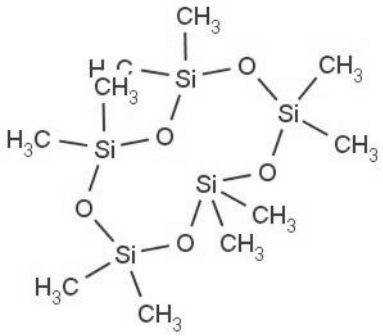
Data sources

The environmental information regarding properties and (eco)toxicity of D5 have been collected from the scientific literature (literature search conducted in March 2017), several reports from regulatory agencies, including the REACH registration dossier (ECHA 2017), the PBT evaluation (ECHA 2012), the Annex XV restriction report (ECHA 2015), the report from the Scientific Committee on Consumer Safety (SCCS 2016), and in assessments performed by UK Environment Agency (EA 2009) and Canada (Environment Canada 2008). Most of the available information was collected from secondary literature and only a few (eco)toxicity studies were publicly available.

Due to the lack of publicly available (eco)toxicity studies, reliability evaluations (based on Klimisch score) were collected from the UK risk assessment (EA 2009) and the REACH registration Dossier (ECHA 2017). Studies were scored as: (1) Reliable without restrictions, (2) Reliable with restrictions, (3) Not reliable or (4) Not assignable.

The following databases were used: Scopus; Web of science; Google Scholar; ETOX; Ekotoxzentrum; UBA; INERIS; RIVM. The following keywords were used: Decamethylcyclopentasiloxane* OMCTS * D5 and ecotoxicity* toxicity* sediment toxicity*mammal toxicity* avian toxicity.

2. CHEMICAL IDENTITY

Common name	**Decamethylcyclopentasiloxane**
Chemical name (IUPAC)	2,2,4,4,6,6,8,8,10,10-decamethylcyclopentasiloxane
Synonym(s)	D5; 2,2,4,4,6,6,8,8,10,10-decamethyl-1,3,5,7,9,2,4,6,8,10- pentaoxapentasilecane
Chemical class	Cyclic volatile methyl siloxanes (cVMS)
CAS number	541-02-6
EU number	208-764-9
Molecular formula	$C_{10}H_{30}O_5Si_5$
Molecular structure	
Molecular weight ($g.mol^{-1}$)	370,77

3. EXISTING EVALUATIONS AND REGULATORY INFORMATION

Annex III EQS Dir. (2008/105/EC)	Not included
Existing Substances Reg. (793/93/EC)	Not included
Pesticides(91/414/EEC)	Not applicable
Biocides (98/8/EC)	Not applicable
PBT substances	PBT assessment under the previous EU chemical legislation (under REACH): D5 is under evaluation.
Substances of Very High Concern(1907/2006/EC)	No
POPs (Stockholm convention)	No
Other relevant chemical regulation	Regulated under Cosmetics products Regulation 1223/2009/EC (not included in any Annex). *"Shall not be placed on the market in wash-off cosmetic products in a concentration equal to or greater than 0.1 % by weight of either substance, after 31 January 2020. "* Commission Regulation (2018/35/EU) amending Annex XVII to Regulation (EC) No 1907/2006. "*Leave- on personal care products and other consumer/professional products (e.g. dry cleaning, waxes and polishes, washing and cleaning products) containing D4/D5 in concentrations > 0.1% shall not be placed on the market.*" (expected submission on 13/04/2018) (REACH)."*D5 in cosmetic products is safe at the reported concentrations, except for the use in hair styling aerosols and sun care spray products*" (SCCS, 2016).
Endocrine disrupter	Not listed on the PACT or SIN-list as ED
CLP-Harmonised hazard classification	No

4. PROPOSED QUALITY STANDARDS (QS)

Protection objective	Unit	Value	Comments
Pelagic community (freshwater)	[µg.L^{-1}]	Not derived	See section 8.1
Pelagic community (marine waters)	[µg.L^{-1}]	Not derived	
Benthic community (freshwater)	[µg.kg^{-1} $_{dw}$]	10 900	See section 8.2
	[µg.L^{-1}]	Not derived	
Benthic community (marine)	[µg.kg^{-1} $_{dw}$]	2180	
	[µg.L^{-1}]	Not derived	
Predators (secondary poisoning)	[µg.kg^{-1} $_{biota\ ww}$]	833	See section 8.3
	[µg.kg^{-1} $_{lipid\ ww}$]	16 660	
	[µg.L^{-1}]	0.13 (freshwaters)	
Human health via consumption of fishery products	[µg.kg^{-1} $_{biota\ ww}$]	15 200	See section 8.3
	[µg.L^{-1}]	2.3 (freshwaters)	
Human health via consumption of water	[µg.L^{-1}]	Not derived	

5. MAJOR USES AND ENVIRONMENTAL EMISSIONS

5.1 Summary of Uses and Quantities

According to the REACH registration dossier (ECHA 2017), 10 000- 100 000 tonnes of D5 is manufactured and/or imported yearly in the European Economic Area. Application areas of D5 include detergents products, polishes (e.g. car cleaning products) and waxes, cosmetics and personal care products (PCPs), textile treatment products and dyes, adhesives and sealants, and laboratory chemicals. The substance is used as an intermediate in industrial processes. D5 is used in formulations of mixtures and/or re-packaging, in the production of chemicals, textiles and leather, as well as electronic and optical products.

The major use of D5 is as an intermediate and as a monomer in the production of silicone polymers (in which D5 can remain as residual impurities). Approximately a quarter of the manufactured volume is used in PCPs (ECHA, 2015). Cosmetic Europe estimated the total amount of D5 used in "wash-off"[2] and "leave-on"[3] products to 750 and 14250 tonnes per year (ECHA 2016). According to Mackay et al. (2015a) the yearly use of D5 in PCPs within Europe and the United Kingdom was approximately 21 000 tonnes in 2004.

5.2 Summary of Estimated Environmental Emissions

Release of D5 to the environment is likely from industrial use, indoor use, and outdoor use (ECHA 2017). Emissions via waste water is the most important route of release to the aquatic environment and the use of PCPs is the dominant contribution (ECHA 2016). The total emission from WWTPs to EU surface water of D5 used in PCPs was estimated to 154.8-185.4 tonnes per year (the most significant release is through the use of D5 in "wash-off" PCPs) (ECHA 2016, Annex B). More than 90% of D5 used in PCPs are antiperspirants and hair-care products, of which less than 10% of the use is estimated to discharge to sewers. The remaining use of D5 in PCPs is in skin care, cosmetics, bath and body products, with 1 % expected to discharge to sewers (results reported in Mackay et al. 2015a).

D5 are efficiently removed in WWTPs under different aerobic and anaerobic conditions (ECHA 2016, Annex B). The removal efficiency from WWTPs was estimated to be 95% (approximately 22% to air and 73% to sludge) (ECHA 2015). It was estimated that 14 814 tonnes of D5 may be emitted to the air every year from the use of PCPs (EA 2009). From the use of PCPs, emissions to the atmosphere accounts for approximately 90 % of the release to the environment (Mackey et al. 2015).

Currently, ECHA calls for evidence to identify the presence of D5 in consumer and professional productions, content of the substance, and emission rates from these articles.

[2] *Rinse-off product* means a cosmetic product which is intended to be removed after application on the skin, the hair or the mucous membranes (Cosmetics Regulation 1223/2009/EC).

[3] *Leave-on product* means a cosmetic product which is intended to stay in prolonged contact with the skin, the hair or the mucous membranes" (Cosmetics Regulation 1223/2009/EC).

6. ENVIRONMENTAL BEHAVIOUR

6.1 Environmental distribution

The high vapour pressure and low water solubility of D5 (table 1) entail a high air-water partition coefficient (K_{AW}) >1000. A high K_{AW} suggests that D5 will prefer to accumulate in the atmosphere rather than aquatic systems. The volatilisation half-life from water was estimated to 2 hours in a river and 183 hours in a shallow lake (modelled) (EA 2009). However, preferential distribution out of aqueous phases may be ameliorated due to adsorption to organic carbon. A relatively high Log K_{OC} value suggests that sorption will be significant.

The most reliable bioconcentration factor (BCF) for D5 in fish is, according to UK EA, 7060 (EA, 2009). This is in excess of the bioaccumuative (B) and very bioaccumulative (vB) criteria in REACH (the criteria are 2000 and 5000, respectively). Kierkegaard et al. (2011) showed that if you defined the bioaccumulation factor in fish as the concentration in the fish normalized to the chemical concentration in the water body (as opposed to the freely dissolved concentration), then D5 was even much more bioaccumulative than suggested by the BCF in fish, with a bioaccumulation behaviour about twice that of PCB 180 (strongly bioaccumulative substance). Trophic magnification factors (TMF) have been measured in several systems for D5, and values >1 and <1 have been measured (Table 1). This suggests considerable variability in TMF between systems and questions whether TMF can be considered an intrinsic property. ECHA has concluded that D5 is very bioaccumulative, largely on the basis of the fish BCF (ECHA 2015).

Regarding long-range atmospheric transport, laboratory studies have shown that D5 reacts with hydroxyl radicals in the atmosphere, and a half-life in the atmosphere of 10 days at average hydroxyl radical concentrations has been estimated (ECHA 2015). Model simulations based on these laboratory reaction rates have shown very good agreement with D5 concentrations measured in ambient air (McLachlan et al., 2010). The same model showed that D5 is present in the atmosphere throughout the Northern Hemisphere, with high concentrations at high latitudes (McLachlan et al., 2010). The model predictions were confirmed with measurements of D5 concentrations at Svalbard (Krogseth et al. 2013), clearly proving that D5 is subject to long-range atmospheric transport (LRAT). The concentrations measured in the Arctic are high compared to many other organic contaminants, ranging from 0.14-4 ng/m^3 (Krogseth et al. 2013). Despite these high concentrations, the potential for deposition to surface water and soil is low due to the high air/water partition coefficient and low octanol/air partition coefficient (ECHA 2015). Considerable concentrations of cyclic volatile methyl siloxanes (cVMS) have been reported in surface media in the Antarctic (Sanchis et al. 2015), but the validity of these data have been questioned (Mackay et al., 2015b; Warner et al., 2015). Chemical properties relevant for environmental distribution and bioaccumulation are presented in table 1.

Table 1. Chemical properties of D5.

		Master reference
Water solubility (mg.L^{-1})	0.017 at 23°C	ECHA 2015
Volatilisation		
Vapour pressure (Pa)	33.2 at 25°C	ECHA 2015
Henry's Law constant (Pa.m^3.mol^{-1})	3.34 x10^6 at 25°C	
n-Octanol/air partition coefficient (Log K_{OA})	4.96 at 24°C	
Air/water partition coefficient (Log K_{AW})	3.13 at 24.6°C	
Adsorption		
Organic carbon – water partition coefficient (Log K_{OC})	5.2-5.4 (natural sediment)	Van Egmond and Sanders, 2010 (in Wang et al. 2013a)
	5.4-5.5 (artificial sediment)	
	5.17 (soil)	Durham 2007 (in ECHA 2015)
	5.6-5.7 (natural soil)	
Suspended matter – water partition coefficient ($K_{suspwater}$)	2100	USEPA EPI (v3.12.) (EA 2009)
Bioaccumulation		
Octanol-water partition coefficient (Log K_{ow})	8.02 at 25 °C (exp) 5.71 (EPI v.3 12)	ECHA 2015 EA 2009
BCF	4450 (*P. promelas*)	Parrott et al 2012
	13 300[b] (*P. promelas*)	Drottar, 2005 (in EA 2009, evaluated as "use with care")
	7060[a] (*P. promelas*)	Drottar, 2005 (In EA 2009, evaluated as "valid")
	1950[a] (*P. promelas*)	Drottar, 2005 (In EA 2009, evaluated as "use with care")
	5260[b] (*P. promelas*)	Drottar, 2005 (In EA 2009, evaluated as "use with care")
	3362 (*O. mykiss*)	Annelin and Frye, 1989 (In EA 2009, evaluated as"use with care")
	1010 (*Pocecilia reticulate*)	Opperhuizen et al. 1987 (In EA 2009, evaluated as "Invalid")
	10500-11048[ac] (Cyprinus carpio)	CERI 2010 (In ECHA 2012)
BMF	0.22[a] (*O. mykiss*)	Dow Corning, 2006 (In EA 2009. "Valid")
	0.63[ac]	
	1.39[b]	
	3.9[bc]	
	0.31[a] (*O. mykiss*)	Woodburn et al. 2012
	1.3[b]	
	0.83[ac]	
	3.4[bc]	
	0.2 (cod-herring) (field)	Powell et al. 2010 (in ECHA 2012)
	0.8-0.9 (cod-shrimp) (field)	
TMF	0.45 (pelagic food web)	Powell et al. 2010
	2.3 (pelagic food web)	Borgå et al. 2012
	2.9 (pelagic food web)	Borgå et al. 2013
	0.59 (marine food web)	Powell 2012

BSAF (Biota-sediment accumulation)	0.46-1,2 (*C. riparius*)	IUCLID (2005) (In EA 2009, evaluated as "use with care")
	0,05 and 0.82 (at low and high organic content) (*H. azteca*)	Norwood et al. 2012
	2.1 organic carbon/kg lipid (Cod)	Warner et al. 2010
	1.5 organic carbon/kg lipid (Sculpin)	
	4.29 kg dry/kg ww (*Lumbriculus variegates*)	Krueger et al. 2010 (in Gobas et al. 2015)
	0.1 (fish) (field)	Hong et al. 2014

a = steady-state. b = kinetic. c = lipid adjusted.

6.2 Abiotic and biotic degradation

D5 has a hydrolysis half-life of 315 days at pH 7 and 12 °C (freshwater), and 64 days at pH 8 and 9 °C (marine water), and is not readily biodegradable (in addition, hydrolysis might be reduced by adsorption to organic matter and particulates). The hydrolysis rate is dependent on the pH and temperature, with a minimum near neutral pH and an increased rate at lower and higher pH. Additionally, the hydrolysis rate decreases with decreasing temperature. The main degradation product is believed to be dimethylsilanediol, which may undergo further degradation to carbon dioxide and silicic acid and/or silica (ECHA 2015).

D5 shows high persistence in sediment with degradation half-times of >1200-3100 days, and is expected to be longer at lower temperatures. D5 meets the criteria for persistent (P) and very persistent (vP) in water and sediment (criteria for vP is 60 days in water and 180 days in sediment) (ECHA 2015). Expected abiotic and biotic degradation half-life are presented in table 2.

Table 2. Abiotic and biotic degradation of D5.

		Master reference
Hydrolysis	DT_{50}= 315 d at 12°C and pH 7 (freshwater)	ECHA 2015
	DT_{50}= 64 d at 9°C and pH 8 (marine water)	ECHA 2015
Photolysis	Not significant in atmosphere	
Degradation	$DT_{50\ (aquatic\ sediment)}$ =2700d (aerobic)	Xu 2010 (In EA 2009)
	$DT_{50\ (aquatic\ sediment)}$ >1200d (aerobic)	ECHA 2015
	$DT_{50\ (aquatic\ sediment)}$ =3100d (anaerobic)	Xu 2010 (In EA 2009)
	$DT_{50\ (dry\ soil)}$ = 9.7-12.4 d	Xu 2007 (in Wang et al. 2013a)
	$DT_{50\ (temp\ soil)}$ = 0.08d	ECHA 2015
Atmospheric degradation	DT_{50}= 20d	Aktinson 1991
	DT_{50}= 10.4 d	ECHA 2015

7. AQUATIC ENVIRONMENTAL CONCENTRATIONS

7.1 Predicted concentrations

Predicted environmental concentrations (PEC) derived by EA (2009) were estimated using EUSES 2.0.3 (table 3). The highest estimations of PECs were from a scenario for formulation of PCPs (at a general non-UK site). PECs of surface water and sediment from the use of PCPs estimated in ECHA (2016) (using EUSES v2.1) are presented in table 4.

Table 3. Predicted environmental concentrations (PEC) of D5 derived by the EA (2009).

Compartment	**PEC (range)**
Surface water (µg/L)	0.10-1.6
Marine waters (coastal and/or transitional) (µg/L)	0.0098-3.2
Sediment (µg/kg ww)	330-5 100
Sediment (marine) (µg/kg ww)	32-10 000
Biota (fish, freshwater) (mg/kg)	3500-24 000
Biota (marine top predators) (mg/kg)	1700-25 000

Table 4. Predicted environmental concentrations (PEC) of D5 from the use of PCPs (ECHA 2016).

Compartment	**Continental PEC**	**Regional PEC**	**Local PEC**
Surface water (µg/L)	0.013 (total) 0.0001 (dissolved)	0.11 (total) 0.081 (dissolved)	1.24
Sediment (µg/kg ww)	61	521	3 985

7.2 Measured concentrations

In aquatic compartments, D5 has been detected in sediment, freshwater and marine fish, benthic organisms, marine predators and seabirds with the highest concentration of 2200 ng/g ww in marine fish. Most of the measured environmental concentrations (MEC) of aqueous phases are from WWTPs effluents (table 5).

In a Swedish screening (Kaj et al. 2005), D5 was the dominant siloxane in most of the samples. All 54 sludge samples from municipal treatment plants had detectable concentrations. D5 was not detected in fish samples (LOD 5 ng/g ww) but in two out of 26 sediment samples (LOD 1-20 ng/g dw). In a regional Nordic screening (which included Kaj et al. 2005), D5 was the dominant siloxane (cyclic and linear) in all measured matrixes except for air (where D4 dominated). Elevated concentration of D5 was found in air samples within STPs as well as in matrixes surrounding the plants. D5 was detected in all sludge samples, 12 out of 24 sediment samples (LOD 1-30 ng/g dw), 15 out of 36 water samples (LOD 0.04-0.08 µg/L), 12 out of 21 fish samples, and in 5 out of 7 marine mammal samples (biota LOD 5 ng/g ww). None of the investigated siloxanes was detected in the two analysed soils from Faroe Islands or in seabird egg samples (LOD 5 ng/g ww). General conclusions from the Nordic screening were that siloxanes in biota were primarily detected in fish liver samples from urban sites (diffuse sources) and only in a few background samples. Water samples with detectable concentrations were from landfills and inlet and outlets from STPs; D5 was not detected in water from background or urban sites (TemaNord, 2005). Kierkegaard et al. (2013a) analysed D5 in fish from six Swedish lakes that did not receive STP effluent, and in fish and sediment from six lakes that received STP effluent. D5 was detected in fish in lakes receiving effluents but all measurements were below the detection limit in

lakes without effluents. D5 concentrations in sediment and fish correlated with how impacted the lakes were from STP effluents.

Retrospective analysis of D5 showed an increased trend (5-6% per year since 1989) in Herring muscle at two different locations in the Baltic Sea (Faxneld et al. 2014). In addition, D5 has been detected in in biota samples from remote regions (Campbell 2010; Evenset et al. 2009).

Table 5. Measured environmental concentrations of D5.

Compartment	**Measured environmental concentration (MEC)**	**Master reference**
Freshwater (µg/L)	<0.03 (Sweden)	Kaj et al. 2005
	<0.01- 0.03 (UK, river)	Sparham et al. 2008
	0.09-0.47 (WWTP recipient, Spain)	Sanchís et al. 2013
	<0.01-1.48 (WWTP recipient, Canada)	Wang et al. 2013b
	0.4 (Downstream industrial WWTP, UK)	Boehmer and Gerhards, 2003 (in EA 2009)
Marine waters	-	
Landfills (µg/L)	3.9-5.4 (Northern[a])	TemaNord 2005
WWTP effluent (µg/L)	<0.03-0.06 (Sweden)[b]	Kaj et al. 2005
	0.45-2.3 (Sweden, Borlänge)	Kaj et al. 2007
	<0.02- 1 (Norway)	Schlabach 2007
	0.2-1 (Norway)	Whelan and Breivik 2013
	0.31- 0.4 (UK)	Sparham et al. 2008
	<0.03-0.98 (Northern)	TemaNord 2005
	<0.01-1.56 (Canada)	Wang et al. 2013b
	0.62-1 (UK)[c]	Boehmer and Gerhards, 2003 (in EA 2009)[3]
	0.1-0.5 (Germany)[c]	
WWTP effluent (industrial, silicone producers) (µg/L)	0.22-26.7 (Germany)[c]	
	<0.02 (France)[c]	
	0,2-07 (UK)[c]	
Sewage sludge (µg/kg)	10 000- 22 000 dw (Sweden)	Kaj et al. 2005
	6900 ww (Sweden, Borlänge)	Kaj et al. 2007
	1900-89 000 dw (Norway)	Schlabach 2007
	220-50 000 dw (Northern)	TemaNord 2005
Sediment (µg/kg dw)	<3.4-190 (Sweden)	Kaj et al. 2005
	124-130 (Baltic Sea) <0.5-1.6 (Mälaren) 30-38 (Hemfjärden) 65-80 (Kyrkviken) 60- 154 (Ekoln) 450-1200 (Runn) (STP recipient, Sweden)	Kierkegaard et al. 2013a
	93-920 (Norway)	Schlabach 2007
	0.07-1.45 (receiving water, Norway)	Sparham et al. 2011
	66.2 and 86.5 (mean in March and June, Norway)	Krogset et al. 2016
	1.8-2000 (Northern)	TemaNord 2005
	<3-91 (River Rhine)	Boehmer and Gerhards, 2003 (in EA 2009)
	33-83 (River Mersey, marine)	
	120-250 (Cardiff Bay)	
	3.39-1270	Sanchis et al. 2013
	0.02-5.84 (WWTP recipient, Canada)	Wang et al. 2013b

	<0.56- 22.7 (China)	Hong et al. 2014
Biota (µg/kg ww)	<5 (fish muscle, Sweden)	Kaj et al. 2005
	0.8 (mean) <0.5-1 (range) (Baltic Sea) 1.5 (mean) <0.5-3.5 (range) (Mälaren) 2.6 (mean) <0.9-3.8 (range) (Hemfjärden) 8.5 (mean) 2.8-9.6 (range) (Kyrkviken) 13.4 (mean) 2.3-19.6 (range) (Ekoln) 14.4 (mean) 6.6-14.4 (range) (Runn) (Peach muscle from STP recipient, Sweden)	Kierkegaard et al. 2013a
	26-2200 (marine fish, Northern)	TemaNord 2005
	6.5-8 (freshwater fish, Northern)	TemaNord 2005
	>0.3-20 (Arctic char muscle, Swedish lakes)	Kierkergaard et al. 2010
	<0.5-4.3 (Herring muscle, Baltic Sea)	Kierkergaard et al. 2010
	0.8-4.2 (Herring muscle, Sweden)	Kierkegaard et al. 2008
	137 (mean) 15-718 (range) lipid weight (Herring muscle, Sweden)	Kierkegaard et al. 2013b
	234-1140 lipid weight (Herring muscle, Sweden)	Kierkegaard et al. 2013b
	0.99-4.13 (Sprat, Skagerrak-Sweden)	Campbell 2010 (in ECHA 2012)
	1491-1979 (cod liver, Oslofjord)	Schalbach et al. 2007
	2.7-4.6 Atlantic cod, Svalbard	Evenset et al. 2009
	1.9-110 (Atlantic cod liver, Svalbard)	Campbell 2010 (in ECHA 2012)
	0.63-2.75 (Bivalve, Svalbard)	Campbell 2010 (in ECHA 2012)
	345 (max) (Sculpin liver, Norway)	Campbell 2010 (in ECHA 2012)
	<6.6-33.1 (Mussels, Europe)	Boehmer et al. 2007 (in ECHA 2012)
	150-2600 (freshwater fish, River Rhine in Germany)	EVONIK industries 2007 (in ECHA 2012)
Biota (marine predators) (µg/kg ww)	9-24 lipid weight (Seal blubber, Sweden)	Kierkegaard et al. 2013b
	17-24 (Seal blubber, Denmark)	TemaNord 2005
	10 (Pilot whale blubber, Faroe Islands)	TemaNord 2005
	32.3-68.8 (Glaucous gulls liver, Bjørnøya)	Knudsen et al. 2007
	0.93-3.5 (Glaucous gulls liver, Svalbard)	Campbell 2010 (in ECHA 2012)
	2.6-3.4 (Glaucous gulls liver, Svalbard)	Campbell 2010 (in ECHA 2012)
	<5 (Seabirds eggs, Sweden and Faroe Islands)	TemaNord 2005
	44 (mean in muscle and fat) 15 (mean in liver) lipid (Mink, US)	Woodburn and Durham, 2009; Woodburn et al. 2011 (in ECHA 2012)

a = Denmark, Faroe Islands, Finland, Iceland, Norway and Sweden. b = Influents 0.1-1.1 µg/L (detected in three out of four samples). c = Municipal WWTP influents 11.2 and 50.1 (UK), and 1.3-8.9 µg/L (Germany). Industrial influents 2900 and 3120 (Germany), 365-3694 µg/L (France), downstream samples were below detection limit of 0.02 µg/L.

8. EFFECTS AND QUALITY STANDARDS

8.1 Aquatic ecotoxicity

None of the aquatic ecotoxicity studies showed adverse effects of D5 exposures close to the water solubility of D5 (17 µg/L) (acute and chronic studies in table 6 and 7, respectively). The available chronic studies for algae, Daphnia and fish were assessed as "reliable without restriction" or "reliable with restrictions" in the REACH registration dossier (ECHA 2017) (although the algae study was assessed as "use with care" in EA, 2009). No mortality or effects on growth were seen in any of the BCF and BAF fish studies at concentrations up to 15 µg/L and at diet doses up 458 mg/kg (Annelin and Frye, 1989; Drottar, 2005; Dow Corning 2006 in EA 2009).

In EA (2009) the toxicity of D5 was estimated using QSAR and EPI (v3.12) with varying results based on different Log K_{OW}. EPI and QSAR calculations using Log K_{OW} of 5.7 and 5.2 suggests toxicity above water solubility for fish, daphnia and algae. However, there was one exception for *Mysid shrimp* which suggested toxicity at 1.8 µg/L (EPI calculations). QSAR calculations with Log K_{OW} 8.0 yielded a predicted toxicity well below the water solubility, with a NOEC of 0.1 µg/L and an EC_{50} of 0.02 µg/L for long term exposure to fish and daphnia.

Taking this together, there were no available empirical indications of toxicity to aquatic organisms at concentrations close to the water solubility of D5. In ECHA (2015), D5 was judged to not meet the REACH legislation's PBT criteria (i.e. NOEC or EC_{10} less than 0.01 mg/L) for "Toxicity" to pelagic organisms based on the available data. As a consequence, MAC or AA-QS for pelagic ecosystems was not derived. However, given the high BCF for D5 in fish there may still be uncertainties regarding long-term exposure e.g. due to the absence of reproduction toxicity studies of fish and due to available evidence suggesting a long depuration half-life for D5 in liver of fish (EA 2009).

Table 6. All acute freshwater ecotoxicity studies of D5.

Species	Endpoint & Duration	Effect value (µg/L)	Guideline & Comments	Reference
Oncorhynchus mykiss	14d NOEC	>16	OECD 204; GLP; Reliability: 1[a]	Sousa 2000 (in ECHA 2017)
Oncorhynchus mykiss	28d NOEC	>5.8	BCF study; endpoint mortality; Reliability: 2[b]	Annelin and Frye (in EA 2009)
Daphnia magna	48h EC_{50}	>2.9	OECD 202; GLP; Reliability:1[a]	ECHA 2017[c]; IUCLID 2005 (study conducted 2002)

a = evaluation from REACH registration dossier (ECHA 2017). b = evaluation from EA (2009). c = Ref. 001 (short-term toxicity to aquatic invertebrates) in REACH registration dossier (ECHA 2017).

Table 7. All chronic freshwater ecotoxicity studies of D5.

Species	Endpoint & Duration		Effect value D5 (µg/L)	Guideline & Comments	Reference
Oncorhynchus mykiss (embryos)	Hatching, survival, growth	90d NOEC	>14	OECD 210; GLP; Reliability: 1[a]	Lee 2009 (in ECHA 2017)
Oncorhynchus mykiss	Survival	45d NOEC	>17	BCF study	Drottar 2009 (in Mackey et al. 2015)
Oncorhynchus mykiss	Survival, growth	45d NOEC	>17	OECD 204; Reliability: 2[a]	ECHA 2017[b] (study conducted 2009)
Pimephales promelas (embryo- juvenile)	Survival, hatching success	65d NOEC	>8.7	OECD 210 with modification	Parrott et al. 2013
Pimephales promelas (embryo- juvenile)	Growth	65d NOEC	>8.7	OECD 210 with modification	Parrott et al. 2013
Pimephales promelas (embryo- juvenile)	Condition Factor (CF)	65d NOEC	1.7	OECD 210 with modification; Increased CF[c]	Parrott et al. 2013
Pimephales promelas	Weight, survival	35d NOEC	>15	OECD 305; BCF study; Reliability: 2[d]	Drottar 2005 (in EA 2009)
Daphnia magna	Reproduction, growth, survival	21d NOEC	>15	OECD 211; GLP; Reliability: 1[a]	ECHA 2017[e] (study conducted 2003)
Pseudokirchneriella subcapitata	Growth	96h NOEC	>12	OECD 201; GLP; single dose test; Reliability: 2[ad]	ECHA 2017[f] (study conducted 2001)

a = Evaluation from REACH registration dossier ECHA (2017). b = Ref. 002 (long-term toxicity to fish) in REACH registration dossier (ECHA, 2017). c = Not considered an adverse effect. d = Evaluation from EA (2009). e = Ref. 001 (long-term toxicity to invertebrates) in REACH registration dossier (ECHA 2017). f = Ref. 001 (toxicity to algae and cyanobacteria) in REACH registration dossier (ECHA 2017).

8.2 Sediment toxicity

The evidence of sorption potential (i.e. Log K_{OC} ≥3) was convincing for D5, with Log K_{OC} varying from 5.2-5.5. There were available environmental measurements suggesting that D5 may be widely present in sediment. Five sediment ecotoxicity studies were found including 24 effect values for three species from three different taxonomic groups (Insect, Annelida and Crustacean) (supporting information, table S1). Critical data for the three species are presented in table 8. All effect values were normalised to a standard organic carbon content of 5% accordingly to European Communities (2011). Norwood et al. (2012) showed that the toxicity to *Hyalella azteca* increased with decreased organic content (from 10 to 0.5%), and it was concluded that D5 is expected to cause higher toxicity in sediment with lower organic content due to increased bioavailability. D5 is toxic to sediment organisms but was not assumed to meet the REACH legislation's PBT criteria for "Toxicity" based on the calculated pore water concentration corresponding to the NOEC of 109.4 mg/kg dw, which was estimated to be around 14 µg/L (just below the water solubility) (ECHA 2015).

Table 8. Sediment ecotoxicity studies with lowest effect values for three different species and taxonomic groups.

Species	**Endpoint & Duration**		**Effect value (mg/kg dw)**	**Normalized to 5% OC (mg/kg dw)**	**Reliability evaluation**	**Reference**
Chironomus riparius	Development rate	28d NOEC	70	109.4	Reliability: 1[a]	Krueger et al. 2008 (in ECHA 2017)
Hyalella azteca	Survival	28d NOEC	130	135.4	Reliability: 1[a] 2[b]	Picard 2009 (in ECHA 2017)
Lumbriculus variegatus	Survival, reproduction, growth	28d NOEC	>1272	>1718.9	Reliability: 1[a]	Krueger et al. 2007 (in ECHA 2017)

a = Evaluation from REACH registration dossier (ECHA 2017). b = Evaluation from ECHA (2012).

$QS_{sediment}$ derivation

The study showing the lowest effect value was *C. riparius* with the endpoint development rate and a NOEC of 109.4 mg/kg dw. Assessment factor (AF) 10 and 50 was used to derive $QS_{sed\text{-}freshwater}$ and $QS_{sed\text{-}marine}$ respectively, since the dataset was considered to include three NOEC values from species representing different living and feeding conditions (European Communities, 2011). The QS for sediment was set to 10.9 and 2.2mg/kg dw for freshwater and marine water, respectively.

8.3 Secondary poisoning

The evidence for bioaccumulation potential (i.e. BMF>1 and BCF≥100) was convincing for D5 (European Communities, 2011). D5 is not classified for harmonised classification and labelling regarding carcinogenicity, mutagenicity, reproductive toxicity or specific target organ toxicity according to the CLP-legislation (ECHA, 2015). In SCCS (2016), it was concluded that D5 does not pose a risk for humans in cosmetic products, except through the use of hair styling aerosols and sun care spray products. D5 was found in 8 of 49 Swedish breast milk samples with a maximum concentration of 4.8 µg/L (Kaj et al. 2005). Six studies and a total of 10 effect values for rats and avian species were available in secondary literature (of which one was published as a peer-review study). All oral toxicity studies found are presented under supporting information, table S2.

General toxicity

There was no evidence of acute toxicity in rats following exposure via oral or dermal routes on rats, while an inhalation study suggested an LD_{50} of 560 ppm (SCCS 2016; ECHA 2017).

The liver has been shown to be the organ most negatively affected, following oral and inhalation administration. The observed effects in liver include increased liver weight (mainly in females), and clinical biochemistry changes (such as decreased urea concentration, increased cholestrole, increased triglycerides, increased total protein, and increased gamma-glutamyltransferase) (SCCS 2016). D5 exposure induces hepatic xenobiotic metabolizing enzymes similar to those induced by phenobarbital (Zhang et al. 2000; Dow Corning 1995). According to EA (2009) the induction of enzyme activity was the most likely reason for increases in liver weight.

Repeated oral dose studies were available for durations up to 90 days and doses up to 1600 mg/kg/day (supporting information, table S2). Dow Corning 1990a (in SCCS, 2016) conducted a repeated dose study (14 days) resulting in 31, 36 and 48 % increased liver weight (absolute and relative weights) at 100, 400 and 1600 mg/kg/day, respectively in females (no effects in males), giving a NOAEL of 25 mg/kg/day. There were no functional or histopathological changes observed, and it was therefore considered unclear if the increased liver weight was relevant on a wildlife population level (ECHA 2016). In a 90 day repeated oral dose study the lowest dose tested, 100 mg/kg/day, resulted in a 30% increase in liver weight (Jäger et al. 1991, in SCCS 2016). Since it was not possible to derive a NOAEL from this study comparisons with the NOAEL from the 14 day study was not possible. In SCCS (2016) it was stated that the increased liver weight in the study by Jäger et al. 1991 was not accompanied by histopathological changes and there was no biological alteration in enzymatic activities, resulting in an uncertainty whether these liver effects were adverse or not. A two-year inhalation study suggests, for example, that treatment related effects of D5 were reversible (EA 2009; SCCS 2016). According to ECHA (2015), an increase in liver weight by more than 10% is considered an adverse effect for human health. A larger increase in liver weight may compress other abdominal organs, and the enzyme induction can modify the normal response to other xenobiotics.

Carcinogenicity, Mutagenicity, Endocrine activity and Reproduction toxicity

D5 showed carcinogenic potential (uterine tumours) in a two-year inhalation study with female rats exposed to 160 mg/m^3 (Young and Morfeld 2016 in EA 2009; SCCS, 2016). According to SCCS (2016) the mode of action for the carcinogenic effects was not fully understood and it was not known whether these effects are relevant to humans.

D5 lacked mutagenic potential in *in vitro* assays and *in vivo* (inhalation) (results reported in EA 2009; SCCS 2016). Quinn et al. (2007) concluded that D5 did not exhibit estrogenic, androgenic or prostagenic activity *in vitro* or *in vivo* (rat whole-body inhalation).

There was no evidence of reproduction toxicity, neonatal toxicity or developmental toxicity in a two-generation whole-body vapour inhalation study on rats exposed to 160 ppm (Siddiqui et al. 2007). However, since the highest dose (160 ppm) used in this study was below the identified NOAEL for D4 (which demonstrates reproduction toxicity) of 300 ppm, it is not possible to exclude reproductive effects at higher doses.

No oral studies investigating reproduction toxicity, carcionogenic or endocrine activity were found for mammals. One avian oral reproduction toxicity study (range-finding study) was found, suggesting no effects at the highest tested doses of 1000 mg/kg (Stafford 2012, in ECHA 2012).

$QS_{biota\ sec\ pois}$ derivation

The critical effect value was 25 mg/kg/day (14 days) (Dow Corning 1990a in SCCS, 2016) for endpoint increased liver weight in rats. According to European Communities (2011) the following conversion factors (CF) can be used:

1. Age/study > 6 weeks = CF 20
2. Age/study < 6 weeks = CF 10

Since no details regarding age of rats were available and due to the short duration (14 days) CF of 10 was used as precaution to convert NOAEL to NOEC. AF 300 was used giving a QS of 833 µg/kg biota ww[4]. A lower AF was not possible since no chronic or 90-day reproduction study is available (European Communities 2011). QS of 833 µg/kg biota ww corresponds to 0.13 µg/L in freshwater using BCF of 7060 and field BMF for cod-shrimp of 0.9 from the study by Powell et al. (2010).

$QS_{biota\ hh}$ derivation

There were no available acceptable daily intake (ADI) or tolerable daily intake (TDI), therefore a human toxicological standard (TL_{hh}) was calculated using the lowest NOAEL (25 mg/kg/day) and AF of 100, giving a TL_{hh} of 0.25 mg/kg/day (European Communities, 2011). Using this TL_{hh}, a body weight of 70 kg, and a daily fish consumption of 115 g, the QS_{hh} was set to 15.2 mg/kg biota ww (corresponding to 2.36 µg/L in freshwater). Using the DNEL of 5 mg/kg/d (table 9) the QS_{hh} was calculated to 304 mg/kg biota ww.

There is no existing drinking water standard for D5 (Directive 98/83/EC). QS for drinking water was not undertaken in the present dossier.

[4] Corresponds to 16 660 µg/kg lipid ww, normalized to 5% lipid weight (QS_{biota} divided by 0.05).

9. EXISTING ECOTOXICOLOGICAL THRESHOLD VALUES

Results from present and previous assessments of D5 are presented in table 9. In Environment Canada (2008) the PNEC was set to 15 µg/L on the basis that this concentration did not cause any effect to *O. mykiss* or *D. magna* (no AF applied). Sediment $PNECs_{fw}$ derived in REACH registrations Dossier and in EA (2009) were both based on *C. riparius* NOEC of 109 mg/kg (Krueger et al. 2008) but with AF of 10 and 50 respectively. A higher AF was used in the UK assessment due to the absence of a third species, which now is available (*H. azteca*). $PNEC_{sec\ pois}$ was derived based on a 90 day inhalation NOEAL extrapolated to oral NOAEL of 19 mg/kg/day (CF 20 and AF 30) in EA (2009).

Table 9. Ecotoxicological threshold values from previous and present assessments.

	REACH registration Dossier (ECHA 2017a)	**UK assessment (EA 2009)**	**Canada assessment (Environment Canada 2008)**	**Proposal from this dossier**
$PNEC_{fw}$ (µg/L)	Not derived	Not derived	15	Not derived
$PNEC_{sw}$	Not derived	Not derived	-	Not derived
$PNEC_{fw}$ sediment (mg/kg dw)	11 (AF 10)	2.2 (AF 50)	-	10.9 (AF 10)
$PNEC_{sw}$ sediment (mg/kg dw)	1.1 (AF 100)	0.2 (AF 500)	-	2.2 (AF 50)
PNEC sec pois (mg/kg)	16 (AF 90)	13 (AF 30)	-	0.83 (AF 300)
$DNEL_{oral}$ (mg/kg bw/d)	5 (AF 200)	-	-	-
QS_{hh} (mg/kg biota ww**)**	-	-	-	15.2 (AF 100)

10. IDENTIFICATION OF ISSUES RELATING TO UNCERTAINTY IN RELATION TO THE QSs DERIVED

Since (eco)toxicity data were collected from secondary literature it has not been possible to evaluate studies for their reliability and relevance.

Uncertainties related to ecotoxicity to pelagic organisms

Sorption and volatilization properties and the low water solubility (17 µg/L) of D5 challenge the assessment of the substance in standard aquatic toxicity tests. Although absence of effects on pelagic organisms there are uncertainties regarding long-term exposure of D5 due to the high BCF in fish and evidence of long depuration half-life in liver of fish (EA 2009).

Uncertainties related to $QS_{sediment}$

Exposure directly through sediment (and not through the overlaying water, e.g. *H. azteca* bioassays) are the most important route when assessing the risks of sediment toxicity of D5 (because of the absence of toxicity through water and given high absorption affinity). Investigating effects of life-long exposure of D5 are necessary to reduce uncertainties regarding sediment toxicity (e.g. OECD 233 for *Chironomus sp*., during >44 days which covers the 1st generation and the early part of the 2nd generation). In addition, the available OECD guideline for macrophytes (OECD 239: Water-Sediment *Myriophyllum Spicatum* Toxicity test) could also provide data for an additional taxonomy to comparisons of species sensitivity.

Uncertainties related to $QS_{biota\ sec\ pois}$

QS for secondary poisoning is coupled with uncertainties since it is based on a non-chronic study (14 days). The ecological or human health consequences caused by increased liver weight is not well defined. A larger increase of liver weight may compress other abdominal organs, and the enzyme induction can modify the normal response to other xenobiotics. Using AF 300 may be too conservative since data from a 90 day oral study is available (NOAEL < 100 mg/kg/d resulting in 30% increased liver weight) and a two year inhalation reproduction study. However, due to the similar structure with D4 (which is classified as toxic to reproduction according to the CLP-legislation) it is believed that further mammal toxicity studies investigating toxicity to reproduction is necessary. The highest inhalation dose in the available reproduction study for D5 (160 ppm) is lower compared to the NOAEL for D4 (300 ppm) thus, it remains unclear whether D5 is toxic to reproduction at similar concentrations as D4 or through 90-day oral exposure.

The QS for secondary poisoning derived in this dossier is more stringent compared to EA (2009) and the REACH registration dossier (ECHA 2017), however, the EA (2009) derivation is based on extrapolations from inhalation to oral exposures which entails large uncertainties. The toxicokinetic pathways between oral and inhalation routes are clearly distinct. In oral exposure D5 is mostly absorbed along with lipids from the diet, which is distributed to the liver (later metabolized or distributed primarily into fat). Inhaled D5 mostly is exhaled due to partitioning between blood and air. D5 that is not exhaled can be metabolized locally or in the liver (SCCS 2015). The reasoning and effect value that the PNEC for secondary poisoning is based on in the REACH registration dossier (ECHA, 2017) is unknown.

Uncertainties related to mixture effects

The homologous structure and similar effects of D4 and D5 raise concerns regarding their mixture effect.

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12. SUPPORTING INFORMATION

Table S1. All available sediment toxicity studies for D5 with effect values normalised to 5% organic content (OC).

Species	Endpoint & Duration		Effect value (mg/kg dw)	Normalised to 5% OC	Guideline & Comments	Reliability Evaluation	Reference
Annelida							
Lumbriculus variegatus	Survival, reproduction, growth	28d NOEC	>1272	>1719	Formulated sediment; EPA guideline; OC 3,7%	1[a]	Krueger et al. 2007 (in ECHA 2017)
Insecta							
Chironomus riparius (larvae)	Survival	10d LC_{50}	450	1125	Formulated sediment; OECD 218; OC 2%	1[a]2[b]	Putt 2003 (in ECHA 2017)
Chironomus riparius (larvae)	Growth rate	10d EC_{50}	410	1025	Formulated sediment; OECD 218; OC 2%	1[a]2[b]	Putt 2003 (in ECHA 2017)
Chironomus riparius (larvae)	Growth rate	10d NOEC	73	182.5	Formulated sediment; OECD 218; OC 2%	1[a]2[b]	Putt 2003 (in ECHA 2017)
Chironomus riparius (larvae)	Growth rate	10d LOEC	180	450	Formulated sediment; OECD 218; OC 2%	1[a]2[b]	Putt 2003 (in ECHA 2017)
Chironomus riparius (larvae)	Development rate	28d NOEC	69	172.5	Formulated sediment; OECD 218; OC 2%	1[a]2[b]	Putt 2003 (in ECHA 2017)
Chironomus riparius (larvae)	Development	28d LOEC	180	450	Formulated sediment; OECD 218; OC 2%	1[a]2[b]	Putt 2003 (in ECHA 2017)
Chironomus riparius (larvae)	Emergence rate	28d EC_{50}	420	1050	Formulated sediment; OECD 218; OC 2%	1[a]2[b]	Putt 2003 (in ECHA 2017)
Chironomus riparius (larvae)	Development rate	28d EC_{50}	>570	>1425	Formulated sediment; OECD 218; OC 2%	1[a]2[b]	Putt 2003 (in ECHA 2017)
Chironomus riparius	Survival	28d LC_{50}	257	401.6	Formulated sediment; OECD 218; OC 3,2%	1[a]	Krueger et al. 2008 (in ECHA 2017)
Chironomus riparius	Development rate	28d NOEC	70	109.4	Formulated sediment; OECD 218; OC 3,2%	1[a]	Krueger et al. 2008 (in ECHA 2017)
Chironomus riparius	Development rate	28d LOEC	160	250	Formulated sediment; OECD 218; OC 3,2%	1[a]	Krueger et al. 2008 (in ECHA 2017)
Chironomus riparius	Development time, emergence ratio	28d NOEC	160	250	Formulated sediment; OECD 218; OC 3,2%	1[a]	Krueger et al. 2008 (in ECHA 2017)
Chironomus riparius	Development time, emergence ratio	28d LOEC	248	382.8	Formulated sediment; OECD 218; OC 3,2%	1[a]	Krueger et al. 2008 (in ECHA 2017)
Crustacean							
Hyalella azteca (juvenile)	Survival	28d LC_{50}	191	1910	Natural sediment; OECD 315; OC 0,5%	1[c]	Norwood et al. 2012
Hyalella azteca (juvenile)	Survival	28d LC_{25}	144	1440	Natural sediment; OECD 315; OC 0,5%	1[c]	Norwood et al. 2012
Hyalella azteca (juvenile)	Survival	28d LC_{50}	857	428	Natural sediment; OECD 315; OC 10%	1[c]	Norwood et al. 2012

Species	Endpoint & Duration		Effect value (mg/kg dw)	Normalised to 5% OC	Guideline & Comments	Reliability Evaluation	Reference
Hyalella azteca (juvenile)	Survival	28d LC_{25}	637	319	Natural sediment; OECD 315; OC 10%	1[c]	Norwood et al. 2012
Hyalella azteca (juvenile)	Growth	28d EC_{25}	821	411	Natural sediment; OECD 315; OC 10%	1[c]	Norwood et al. 2012
Hyalella azteca	Survival	28d LC_{50}	310	323	Natural sediment; EPA guideline; OC 4,8%	1[a]	Picard 2009 (in ECHA 2017)
Hyalella azteca	Survival	28d LOEC	230	240	Natural sediment; EPA guideline; OC 4,8%	1[a]	Picard 2009 (in ECHA 2017)
Hyalella azteca	Survival	28d NOEC	130	135	Natural sediment; EPA guideline; OC 4,8%	1[a]	Picard 2009 (in ECHA 2017)
Hyalella azteca	Growth	28d EC_{50}	>130	>135	Natural sediment; EPA guideline; OC 4,8%	1[a]	Picard 2009 (in ECHA 2017)
Hyalella azteca	Growth	28d LOEC	>130	>135	Natural sediment; EPA guideline; OC 4,8%	1[a]	Picard 2009 (in ECHA 2017)

a = evaluation from REACH registration dossier (ECHA 2017). b = evaluation from EA (2009). c = evaluation from ECHA (2012).

Table S2. Mammal (oral) and avian toxicity studies for D5.

Species	Endpoint & Duration		Effect value (mg/kg bw)	Guideline & Comments	Reliability evaluation	Reference
Rat (Sprague-Dawley) (8-12 weeks old)	Survival	14d LD_{50}	>5000	OECD 401; GLP	1[ab]	ECHA 2017; EA 2009; SCCS 2016
Rat (Sprague-Dawley)	Enzymatic induction	4d NOAEL	5	CYP2B1/2, PROD, EROD, CYP3A1/2 was induced		Zhang et al. 2000
Rat (Sprague-Dawley) (female)	Liver to body ration	4d LOAEL	20	15% increased relative liver weight.		Zhang et al. 2000
Rat (Sprague-Dawley) (male)	Liver to body ration	4d LOAEL	100	40% increased relative liver weight.		Zhang et al. 2000
Rat (Sprague-Dawley) (female)	Liver weight	14d NOAEL/ LOAEL	25	25, 100, 400 and 1600 mg/kg/day resulted in 13, 34, 33 and 50% increased weight, respectively (in EA 2009). 100, 400 and 1600 mg/kg/day resulted in 31, 36 and 48% increased liver weight (in SCCS, 2016).		Dow Corning, 1990a (in EA 2009; SCCS 2016)
Rat (Sprague-Dawley) (male)	Liver weight	14d NOAEL	400	13% increased liver weight.		Dow Corning, 1990a (in EA 2009)
Rat (Sprague-Dawley) (female)	Liver weight	28d NOAEL	<1500	Single dose administration. Significant increase in liver weight (23% compared to control). No effect in males.	-	Dow Corning 1990b (in SCCS 2016)
Rat (Wistar)	Liver weight	90d NOAEL "For the purposes of human hazard assessment"	>1000	OECD 408/GLP; Increased liver weight at all doses (100, 330, 1000) in females. No histapathological changes. At 1000 mg/kg/day the appearance of hepatocyte cytoplasma changed (histological observations both male and female). Assessed as reliable without restrictions (Echa Dossier).	1[a]	Jäger et al. 1991 (in ECHA 2017)
Rat (Wistar)	Liver weight	90d NOAEL /LOAEL	100	OECD 408/GLP; Increased liver weight at all doses (100, 330, 1000) in females. 100 mg/kg/bw resulted in an increase of 30%. No effect in males.		Jager et al. 1991 (in SCCS 2016)
Bird (*Coturnix coturnix japonica*)	Reproduction toxicity	8 weeks	>1000	Range finding study. Endpoints: food consumption, total eggs laid, total eggs cracked, total eggs set, egg set of laid, total eggs viable, eggs viable of set, total surviving embryos, surviving embryos of viable eggs, total hatchlings, total hatchlings of surviving embryos, average hatchling weight, body weights, weight gain. The proportion of viable eggs was low in the control compared to treatment groups.	2[c]	Stafford, 2012 (in ECHA 2012)

a = evaluation from Reach registration dossier (ECHA 2017). b = evaluation from EA (2009). c = evaluation from ECHA (2012).

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