SUBSTANCE EVALUATION CONCLUSION

As required by REACH Article 48

And

EVALUATION REPORT

For

Medium-chain chlorinated paraffins / alkanes, C_{14-17}, chloro

EC No 287-477-0

CAS No 85535-85-9

Evaluating Member State(s): United Kingdom

Dated: 09 December 2019

Evaluating Member State Competent Authority

United Kingdom

This report was produced by a delegated national authority working in partnership with the national Competent Authority (the Health & Safety Executive).

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Year of evaluation in CoRAP: 2012

Before concluding the substance evaluation a Decision to request further information was issued on: 25 February 2014

Further information on registered substances here:
http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances

DISCLAIMER

This document has been prepared by the evaluating Member State as a part of the substance evaluation process under the REACH Regulation (EC) No. 1907/2006. The information and views set out in this document are those of the author and do not necessarily reflect the position or opinion of the European Chemicals Agency or other Member States. The Agency does not guarantee the accuracy of the information included in the document. Neither the Agency nor the evaluating Member State nor any person acting on either of their behalves may be held liable for the use which may be made of the information contained therein. Statements made or information contained in the document are without prejudice to any further regulatory work that the Agency or Member States may initiate at a later stage.

Foreword

Substance evaluation is an evaluation process under REACH Regulation (EC) No. 1907/2006. Under this process the Member States perform the evaluation and ECHA secretariat coordinates the work. The Community rolling action plan (CoRAP) of substances subject to evaluation, is updated and published annually on the ECHA web site[1].

Substance evaluation is a concern driven process, which aims to clarify whether a substance constitutes a risk to human health or the environment. Member States evaluate assigned substances in the CoRAP with the objective to clarify the potential concern and, if necessary, to request further information from the Registrant(s) concerning the substance. If the evaluating Member State concludes that no further information needs to be requested, the substance evaluation is completed. If additional information is required, this is sought by the evaluating Member State. The evaluating Member State then draws conclusions on how to use the existing and obtained information for the safe use of the substance.

This Conclusion document, as required by Article 48 of the REACH Regulation, provides the final outcome of the Substance Evaluation carried out by the evaluating Member State. The document consists of two parts i.e. A) the conclusion and B) the evaluation report. In the conclusion part A, the evaluating Member State considers how the information on the substance can be used for the purposes of regulatory risk management such as identification of substances of very high concern (SVHC), restriction and/or classification and labelling. In the evaluation report part B the document provides explanation how the evaluating Member State assessed and drew the conclusions from the information available.

With this Conclusion document the substance evaluation process is finished and the Commission, the Registrant(s) of the substance and the Competent Authorities of the other Member States are informed of the considerations of the evaluating Member State. In case the evaluating Member State proposes further regulatory risk management measures, this document shall not be considered initiating those other measures or processes. Further analyses may need to be performed which may change the proposed regulatory measures in this document. Since this document only reflects the views of the evaluating Member State, it does not preclude other Member States or the European Commission from initiating regulatory risk management measures which they deem appropriate.

[1] http://echa.europa.eu/regulations/reach/evaluation/substance-evaluation/community-rolling-action-plan

Contents

Part A. Conclusion

1 CONCERNS SUBJECT TO EVALUATION

Alkanes, C_{14-17}, chloro – more commonly referred to as medium-chain chlorinated paraffins (MCCPs, CAS no. 85535-85-9) – was originally selected for substance evaluation in order to clarify concerns about:

- Persistent, Bioaccumulative and Toxic (PBT) properties; and

- Exposure scenarios.

During the first evaluation initiated in 2012, other concerns were identified regarding:

- Substance identity; and

- Aspects of environmental hazard classification under the CLP Regulation EC No. 1272/2008.

2 OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

The United Kingdom Competent Authority (UK CA) was the rapporteur for MCCPs under the Existing Substances Regulation EC No. 793/93 (ESR), producing two environmental risk assessments (EC, 2005; EC, 2007), and a transitional Annex XV dossier (including the human health risk assessment) once the REACH Regulation was introduced (HSE, 2008a & b). The Annex XV dossier included an analysis of risk management options for scenarios that had been identified as posing an environmental risk in the earlier assessments. In particular, a restriction on the marketing and use of MCCPs in leather fat liquors was agreed at the 15th Risk Reduction Strategy meeting, and this was communicated to ECHA in this dossier. Subsequently, further data were provided by Industry in compliance with Commission Regulation (EC) No. 466/2008, and these were evaluated and reported to ECHA by the UK CA (EA, 2010). That evaluation identified further data needs but, as Industry was performing additional biodegradation studies and the REACH registration deadline was imminent, it was decided to leave it to Registrants to take the conclusions of the various UK CA reports into account and propose further testing or risk management measures as necessary.

3 CONCLUSION OF SUBSTANCE EVALUATION

The evaluation of the available information on the substance has led the evaluating Member State Competent Authority (eMSCA) to the following conclusions in Table 1.

Table 1

CONCLUSION OF SUBSTANCE EVALUATION	
Conclusions	**Tick box**
Need for follow-up regulatory action at EU level	✓
Harmonised Classification and Labelling	
Identification as SVHC (authorisation)	✓
Restrictions	✓
Other EU-wide measures	
No need for regulatory follow-up action at EU level	

4 FOLLOW-UP AT EU LEVEL

4.1 Need for follow-up regulatory action at EU level

4.1.1 Harmonised Classification and Labelling

No multiplication factors (M-factors) for mixtures are given in the harmonised classification of MCCPs under the CLP Regulation. The self-classification given in the Lead Registrant's latest dossier update includes an M-factor of 100 and 10 for acute and chronic aquatic hazards, respectively. This is discussed further in Section 6.6. The eMSCA considers it a relatively low priority to update the harmonized classification to include M-factors given the conclusion on PBT properties, which is likely to have a greater impact on risk management (see next section). This could be reconsidered following the completion of the further risk management work.

4.1.2 Identification as a substance of very high concern, SVHC (first step towards authorisation)

MCCPs is a substance of unknown or variable composition, complex reaction products or biological materials (hereinafter 'UVCB'). It contains linear chloroalkanes with carbon chain lengths predominantly in the range of C_{14-17} with chlorination levels that can differ depending on the application. MCCPs therefore contains thousands of constituents and it is neither feasible nor justifiable to experimentally determine key properties for every constituent separately. The assessment approach has therefore been to select test substances that provide a representative structural match for a significant number of constituents, described by carbon chain length and degree of chlorination.

The Registrants do not consider that MCCPs meets the Annex XIII PBT or 'very persistent very bioaccumulative' (vPvB) criteria. In particular, they consider that evidence of aerobic mineralisation in screening level studies outweighs evidence from environmental simulation tests, and that limited evidence of trophic magnification from field studies outweighs data from aquatic bioaccumulation tests. The eMSCA disagrees with this assessment, and considers that MCCPs meets the Annex XIII PBT and vPvB criteria (it is possible that lower chlorine content MCCP products (≤45% Cl wt.) might not be persistent within the meaning of the Annex XIII criteria, but definitive data to confirm this are not available).

In addition, the registered substance contains unintentional C_{10-13} constituents that are structural analogues of alkanes, C_{10-13}, chloro (short-chain chlorinated paraffins or SCCPs, CAS no. 85535-84-8). These are typically present in the range 0.1 -1% weight by weight (w/w). SCCPs is on the Candidate List due to its PBT properties, and is also listed as a persistent organic pollutant under the United Nations' Stockholm Convention on Persistent Organic Pollutants (although evidence provided for this evaluation indicates that SCCPs with chlorine contents below 50% wt. are unlikely to be persistent). The C_{10-13} constituents of MCCPs are likely to have the same PBT properties as SCCPs. As they are present above 0.1% w/w, MCCPs with a chlorine content equal to or greater than 50% wt. is therefore also a "PBT-containing substance".

The eMSCA considers that a restriction is the most appropriate regulatory risk management measure. There is no formal requirement to identify MCCPs as an SVHC prior to a restriction proposal. However, it would provide legal certainty to all stakeholders to do so.

4.1.3 Restriction

REACH calls for minimisation of emissions and exposures of PBT/vPvB substances as far as technically and practically possible (recital 70). The Registrants' Chemical Safety Reports (CSR) assess environmental risk on the basis of PEC/PNEC ratios. The CSRs indicate that there will be environmental releases from various life cycle stages for all registered uses. There is therefore an unacceptable risk, since releases do not appear to be minimised to the greatest extent technically and practically feasible.

A restriction would be able to target the uses giving rise to the greatest exposure, and could take account of the fact that not all MCCP product types meet the PBT criteria. It would also address imported articles, creating a level playing field for all European stakeholders.

Further information can be found in the separate Risk Management Options Analysis (RMOA) (See the ECHA website; https://echa.europa.eu/pact?p_p_id=disspact_WAR_disspactportlet&p_p_lifecycle=0&p_p_state=normal&p_p_mode=view&p_p_col_id=column-1&p_p_col_pos=1&p_p_col_count=2&_disspact_WAR_disspactportlet_substanceId=100.079.497&_disspact_WAR_disspactportlet_jspPage=%2Fhtml%2Fportlet%2Fdisspact%2FdetailsPage%2Fview_detailsPage.jsp)

4.1.4 Other EU-wide regulatory risk management measures

A proposal has been made to add MCCPs to the Restriction of the Use of Certain Hazardous Substances (RoHS) in Electrical and Electronic Equipment (EEE) Directive (2011/65/EU). No additional EU-wide regulatory risk management measures are foreseen.

5 TENTATIVE PLAN FOR FOLLOW-UP ACTIONS (IF NECESSARY)

Indication of a tentative plan is not a formal commitment by the evaluating Member State. A commitment to prepare a REACH Annex XV dossier (SVHC, restrictions) and/or CLP Annex VI dossier should be made via the Registry of Intentions.

Table 2

FOLLOW-UP		
Follow-up action	**Date for intention**	**Actor**
Annex XV dossier for SVHC identification	Q1 2020	To be confirmed
Annex XV dossier for restriction	Q1 2021	To be confirmed

Note: The timing of the UK's exit from the EU is likely to affect which actors would be involved in the formal submission of any dossier. This requires further discussion.

Part B. Substance evaluation

6 EVALUATION REPORT

This evaluation is targeted on environmental hazard and risks.

6.1 Overview of the substance evaluation performed

MCCPs was included on the first Community Rolling Action Plan (CoRAP) in 2012 to check the environmental exposure scenarios to ensure that the risk characterization ratios were all below one, and to review the Registrants' assessment of persistence, bioaccumulation and toxicity (PBT).

Table 3

EVALUATED ENDPOINTS	
Endpoint evaluated	**Outcome/conclusion**
Persistence	MCCPs meets the Annex XIII criteria for persistence (P), with some constituents potentially meeting the very persistent criteria (vP).
Bioaccumulation	The substance meets the Annex XIII criteria for bioaccumulation (B), with some constituents meeting the very bioaccumulative criteria (vB).
Toxicity	The substance meets the Annex XIII criteria for toxicity (T), based on environmental effects.
CLP	M-factors could be added to the existing harmonised classification for acute and chronic aquatic hazards.
Exposure scenarios	The environmental exposure scenarios are well described. No PEC/PNEC ratios are above one, but due to the conclusion that this substance meets the PBT/vPvB criteria a qualitative risk exists, and the Registrants should take steps to minimise environmental emissions.

6.2 Procedure

The initial substance evaluation carried out during 2012/3 was based on the combined REACH registration dossiers and a literature search. The MCCPs REACH Consortium confirmed that it represented all Registrants of MCCPs, including non-EU manufacturers that have registered via Only Representatives. ECHA sent a decision letter on 25 February 2014 to the Registrants requesting more detailed substance identity information (including how this related to use pattern), addition of robust study summaries of scientific studies available in the academic literature, tiered environmental simulation and fish bioaccumulation testing, and additional information on the exposure scenarios used (ECHA, 2014). The Registrants appealed this decision on 16 May 2014. The ECHA Board of Appeal dismissed the appeal on 9 September 2015 but extended the deadline for dossier update to 9 September 2018 (ECHA, 2015).

The Lead Registrant submitted a registration dossier update on 7 September 2018 (accepted by ECHA on 28 September). This did not include all of the information that had been requested by ECHA. A further update was submitted on 4 June 2019 (accepted by ECHA on 20 June). This contained the missing information so the second evaluation period formally started in June 2019.

Technical work on the second phase of this substance evaluation was carried out between October 2018 and July 2019 using the Lead Registrant dossier submitted in September 2018 and June 2019. The report was peer reviewed by the 22nd ECHA PBT Expert Group, the REACH Consortium and an independent Swiss academic during September 2019. A draft RMOA was also circulated for comment to the Registrants' representatives and the EU Risk Management Expert Group in September 2019.

Unpublished studies that have already been cited in previous published assessments (EC, 2005; EC 2007; HSE, 2008a & b; EA, 2010) are given the same citation in this report for ease of comparison.

6.3 Identity of the substance

Table 4

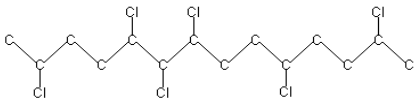
SUBSTANCE IDENTITY	
EC name:	Alkanes, C_{14-17}, chloro
EC number:	287-477-0
CAS number:	85535-85-9
Index number in Annex VI of the CLP Regulation:	602-095-00-X
Molecular formula:	$C_xH_{(2x - y+2)}Cl_y$, where x = 14 - 17 and y = 1 - 17
Molecular weight range:	300 - 600 g/mole (approximately)
Synonyms:	Medium-chain chlorinated paraffins (MCCPs); Chlorinated paraffins, C_{14-17} (used in Annex VI of the CLP Regulation)

Note: The abbreviation MCCPs will be used for the substance throughout this report.

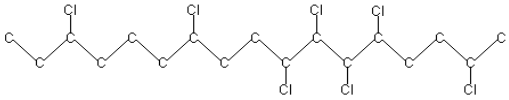
Type of substance ☐ Mono-constituent ☐ Multi-constituent ☒UVCB

Structural formula:

Example structures (hydrogen atoms removed for simplicity) include



$C_{14}H_{24}Cl_6$



$C_{17}H_{29}Cl_7$

UVCB substance

The identity of MCCPs can be defined by the chlorination of the paraffin feedstock which then defines the composition of the substance. It is a UVCB substance containing linear chloroalkanes predominantly in the range of C_{14-17} (governed by the feedstock). The chlorination process is random, and so MCCPs contains many thousands of constituents[2]. A UVCB substance technically

[2] Tomy *et al*. (1997) includes a formula for the calculation of the number of isomers.

does not contain impurities but some constituents outside of the C_{14-17} range are present in small amounts.

The ECHA dissemination portal (checked July 2019) lists 10 active Registrants and 3 inactive Registrants. Of the 10 active Registrants, 7 have submitted dossiers since 2017, 2 Registrants last submitted dossiers in 2013 and one has not submitted a dossier update since 2010. Most Registrants have listed their composition as 100% alkanes, C_{14-17}, chloro (Table 5). Two Registrants have indicated their composition as > 95% alkanes, C_{14-17}, chloro with additives making up the remaining 5%.

Table 5

ConstituentConstituentConstituent **Constituents**	**Typical concentration**	**Concentration range**	**Remarks**
Alkanes, C_{14-17}, chloro	≤100% w/w	Not specified	Based on information in the registration dossiers

The percentage chlorine content of the commercially available product types varies according to the applications they are used for. Table 6 indicates the structural formulae of possible constituents of different MCCP product types (adapted from information originally presented in EC (2000) and EC (2005)).

Table 6

THEORETICAL CHLORINE CONTENT OF CONSTITUENTS IN MCCPS								
Chlorine content,% w/w	**Constituent formula**							
	C_{10}	**C_{11}**	**C_{12}**	**C_{13}**	**C_{14}**	**C_{15}**	**C_{16}**	**C_{17}**
<40	$C_{10}H_{21}Cl$ & $C_{10}H_{20}Cl_2$	$C_{11}H_{23}Cl$ & $C_{11}H_{22}Cl_2$	$C_{12}H_{25}Cl$ to $C_{12}H_{27}Cl_3$	$C_{13}H_{27}Cl$ to $C_{13}H_{25}Cl_3$	$C_{14}H_{29}Cl$ to $C_{14}H_{27}Cl_3$	$C_{15}H_{31}Cl$ to $C_{15}H_{29}Cl_3$	$C_{16}H_{33}Cl$ to $C_{16}H_{30}Cl_4$	$C_{17}H_{35}Cl$ to $C_{17}H_{32}Cl_4$
40 - 45	$C_{10}H_{19}Cl_3$	$C_{11}H_{21}Cl_3$	-	$C_{13}H_{24}Cl_4$	$C_{14}H_{26}Cl_4$	$C_{15}H_{28}Cl_4$	$C_{16}H_{29}Cl_5$	$C_{17}H_{31}Cl_5$
45 - 50	$C_{10}H_{19}Cl_3$	$C_{11}H_{20}Cl_4$	$C_{12}H_{22}Cl_4$	$C_{13}H_{23}Cl_5$	$C_{14}H_{25}Cl_5$	$C_{15}H_{27}Cl_5$	$C_{16}H_{28}Cl_6$	$C_{17}H_{30}Cl_6$
50 - 55	$C_{10}H_{18}Cl_4$	$C_{11}H_{19}Cl_5$	$C_{12}H_{21}Cl_5$	$C_{13}H_{22}Cl_6$	$C_{14}H_{24}Cl_6$	$C_{15}H_{26}Cl_6$ & $C_{15}H_{25}Cl_7$	$C_{16}H_{27}Cl_7$	$C_{17}H_{29}Cl_7$
55 - 65	$C_{10}H_{16}Cl_6$& $C_{10}H_{17}Cl_7$	$C_{11}H_{18}Cl_6$& $C_{11}H_{17}Cl_7$	$C_{12}H_{20}Cl_6$ to $C_{12}H_{18}Cl_8$	$C_{13}H_{21}Cl_7$ to $C_{13}H_{19}Cl_9$	$C_{14}H_{23}Cl_7$ to $C_{14}H_{21}Cl_9$	$C_{15}H_{24}Cl_8$ to $C_{15}H_{22}Cl_{10}$	$C_{16}H_{26}Cl_8$ to $C_{16}H_{23}Cl_{11}$	$C_{17}H_{28}Cl_8$ to $C_{17}H_{25}Cl_{11}$
>65	$C_{10}H_{14}Cl_8$ and higher no. of Cl atoms	$C_{11}H_{16}Cl_8$ and higher no. of Cl	$C_{12}H_{17}Cl_9$ and higher no. of Cl atoms	$C_{13}H_{18}Cl_{10}$ and higher no. of Cl atoms	$C_{14}H_{20}Cl_{10}$ and higher no. of Cl atoms	$C_{15}H_{21}Cl_{11}$ and higher no. of Cl atoms	$C_{16}H_{22}Cl_{12}$ and higher no. of Cl atoms	$C_{17}H_{24}Cl_{12}$ and higher no. of Cl atoms

Note: The grey columns refer to constituents potentially present at ≥0.1% w/w and <1% w/w. They are structurally analogous to short-chain chlorinated paraffins (SCCPs).

The chlorine content of the commercially available product types is generally within the range 40% to 63% by weight, with the majority of product types having a chlorine content between 45% and 52% by weight. The main constituents in the majority of product types have between five and seven chlorine atoms per molecule. Nevertheless, it should be noted that percentage chlorine content only represents an average level of chlorination, and so a wider range of constituents may be present in any particular product.

Petersen *et al.* (2006) produced a graph showing the chain length and chlorine distribution of an unnamed MCCP product with a 52% chlorine content. C_{14} chlorinated n-alkane dominated, followed by decreasing amounts of C_{15}, C_{16} and C_{17} (no information was shown on chain lengths shorter than C_{14}). There were mainly 6 – 9 chlorine atoms per molecule, but substances with 5 chlorine atoms per molecule were also evident. Similar findings were also reported by Hüttig and Oehme (2006) for a 57% Cl wt. MCCP.

Chen *et al.* (2011) reported that the commercial MCCP product CP52 (stated to be used in China) had the following carbon chain length distribution: 60.3% C_{14}, 21.1% C_{15}, 12.2% C_{16} and 6.3% C_{17} (in the supporting information to their paper). The predominant number of chlorine atoms per molecule was around 7 – 9, with a lower relative abundance of substances with 6 or 10 chlorine atoms per molecule.

Steinberg and Emerson (2012) presented a carbon chain length distribution of a commercial product called OS-52, with the CAS number 68920-70-7. It is not clear where this was manufactured (it is not stated in the paper and the REACH Registrants have not been able to identify the manufacturer (pers. comm.)). The paper presented gas chromatograms of carbon chain lengths following dechlorination-hydrogenation of the chlorinated paraffin. The predominant chain length was C_{14}, followed by C_{15} with much smaller amounts of C_{16} and C_{17}. Traces of C_{10}, C_{11}, C_{12} and C_{13} were also present. Whilst this distribution matches MCCPs (e.g. as determined by Petersen *et al.*, 2006), the CAS number given in the paper is for alkanes, $C_{6\text{-}18}$, chloro, and no registrations under this CAS number appear on ECHA's public dissemination database. Therefore, the relevance of this information to the current evaluation is unclear.

The Registrants have stated that they are not aware of any commercially viable $C_{14\text{-}17}$ n-alkane feedstock that does not contain significant amounts of C_{14} constituents (pers. comm.).

Table 7

CONSTITUENTS PRESENT IN AMOUNTS <1% BY WEIGHT			
Constituent	**Typical concentration**	**Concentration range**	**Remarks**
Chlorinated alkanes with carbon chain lengths $<C_{14}$	<1%	Not specified	Based on information in EC (2005) and information in the registration dossiers, assuming that the alkanes in the feedstock are chlorinated during manufacture of MCCPs
Chlorinated aromatics	<100 mg/kg	Not specified	Based on information in EC (2005) assuming that aromatics and isoparaffins in the feedstock are chlorinated during manufacture of MCCPs.
Chlorinated isoparaffins	<1 - 2%	Not specified	

All constituents in commercial chlorinated paraffins are likely to be related to those present in the n-paraffin feedstock, in which the major non-paraffinic constituent is a small proportion of aromatics (generally less than 100 mg/kg). The isoparaffin content of the feedstock is less than 1 - 2% (Table 7).

Producers of MCCPs represented by Euro Chlor have, since 1991, used paraffin feedstocks in the production process with a $C_{<14}$ content of <1% by weight and reported that the actual levels are often much lower than this (EC, 2005).

Table 8

ADDITIVES		
Constituent	**Typical concentration**	**Remarks**
Epoxidised soya oil	<1%	Based on information in EC (2005)
Glycidyl ethers	<1%	Based on information in EC (2005)

Various stabilisers can be added to commercial chlorinated paraffins at <1% by weight to improve thermal or light stability (EC, 2005). Some of the registration dossiers list additives as part of their composition. This is confidential information. It is possible that other Registrants have not mentioned them because they are added post-reaction and so are considered to create an intentional mixture.

Identity and composition of structurally related substances (used in a benchmarking or read-across approach)

Around forty CAS numbers have been used to describe the whole chlorinated paraffin family at one time or another. Some of these are now historical, and others may be in use for the sole purpose of compliance with national or regional chemical inventories. It is possible that some may contain chlorinated alkanes in the C_{14} to C_{17} range, so these are presented in Table 9 (this list may not necessarily be exhaustive).

Table 9

OTHER CAS NUMBERS ASSOCIATED WITH MEDIUM CHAIN CHLOROPARAFFINS		
Substance	**CAS number**	**EC number**
Alkanes, chloro	61788-76-9	263-004-3
Alkanes, C_{6-18}, chloro	68920-70-7	272-924-4
Alkanes, C_{10-14}, chloro	85681-73-8	288-211-6
Alkanes, C_{10-21}, chloro	84082-38-2	281-985-6
Alkanes, C_{10-26}, chloro	97659-46-6	307-451-5
Alkanes, C_{10-32}, chloro	84776-06-7	283-930-1
Alkanes, C_{12-14}, chloro	85536-22-7	287-504-6
Alkanes, C_{14}, chloro	-	-
Alkanes, C_{14-16}, chloro	1372804-76-6	-
Alkanes, C_{16-27}, chloro	84776-07-8	283-931-7
Alkanes, C_{16-35}, chloro	85049-26-9	285-195-2
Reaction mass of Alkanes, C_{14-17}, chloro and Paraffin waxes and Hydrocarbon waxes, chloro	915-934-2	-
Paraffin oils and hydrocarbon oils, chloro	85422-92-0	287-196-3
Paraffins (petroleum), normal $C_{>10}$, chloro	97553-43-0	307-202-0
Slackwax (petroleum), chloro	2097144-44-8	-
Tetradecane, chloro derivatives	198840-65-2	-

No REACH registrations had been made for any of the CAS numbers in Table 11 when the eMSCA checked ECHA's public dissemination database on 23 July 2019.

The details of the registrations for short-chain chlorinated paraffins (SCCPs) and long-chain chlorinated paraffins (LCCPs) can be found in Table 10.

Table 10

SUBSTANCE IDENTITY OF RELEVANT STRUCTURAL ANALOGUES		
EC name	Alkanes, C_{10-13}, chloro	Paraffin waxes and Hydrocarbon waxes, chloro
EC number	287-476-5	264-150-0
CAS number	85535-84-8	63449-39-8
Index number in Annex VI of the CLP Regulation	602-080-00-8	-
Molecular formula	$C_xH_{(2x - y+2)}Cl_y$, where x = 10 - 13 and y = 1 – 13	$C_xH_{(2x - y+2)}Cl_y$, where x = 18 - 30 and y = 1 - 30
Molecular weight range	320 - 500 g/mole (approximately)	420 - 1355 g/mole (approximately)
Synonyms	Short-chain chlorinated paraffins (SCCPs); alkanes, C_{10-13}, chloro; chlorinated paraffins, C_{10-13} (used in Annex VI of the CLP Regulation)	Long-chain chlorinated paraffins (LCCPs); alkanes, C_{18-30}, chloro; chlorinated paraffins, C_{18-30}

Note: The abbreviations SCCPs and LCCPs will be used for the substance throughout this report.

Table 11 contains CAS numbers that have been used to describe chlorinated paraffins that contain chlorinated alkanes with carbon chain lengths $<C_{14}$ and $>C_{17}$. This list is not necessarily exhaustive. No REACH registrations had been made for any of the CAS numbers in Table 11 when the eMSCA checked ECHA's public dissemination database on 23 July 2019.

Table 11

OTHER CAS NUMBERS ASSOCIATED WITH SHORT- AND LONG-CHAIN CHLOROPARAFFINS		
Substance	**CAS number**	**EC number**
Alkanes, C_{12-13}, chloro	71011-12-6	-
Alkanes, C_{18-28}, chloro	85535-86-0	287-478-6
Alkanes, C_{18-20}, chloro	106232-85-3	-
Alkanes, C_{22-40}, chloro	106232-86-4	600-725-8
Alkanes, C_{10-12}, chloro	108171-26-2	600-857-6
Alkanes, C_{22-26}, chloro	108171-27-3	600-858-1
Alkanes, C_{22-30}, chloro	288260-42-4	-
Alkanes, C_{20-24}, chloro	2097144-45-9	-
Alkanes, C_{20-28}, chloro	2097144-43-7	-
Alkanes, C_{21-34}-branched and linear, chloro.	1417900-96-9	-
Alkanes, C_{22-30}-branched and linear, chloro.	1401974-24-0	-
Alkanes, C_{24-28}, chloro	1402738-52-6	-
Hexacosane, chloro derivs.	2097144-46-0	-
Octacosane, chloro derivs.	2097144-47-1	-

6.3.1 Analytical challenges

Due to the complex nature of this UVCB substance, considerable challenges were encountered by the Registrants and the laboratories commissioned to perform chemical analysis. van Mourik *et al.* (2018) conducted an inter-laboratory study using 33 laboratories to assess the consistency of measured concentrations of the related substance SCCPs. Each laboratory was asked to analyse test solutions, fish extract (pooled yellow eel fillets), sediment extract, house dust extract and soil extract spiked with a standard solution provided by Vrije Universiteit (VU) Amsterdam. This eliminated uncertainties related to extraction and clean-up procedures. Each participating laboratory received ampoules with test materials and quantification standards, guidelines and report forms. All participating laboratories provided a short description of the analytical method used and reported back three independent values for the total concentration of SCCPs. The main analytical methods used by the participating laboratories were:

- Gas Chromatography-Electron-Capture Negative Ionisation - Mass Spectrometry (GC-ECNI-MS), low and high resolution mass spectrometry (LRMS and HRMS, respectively) were used.
- Gas Chromatography Electron Ionisation Mass Spectrometry (GC-EI-MS/MS)
- Carbon Skeleton Gas Chromatography Electron Ionisation Mass Spectrometry (Csk-GC-EI-MS). Both Tandem mass spectrometry and low resolution mass spectrometry (MS/MS and LRMS) were used.
- Atmospheric Pressure Chemical Ionization Quadrupole Time-Of-Flight Mass Spectrometry (APCI-QTof-MS).
- Two Dimensional Gas Chromatography Electron-Capture Negative Ionisation Time-Of-Flight Mass Spectrometry (GC x GC-ECNI-ToF-MS).

Large differences in results between laboratories were found (coefficient of variation 23 – 137%). The authors noted that the most commonly used analytical technique for analysis of SCCPs (GC-ECNI-LRMS) showed the largest variation. Low Resolution Mass Spectrometry (LRMS) cannot distinguish between chlorinated paraffins and chlorinated olefins. As chlorinated paraffins and chlorinated olefins differ only by the presence of a double bond, an analytical technique that can distinguish between these two structures is likely to be able to distinguish between any other structurally similar organohalogen impurities within MCCPs. High Resolution Mass Spectrometry (HRMS) can make this distinction so it was recommended that HRMS is used in the future. The same conclusion is likely to apply to MCCPs.

GC-ECNI-MS was also investigated by Schinkel *et al.* (2018) who noted that it is highly sensitive to the degree of chlorination of a compound. If environmental mixtures of chloroparaffins have a different degree of chlorination than the analytical standards, the reported value can differ from the target values by orders of magnitude. The authors presented the development of new analytical methods based on deconvolution of homologue patterns into linear combinations of patterns using complex chloroparaffin mixtures as standards. In addition, there are methods available that allow quantification using single-chain chloroparaffin mixtures that include homologues of only one carbon chain length with different degrees of chlorination.

These analytical findings have led to a concern that a large proportion of the measured values (both for environmental monitoring and experimental studies) reported in the academic literature may not be accurate. The analyses of samples resulting from the three studies performed in response to the initial Substance Evaluation decision[3] were all conducted by the same contract laboratory on behalf of the Registrants. The analytical method used was APCI-ToF-HRMS, which was found to provide measured values that were in good agreement with the

[3] Aerobic and Anaerobic Transformation in Aquatic Sediment Systems (OECD TG 308); Bioaccumulation in Fish: Aqueous and Dietary Exposure (OECD TG 305); and Partition Coefficient (1-Octanol/Water): Slow-Stirring Method (OECD TG 123).

consensus value as part of the inter-laboratory study. Therefore, the analytical measurements from these studies are considered to be reliable.

In contrast, analytical data for the available ecotoxicity studies were generated over ten years ago. All the key ecotoxicity studies cited in the registration dossiers employed radiolabelled test materials to confirm concentrations in the test media. This technology was very well evolved by the time these studies were conducted (generally after 1996, though the 1983 fish toxicity study also used radiolabelled test material). As they are considered to be the best data available to assess the required endpoints, and are cited by the Registrants for use in their CSRs, the eMSCA has no reason to believe that the analytical methods were deficient.

6.4 Physico-chemical properties

Only physico-chemical properties that are relevant for the environmental risk assessment and PBT assessment were considered for this substance evaluation. Key data are summarised in Table 12.

Table 12

OVERVIEW OF PHYSICOCHEMICAL PROPERTIES		
Property	**Value**	**Reference/source of information/remarks**
Physical state at 20 °C and 101.3 kPa	Liquid	
Melting / freezing point	The pour point of C_{14-17} chlorinated paraffins vary between -50 °C and +25 °C	0 °C was used for EUSES modelling in the CSRs, based on EC (2005). The eMSCA considers this to be acceptable.
Boiling point	MCCPs begin to decompose at around 200 °C before boiling	200 °C was used for EUSES modelling in the CSRs, based on EC (2005). The eMSCA considers this to be acceptable.
Vapour pressure	1.3 to 2.7 x 10^{-4} Pa at 20 °C for C_{14-17} chlorinated n-alkane 52% Cl wt. 1.07 x 10^{-3} Pa at 45 °C, 6 x 10^{-3} Pa at 60 °C and 0.051 Pa at 80 °C for C_{14-17} chlorinated n-alkane 52% Cl wt.; 2.27 x 10^{-3} Pa at 40 °C and 0.16 Pa at 80 °C for C_{14-17} chlorinated n-alkane 45% Cl wt.	Campbell and McConnell, 1980 BUA, 1992 as cited in EC, 2005 2.7 x 10^{-4} Pa at 20 °C was used for EUSES modelling in the CSRs. The eMSCA considers this to be acceptable.

OVERVIEW OF PHYSICOCHEMICAL PROPERTIES		
Property	**Value**	**Reference/source of information/remarks**
Water solubility	0.0061 mg/L at 20 °C for C_{14} chlorinated n-alkane 50% Cl wt.	Unpublished, 2019a; non-GLP OECD Test Guideline (TG) 105. Analytical method: APCI-ToF-HRMS. Key study cited by Registrants
	0.005 - 0.027 mg/L at 20 °C for C_{15} chlorinated n-alkane 51% Cl wt.	Madeley, *et al*., 1983; non-standard method. Analytical method: thin-layer chromatography and radioactivity measurements. Key study used in EC (2005)
	0.01 mg/L in freshwater and 0.004 mg/L in seawater at 16-20 °C for C_{16} chlorinated n-alkane 52% Cl wt.	Campbell and McConnell, 1980; method unknown. Analytical method: radioactivity measurements The eMSCA considers that 0.027 mg/L is still a realistic upper limit for this substance.
Partition coefficient n-octanol/water (log K_{OW})	6.58 ± 0.09 for C_{14} chlorinated n-alkane 50% Cl wt.	Unpublished, 2019b; non-GLP OECD TG 123 (slow stir). Analytical method: APCI-ToF-HRMS. Very little variability in K_{OW} was observed between differently chlorinated congener groups
	7.2 (4.7-8.3) for C_{16} chlorinated n-alkane 35% Cl wt.	Fisk, 1998b; key study used in EC (2005). Analytical method: high performance liquid chromatography (HPLC)
	5.52 to 8.21 for C_{14-17} chlorinated n-alkane 45% Cl wt.; 5.47 to 8.01 for C_{14-17} chlorinated n-alkane 52% Cl wt.	Renberg *et al*. (1980); non-GLP non-guideline study. Analytical method: reversed-phase high performance thin layer chromatography (RP-HPTLC) An average value of 7 is used for EUSES modelling in the CSRs. The eMSCA considers this to be acceptable.

The variable composition of MCCPs and the analytical challenges described in Section 6.3.1 make it difficult to assess the accuracy/precision and relevance of physico-chemical end points without detailed information about the test item identity/composition and analytical methods.

6.4.1 Vapour pressure

Measured data

The registration dossiers contain a robust study summary (RSS) for an experimentally determined vapour pressure of 1.3 – 2.7 x 10^{-4} Pa at 20 °C for a C_{14-17} chlorinated n-alkane, 52% Cl wt. (Campbell and McConnell, 1980). This study was considered previously in EC (2005).

Experimentally derived vapour pressures have also been reported for C_{14-17} chlorinated n-alkanes with chlorine contents of 45 and 52% Cl wt. at higher temperatures (BUA, 1992, as cited by EC, 2005). The registrations do not include this information.

There is no experimental information available on the variation of vapour pressure with carbon chain length and chlorine content for MCCPs. A study by Drouillard *et al.* (1998) found that vapour pressure of a series of short-chain chlorinated paraffins (C_{10} to C_{13}) decreased with both increasing carbon chain length and chlorine content and so the same trend can be assumed for MCCPs.

Predicted data

The eMSCA has predicted vapour pressures for a series of hypothetical chlorinated paraffin structures with carbon chain lengths of C_{10}-C_{18} and chlorine contents of 45, 52 and 60% Cl wt. using the MPBPVP v1.43 model contained within the EPI Suite™ v4.11 platform (US EPA, 2012) (Appendix A). Values range from 1.4 x 10^{-10} to 0.022 mm Hg (1.9 x 10^{-8} to 3.0 Pa) at 25 °C. The complete training set for this model is not available, so it is not possible to describe a precise estimation domain. However, the guidance provided with the model indicates that the relationship between the experimental and predicted vapour pressure values for a test set of 1 642 compounds was good, with an R^2 of 0.949, standard deviation of 0.59 and an average deviation of 0.32. The eMSCA considers it unlikely that the training set will have contained close analogues of MCCPs. The reliability of these predicted values is therefore uncertain.

Glüge *et al.* (2013) calculated subcooled-liquid vapour pressure for 29 constituents of MCCPs using COSMO*therm*, SPARC and EPI Suite™, and compared the results to experimental data from the literature. A series of recommended values were presented (see Table 13), which indicate that vapour pressure is likely to decrease with increasing carbon chain length and chlorine content.

Value recommended by eMSCA

Constituents of the substance have a very low vapour pressure at environmentally relevant temperatures. A vapour pressure of 2.7 x 10^{-4} Pa at 20 °C is used by the Registrants for EUSES modelling in their CSR, and the eMSCA agrees that this is an acceptable compromise to avoid unnecessary complexity.

Table 13

KEY PHYSICO-CHEMICAL PROPERTY VALUES FOR MCCPs RECOMMENDED BY GLÜGE *ET AL.* (2013)				
Molecular formula	**Vapour pressure, Pa**	**Water solubility, µg/L**	**n-Octanol solubility, g/L**	**log K_{OW}**
$C_{14}H_{29}Cl_1$	0.11 – 0.12	3.65 – 4.57	274 – 275	7.66 – 7.76
$C_{14}H_{27}Cl_3$	1.3×10^{-4} – 0.013	5.02 – 40.4	297 – 412	6.77 – 7.80
$C_{14}H_{25}Cl_5$	7.9×10^{-5} – 0.0014	3.86 – 34.4	329 – 550	6.88 – 7.89
$C_{14}H_{23}Cl_7$	$<1 \times 10^{-6}$ – 1.5×10^{-4}	3.16 – 44.5	219 – 524	6.57 – 7.97
$C_{14}H_{21}Cl_9$	$<1 \times 10^{-6}$ – 1.5×10^{-5}	2.78 – 272	366 – 560	6.21 – 7.99
$C_{14}H_{19}Cl_{11}$	$<1 \times 10^{-6}$	2.60 – 87.0	431 – 670	6.87 – 8.09
$C_{14}H_{18}Cl_{12}$	$<1 \times 10^{-6}$	1.90 – 68.2	291 – 668	6.94 – 8.03
$C_{15}H_{31}Cl_1$	0.035 – 0.04	1.02 – 1.20	265 – 267	8.22 – 8.29
$C_{15}H_{29}Cl_3$	1.0×10^{-4} – 0.0039	1.56 – 9.88	297 – 403	7.37 – 8.30
$C_{15}H_{27}Cl_5$	7.6×10^{-6} – 5.1×10^{-4}	1.12 – 13.8	251 – 486	7.14 – 8.41
$C_{15}H_{25}Cl_7$	$<1 \times 10^{-6}$ – 5.2×10^{-5}	0.93 – 17.0	228 – 484	6.99 – 8.48
$C_{15}H_{23}Cl_9$	$<1 \times 10^{-6}$ – 5.6×10^{-6}	0.72 – 7.38	300 – 579	7.61 – 8.55
$C_{15}H_{21}Cl_{11}$	$<1 \times 10^{-6}$	0.89 – 68.1	384 – 596	6.88 – 8.54
$C_{15}H_{19}Cl_{13}$	$<1 \times 10^{-6}$	0.50 – 16.1	287 – 639	7.53 – 8.62
$C_{16}H_{33}Cl_1$	0.011 – 0.014	0.26 – 0.35	256 – 256	8.73 – 8.84
$C_{16}H_{31}Cl_3$	1.5×10^{-5} –0.0014	0.38 – 3.13	296 – 390	7.86 – 8.87
$C_{16}H_{29}Cl_5$	5.2×10^{-6} – 1.7×10^{-4}	0.29 – 4.81	263 – 541	7.61 – 8.96
$C_{16}H_{27}Cl_7$	$<1 \times 10^{-6}$ – 1.7×10^{-5}	0.28 – 6.89	206 – 534	7.34 – 9.00
$C_{16}H_{25}Cl_9$	$<1 \times 10^{-6}$ – 2.0×10^{-6}	0.22 – 11.8	294 – 547	7.27 – 9.06
$C_{16}H_{23}Cl_{11}$	$<1 \times 10^{-6}$	0.19 – 27.8	333 – 522	7.20 – 9.09
$C_{16}H_{21}Cl_{13}$	$<1 \times 10^{-6}$	0.15 – 42.2	289 – 1 070	7.45 – 9.12
$C_{17}H_{35}Cl_1$	0.0035 – 0.0042	0.07 – 0.09	247 – 248	9.28 – 9.37
$C_{17}H_{33}Cl_3$	1.3×10^{-5} – 4.8×10^{-4}	0.10 – 0.84	292 – 374	8.41 – 9.43
$C_{17}H_{31}Cl_5$	5.2×10^{-6} – 5.0×10^{-5}	0.08 – 1.51	230 – 556	8.04 – 9.52
$C_{17}H_{29}Cl_7$	$<1 \times 10^{-6}$ – 6.2×10^{-6}	0.08 – 3.28	179 – 497	7.59 – 9.53
$C_{17}H_{27}Cl_9$	$<1 \times 10^{-6}$	0.08 – 12.7	364 – 557	7.35 – 9.58
$C_{17}H_{25}Cl_{11}$	$<1 \times 10^{-6}$	0.04 – 11.5	318 – 587	7.57 – 9.72
$C_{17}H_{23}Cl_{13}$	$<1 \times 10^{-6}$	0.04 – 5.37	289 – 508	7.87 – 9.69
$C_{17}H_{21}Cl_{15}$	$<1 \times 10^{-6}$	0.02 – 1.71	259 – 980	8.74 – 9.85

Note: Data represent the range of the four isomers considered for each structure.

6.4.2 Water solubility

Measured data

A new OECD TG 105 (column elution method) study has been performed voluntarily by the Registrants (Unpublished, 2019a). The Registrants assign this study a reliability score of 1 (reliable without restriction) in their RSS, although it is not subject to Good Laboratory Practice (GLP). The finalised study report has been made available to the eMSCA for review.

C_{14} chlorinated n-alkane, 50 % Cl wt. was applied to silica gel as a solution in pentane. A certificate of analysis for the test substance is not included in the report. The silica gel was then agitated overnight prior to removal of the solvent using gentle heat and air. Columns were loaded with 600 mg of prepared silica gel, then flushed with de-ionised water under controlled conditions. Two test runs were performed in duplicate with flow rates of 12.5 mL/h and 25 mL/h, together with a blank. Fractions of 5 mL eluted water were collected for each of the flow rates for chemical analysis. The report states that test columns were allowed to equilibrate for 'at least' 2 hours. It is not known whether this gave sufficient time for all congeners to dissolve to their greatest extent (compared with an equilibration time of six months in earlier experiments – see later text).

Each 5 mL fraction was centrifuged and the upper portion transferred to a clean vessel to ensure that no silica gel was still present. These centrifuged solutions were then extracted using a solid phase extraction (SPE) method. It is reported that three spiked recoveries were performed alongside sample extractions and yielded ~ 85% recoveries. Ten blanks were also prepared to assess background levels of the test substance. Analysis of the samples was performed using an APCI-ToF-HRMS method with external calibration, detailed in Brandsma *et al*. (2017) (citing Bogdal *et al*., 2015), which is currently the best available technique. The eMSCA recognises the expertise of the laboratory (VU Amsterdam) with regard to the analyses of these samples. Measured solubilities were reported over a range of C_{14} congeners (with 4 to 14 chlorine atoms), and added together to provide a total water solubility value. Instrumental detection limits were calculated for individual congener groups from $C_{14}Cl_4$ to $C_{14}Cl_{11}$ (range 0.035 – 0.135 µg/L). The total instrumental detection limit was calculated from the sum of the individual values to be 0.52 µg/L.

The study is well reported and meets the validity criterion of less than 30% difference between the mean values obtained from two tests with different flows (the coefficient of variation (%RSD) was 29%). The water solubility of C_{14} congeners with different chlorine numbers varied from 0.011 to 2.3 µg/L at 19 °C. Total water solubility values ranged from 3.56 to 11.11 µg/L, with an average of 6.1 µg/L (0.0061 mg/L). Other chain length constituents of MCCPs were not addressed, so the total solubility of the test substance in this study underestimates the total solubility of the registered substance. For comparison, a 59% Cl wt. SCCP product had a measured water solubility of 150-470 µg/L at 20 °C (ECHA, 2008). This suggests that shorter carbon chain lengths are more water soluble than longer chain lengths for a given degree of chlorination.

Variation of water solubility with chlorine content was also assessed as part of this study. The results indicate that the water solubility of C_{14} substances increases with increasing chlorine content up to 53% Cl wt. (6 chlorine atoms) and then declines.

The eMSCA notes that the lack of GLP certification is a concern for a formal regulatory study[4]. The report lacks detail about the preparation of spiked recovery samples. For example, if the test item was applied to the cartridge in a solution containing any polar/apolar solvents to enhance solubility, this could potentially cause breakthrough from the cartridges and a subsequent loss of material. No details are provided about adjustments made to the reported results because of the extraction efficiency. In addition, the report states that an approximate

[4] The laboratory indicated that it was accredited to ISO17025 from 2010 until January 2015.

volume of 3 mL of centrifuged sample was applied to the SPE cartridge; this volume should have been consistent and accurately measured for each retained 5 mL fraction that eluted from the column. These factors lead to some uncertainty about the accuracy of the results. Overall, the eMSCA considers that the results of this study are reliable with restrictions.

EC (2005) cited Madeley *et al*. (1983) as the key study at the time, which is also included as a RSS in the registration dossier with a reliability score of 1 (reliable without restriction). The test substance was prepared by mixing n-pentadecane-8-^{14}C with unlabelled C_{14-17} paraffin prior to chlorination to 51% Cl wt. The test was performed using a non-standard method. Approximately 50 mg of the test substance was weighed out onto a glass microscope slide and this was then placed in 5 litres of water. The test vessels were stirred for 91 days and then the solution was allowed to settle (without stirring) for a further 87 days to ensure that equilibrium was reached. Light was excluded. Samples were analysed by radiochemical analysis and by analysis for the parent compound by thin-layer chromatography (the method of chemical analysis is not mentioned in the RSS). The water solubility determined by the two methods was 0.005 mg/L (parent compound) and 0.027 mg/L (radiochemical) at 20 °C. The Registrants suggest that as the higher result is outside the range of other studies, it may represent both dissolved and undissolved fractions and therefore overstates the water solubility of MCCPs. However, the eMSCA considers that the presence of undissolved substance is highly unlikely given the very long settling time. Suspended or emulsified portions of the substance (if any) would have been located at the base of the test vessel. In the absence of a study report to review, the eMSCA does not know how samples were taken from the test vessels. In addition, although the water solubility result obtained using thin-layer chromatography is within the range of the values measured in the more recent study for C_{14} congeners, the reliability of the analytical method is unknown (see Section 6.3.1). The solubility measured using the radiolabel could therefore be a more accurate measurement of the total solubility.

The summary of water solubility in the registrations also mentioned Campbell and McConnell (1980) but no RSS has been prepared. This study was cited in EC (2005), which noted that the reported water solubility values for a C_{16} chlorinated n-alkane 52% Cl wt. was 0.01 mg/L in freshwater and 0.004 mg/L in seawater at 16-20 °C, but few details were available so its validity cannot be determined.

Predicted data

The eMSCA has predicted water solubility for a series of hypothetical chlorinated paraffin structures with carbon chain lengths of C_{10}-C_{18} and chlorine contents of 45, 52 and 60% Cl wt. using the WSKOWWIN v1.41 and WATERNT v1.01 models contained within the EPI Suite™ v4.11 platform (US EPA, 2012) (see Appendix A). Water solubility values ranging from 2.4×10^{-8} to 0.28 mg/L are predicted using WSKOWWIN v1.41, which is based on estimated log K_{OW} values. The WATERNT v1.01 model results in water solubility values of 6.3×10^{-7} to 0.73 mg/L, using a "fragment constant" method similar to that used to estimate log K_{OW} values. As noted in Section 6.4.3, fragment-based methods may not estimate actual log K_{OW} values of chlorinated paraffins very well, which therefore casts uncertainty about the relevance of these predictions. In addition, there is no universally accepted definition of applicability domain for either model. The maximum molecular weight for substances in the training set for both models is 627.6 g/mol. Only one of the theoretical structures that were used to make the predictions has a molecular weight greater than this. However, the lowest predicted solubility is less than the minimum solubility of the lowest solubility substance in the test set (4×10^{-7} mg/L for both models). The eMSCA considers it unlikely that the training set will have contained close analogues of MCCPs. The reliability of these predicted values is therefore highly uncertain.

Glüge *et al.* (2013) calculated subcooled-liquid solubility in water for 29 constituents of MCCPs using COSMO*therm*, SPARC and EPI Suite™, and compared the results to experimental data from the literature. In general, good or very good agreement between calculated and measured data was obtained for COSMO*therm* whilst EPI Suite™ showed the largest discrepancies. A series of recommended values were presented (see Table 13), which suggest that water solubility is likely to decrease with increasing carbon chain length, but appears to be relatively independent

of the chlorine content for a given carbon chain length, up to a chlorine content of 55% Cl wt. The C_{14} substance tested in Unpublished (2019a) had between 4 and 14 chlorine atoms per molecule. The predictions by Glüge *et al.* (2013) suggest that the range of water solubility for these constituents is 1.9 – 272 µg/L (compared to measured values of 3.56 to 11.11 µg/L in Unpublished, 2019a). In addition, the solubility maximum is predicted for a substance with 9 chlorine atoms (rather than 6 as found experimentally).

Value recommended by eMSCA

The eMSCA concludes that there are difficulties in reliably predicting or measuring the water solubility of this complex UVCB, and that citing a single value is potentially misleading. A measured total water solubility value of 0.027 mg/L [27 µg/L] at 20 °C appears to be a realistic upper limit and will therefore be used in this substance evaluation.

6.4.3 Partition coefficient n-octanol/water (log K_{OW})

Measured data

The registrations include a RSS for a new non-GLP OECD 123 (slow-stirring method) study performed voluntarily by the Registrants (Unpublished, 2019b). The Registrants assign this study a reliability score of 1 (reliable without restriction). The study report has been made available to the eMSCA for review.

The test substance was a C_{14} chlorinated n-alkane, 50% Cl wt. (the same as that used for the Unpublished (2019a) water solubility study), containing a range of C_{14} congeners with 4 to 14 chlorine atoms. A certificate of analysis for the test substance is not included in the report. The Triplicate 5 L test systems were prepared in glass vessels that had taps fitted to aid with sampling. Each test vessel contained 4 900 mL of MilliQ water and 100 mL of water saturated 1-octanol. One millilitre of a 50 mg/mL solution of test substance dissolved in 1-octanol was added to each test vessel by slowly pipetting down the wall of the test vessel. Slow-stirring (with maximum vortices between 0.5 – 2.5 cm) was performed for 5 days prior to sampling. Sampling from the test systems was performed daily from day 5 to 8. Sampling was performed with stirring stopped. Water was sampled from the tap, the first 5 mL was discarded, and the next 500 mL retained. The 1-octanol layers were sampled using 200 µL glass syringes with care taken not to disturb the organic-aqueous interface. Liquid-liquid extraction using dichloromethane was performed in the retained water samples three times. These consisted of an initial 50 mL, followed by two 25 mL extracts. These extracts were combined and reduced to dryness in an evaporator. Samples were brought up in 225 µL of acetonitrile and an internal standard of Dechlorane Plus™ (anti isomer) was added (25 µL). The 1-octanol samples (200 µL) were prepared by diluting 100 fold with acetonitrile and adding internal standard (not defined). All samples were analysed in duplicate using the same APCI-TOF-HRMS method as used in the water solubility study (see Section 6.4.2), with quantification against external standards produced from the original test substance. The limit of detection was the sum of the chlorinated paraffin congeners in the test substance (0.005 µg/L). The analytical method used is currently the best available technique, and the eMSCA recognises the expertise of the laboratory (VU Amsterdam) with regard to the analyses of these samples.

The average log K_{OW} value was 6.58 ± 0.09 at 19 °C. Other chain length constituents of MCCPs were not included in this study, so the reported value only represents a proportion of the possible constituents of commercial products. Variation of log K_{OW} for C_{14} congeners with different chlorine numbers was specifically assessed as part of the study. No trend was found. EC (2005 and 2007) also assessed how the log K_{OW} value for MCCPs varies with both chlorine content and carbon chain length, based on the studies of Sijm and Sinnige (1995) (using a slow stirring method) and Hilger *et al.* (2011a). Neither study is included in the registration dossiers. The latter study is discussed in more detail below.

The eMSCA notes that the lack of GLP certification is a concern for a formal regulatory study[5]. The following deviations from the OECD test guideline have not been acknowledged nor explained in the report:

- The experiment should be performed in the absence of light, but this is not confirmed;
- Both liquid phases should be pre-saturated with each other, but the text suggests that this was only performed for the organic phase. No reason is given for the lack of pre-saturation of the water phase;
- No details are provided about the method of stirring;
- It is not explained why Dechlorane Plus™ was chosen as the internal standard, and no results are reported for this substance;
- No details are provided about any recovery experiments performed to allow the extraction method to be assessed for efficiency.

The eMSCA therefore considers the Unpublished (2019b) study to be reliable with restrictions.

The registrations include RSS for two additional studies (Renberg *et al*., 1980; Fisk *et al*., 1998a), both previously considered in EC (2005). The Registrants rate them as reliable with restrictions. These studies measured the log K_{OW} of four substances with different degrees of chlorination (two of which had a single C_{16} carbon chain length) using either a high performance thin layer chromatography method or a HPLC technique (with radiochemical analysis). The measured log K_{OW} values were in the range 4.7-8.3. No information is provided about the internal standards or reference substances, and so the eMSCA considers that these studies provide indicative information only.

Hilger *et al.* (2011a) used a reversed-phase HPLC method with a UV detector to investigate the effects of carbon chain length, degree of chlorination and structure on log K_{OW} values for 40 chlorinated n-alkanes with carbon chain lengths between C_{10} and C_{28}, 15 individual chlorodecanes, chloroundecanes and chlorododecanes with defined chlorine positions, and a technical SCCP product. Most, but not all, of these data were obtained with substances in the C_{10} to C_{13} range with chlorine contents of 45 – 70% by weight. The reference compounds used to calibrate the method had reported log K_{OW} values of 2.34 to 7.86 and include benzene, toluene, *p*-xylene, biphenyl, *p,p'*-DDD, *p,p'*-DDT, *p,p'*-DDE, benzo[*a*]pyrene, hexachlorobenzene and diethylhexylphthalate. Log K_{OW} values were based on retention times of HPLC chromatographic peak(s)/band(s) of each substance, and the range of log K_{OW} values corresponding to the start and end of the peak(s)/band(s) was also given.

For chlorinated n-alkanes in the C_{14} to C_{17} range, corresponding log K_{OW} values were as follows (the range is given in brackets):

C_{14}, 47.0% Cl wt.	6.30	(5.56 - 7.71)
C_{15}, 50.4% Cl wt.	6.65	(5.84 - 7.81)
C_{16}, 61.0% Cl wt.	6.81	(5.78 - 8.38)
$C_{14\text{-}17}$, 46.7% Cl wt.	6.67	(5.57 - 7.90)

When the entire data set was considered, it was apparent that the log K_{OW} value was relatively independent of the chlorine content for a given carbon chain length for chlorine contents between approximately 45 and 55% Cl wt., which is consistent with the findings of Unpublished (2019b). For higher chlorine contents (up to 70% Cl wt.), the log K_{OW} increased with increasing chlorine content in a non-linear fashion[6].

[5] The laboratory indicated that it was accredited to ISO17025 from 2010 until January 2015.

[6] The correlation between chlorination degree and log K_{OW} was found to follow a second order polynomial relationship.

The effect of carbon chain length on the log K_{OW} was investigated by grouping the substances tested by similar chlorine contents (groupings of < 60% Cl wt. (45% Cl wt. - 55% Cl wt.), ca. 60% Cl wt., ca. 65% Cl wt. and ca. 70% Cl wt.; as noted above, most of the substances had carbon chain lengths in the C_{10} to C_{13} range). It was found that for a given chlorine content, the log K_{OW} values increased at an approximately constant rate for every addition of a carbon (the average increase in log K_{OW} was estimated to be around 0.29 per carbon).

Hilger *et al.* (2011a) also derived regression equations for different chlorine contents from the data generated (n stands here for carbon number):

ca. 44.8% Cl wt. and 57.7% Cl wt.	$\log K_{OW} = 0.281 \times n + 2.280$	$R^2 = 0.9967$
ca. 60% Cl wt.	$\log K_{OW} = 0.269 \times n + 2.515$	$R^2 = 0.9979$
ca. 65% Cl wt.	$\log K_{OW} = 0.276 \times n + 2.621$	$R^2 = 0.9774$
ca. 70% Cl wt.	$\log K_{OW} = 0.321 \times n + 2.576$	$R^2 = 0.9812$

The last three equations were derived with data in the C_{10} to C_{13} range only.

The eMSCA notes that this study used an indirect method for the determination of log K_{OW}. The reference substances were aromatic (monopolar) compounds, and so are not close structural analogues of chlorinated paraffins, which are apolar. Since the mobile phase was methanol/water (90:10 v/v), it is likely that the log K_{OW} values of the chlorinated paraffins were underestimated. Nevertheless, the conclusions about trends are likely to be relatively unaffected because all the values would be expected to be biased in a similar way.

Predicted data

The eMSCA has predicted log K_{OW} values for a series of hypothetical chlorinated paraffin structures with carbon chain lengths of C_{10}-C_{18} and chlorine contents of 45, 52 and 60% Cl wt. using the KOWWIN v1.68 model contained within the EPI Suite™ v4.11 platform (US EPA, 2012) (see Appendix A). This is a fragment constant method, and the range of predicted log K_{OW} is 5.79 – 11.24. Currently, there is no universally accepted definition of the applicability domain of this model. None of the test structures exceed the maximum molecular weight of the training set. The maximum number of chlorine atoms contained in a substance in the training set is 12. All of the theoretical chloroparaffins contain less than 12 chlorine atoms. On the other hand, the eMSCA considers it unlikely that the training set will have contained close analogues of MCCPs.

Appendix A compares the predicted log K_{OW} values from KOWWIN v1.68 with the data from Sijm and Sinnige (1995) and Hilger *et al.* (2011a). Table 14 shows that as the carbon chain length increases, the difference between the predicted values from KOWWIN and the values reported by Sijm and Sinnige (1995) and Hilger *et al.* (2011a) also increases.

Table 14

AVERAGE DIFFERENCE BETWEEN THE PREDICTED LOG K_{OW} VALUE FROM KOWWIN AND THE VALUE REPORTED BY SIJM AND SINNIGE (1995) AND HILGER *ET AL.* (2011a)

Chain length of chloroparaffins	Sijm and Sinnige (1995)	Hilger *et al.* (2011a)
C10	0.18	0.90
C11	0.40	1.35
C12	0.62	1.51
C13	0.98	1.90
C14	1.31	2.10
C15	1.66	2.38
C16	2.08	2.66
C17	2.59	2.95
C18	3.15	3.29

As the chlorine content increases, the difference between the predicted values from KOWWIN and the values reported by Sijm and Sinnige (1995) and Hilger *et al*. (2011a) also increases (Table 15).

Table 15

AVERAGE DIFFERENCE BETWEEN THE PREDICTED LOG K_{OW} VALUE FROM KOWWIN AND THE VALUE REPORTED BY SIJM AND SINNIGE (1995) AND HILGER *ET AL.* (2011a)		
Chlorine content of chloroparaffins	**Sijm and Sinnige (1995)**	**Hilger *et al.* (2011a)**
45	1.33	1.82
52	1.38	2.10
60	1.62	2.43

This analysis casts doubt over the reliability of the KOWWIN predictions, although the reliability of the two experimental studies is also uncertain. For example, Glüge *et al.* (2013) point out that the Sijm and Sinnige (1995) study did not correct the concentrations for recovery, so losses of the analyte during the analytical extraction might have resulted in slight over-estimates of the log K_{OW}.

Glüge *et al.* (2013) calculated log K_{OW} values for 29 constituents of MCCPs using COSMO*therm*, SPARC and EPI Suite™, and compared the results to experimental data from the literature. In general, good or very good agreement between calculated and measured data was obtained for COSMO*therm* whilst EPI Suite™ showed the largest discrepancies. A series of recommended values were presented (see Table 13). The C_{14} substance tested in Unpublished (2019b) had between 4 and 14 chlorine atoms per molecule. The predictions by Glüge *et al.* (2013) suggest that the range of log K_{OW} values for these constituents is 6.2 – 8.1, which is somewhat higher than the experimental findings. The predictions suggest that log K_{OW} values are relatively independent of chlorine content for a given carbon chain length, up to a chlorine content of 55% Cl wt. (consistent with the findings of Unpublished, 2019b). Log K_{OW} is likely to increase with chlorine content above 55% Cl wt. for a given chain length, and also to increase with increasing carbon chain length.

Value recommended by eMSCA

The eMSCA considers that the large number of constituents contained within MCCPs will lead to a range of log K_{OW} values, many of which are likely to be equal to or exceed 6.5. The Registrants' use of an average value of 7 for EUSES modelling in their CSRs is an acceptable compromise to avoid unnecessary complexity.

6.5 Manufacture and uses

6.5.1 Quantities

There are 10 active REACH Registrants listed on the ECHA dissemination portal (checked July 2019), of which six are manufacturers. The ECHA public dissemination website indicates that the registered tonnage lies in the band 10 000 – 100 000 tonnes per year.

Table 16

AGGREGATED TONNAGE (PER YEAR)				
☐ 1 – 10 t	☐ 10 – 100 t	☐ 100 – 1000 t	☐ 1000 - 10 000 t	☒ 10 000 - 50 000 t
☒ 50 000 – 100 000 t	☐ 100 000 – 500 000 t	☐ 500 000 – 1 000 000 t	☐ > 1 000 000 t	☐ Confidential

6.5.2 Overview of uses

Table 17

OVERVIEW OF USES		
Applications in the CSRs	**Exposure Scenario**	**Percentage of total tonnage assumed for the scenario**
Manufacturing	ES1: Manufacturing	100%
PVC, Polymer and Rubber	ES2: Formulation ES3: Conversion ES4: Service life	63.8%
Sealants and Adhesives	ES5: Formulation and use ES6: Outdoor service life ES7: Indoor service life	27.0%
Metalworking Fluids	ES8: Formulation ES9: Use (emulsion) ES10: Use (neat oil)	7.0%
Paints	ES14: Formulation and use ES15: Outdoor service life ES16: Indoor service life	1.3%
Textiles	ES11: Formulation and use ES12: Outdoor service life ES13: Indoor service life	0.9%
Paper Products	ES17: Manufacture of paper and recycled paper	0.3%

Former uses reported in EC (2005) were for leather fat liquors and carbonless copy paper. They are no longer included in the latest registration dossiers. No uses are advised against.

6.6 Classification and Labelling

6.6.1 Harmonised Classification (Annex VI of CLP)

Table 18 details the current harmonised classification for this substance.

Table 18

HARMONISED CLASSIFICATION ACCORDING TO ANNEX VI OF CLP REGULATION (REGULATION (EC) 1272/2008)					
Index No	**International Chemical Identification**	**Classification**		**Spec. Conc. Limits, M-factors**	**Notes**
		Hazard Class and Category Code(s)	**Hazard statement code(s)**		
602-095-00-X	Alkanes, C_{14-17}, chloro; Chlorinated paraffins, C_{14-17}	Lact. Aquatic Acute 1 Aquatic Chronic 1	H362 H400 H410	-	-

No multiplication factors (M-factors) for mixtures are given in the harmonised classification since it was introduced before the CLP Regulation was adopted.

6.6.2 Self-classification

The latest update for the Lead Registrant dossier includes an M-factor for acute and chronic aquatic hazards of 100 and 10, respectively. This is discussed further in Section 6.6.

The self-classification for physical or human health hazards is not considered in this evaluation.

6.7 Environmental fate properties

6.7.1 Degradation

The ECHA decision letter issued in 2014 requested a tiered testing approach using OECD TG 308 studies to establish if concerns over the persistent nature of some of the MCCP constituents were justified (specifically, by measuring environmental half-lives under relevant conditions). In response, the Registrants have completed the first tier of testing by conducting an OECD TG 308 water-sediment simulation study using non-radiolabelled C_{14} chlorinated n-alkane (50% Cl wt.) (Unpublished, 2019c) with further congener specific analyses performed and reported in Unpublished (2019d). A number of additional tests based on the OECD TG 301D test guideline have been included in the dossier update. These are all considered in more detail below.

6.7.1.1 Abiotic degradation

6.7.1.2 Hydrolysis

EC (2005) concluded that MCCPs is not expected to hydrolyse significantly. The registration dossiers are consistent with this information. Data waiving has been applied to the endpoint as the substance constituents have varying but low solubility in water (see Section 6.4.2).

6.7.1.3 Phototransformation/photolysis

The atmospheric half-life has been estimated to be 1 - 2 days (EC, 2005) using AOPWIN (part of the EPI Suite™ platform; US EPA, date unknown). This is based on estimated values for the second order rate constant for reaction with atmospheric hydroxyl radicals for MCCPs with chlorine contents between around 40 and 56% by weight. The registration dossiers are consistent with this information. However, it should be noted that MCCPs with >65% Cl wt. have estimated half-lives which are longer than 2 days. The longest half-life is predicted for C_{14} n-alkane, 70% Cl wt. which has a predicted half-life in air of 6.75 days.

No data are included in the registration dossiers on phototransformation of MCCPs in water or soil. Koh and Thiemann (2001) investigated the degradation of chloroparaffins in water through photochemical dechlorination. The reported half-life in water was 9.6 h and 12.8 h for a $C_{17\text{-}24}$ n-alkane, 35% Cl wt. and a $C_{12\text{-}18}$ n-alkane, 52% Cl wt., respectively. The relevance of photodegradation is likely to be low in most natural waters due to depth, turbidity, quenching agents, etc.

6.7.2 Biodegradation

6.7.2.1 Biodegradation in water

6.7.2.2 Estimated data

No estimated data were included in the registration dossiers.

The available degradation screening tests suggest that the persistence of MCCPs depends on the chlorine content of the substance (see Section 6.7.2.3). In order to explore the possible variation in degradation with structure, it is relevant to consider a weight of evidence approach based on read-across and quantitative structure-activity relationships (QSAR; see the REACH Guidance, Chapter R.7b, p. 201). The following criteria are given for the identification of a persistent substance based on BIOWIN predictions:

BIOWIN 2 <0.5 or BIOWIN 6 <0.5 and BIOWIN 3 <2.2: persistent

BIOWIN 2 <0.5 or BIOWIN 6 <0.5 and BIOWIN 3 between 2.2 and 2.7: more information needed

BIOWIN v4.10 calculations have been carried out for example structures representing each possible chlorine content within the C_{13} to C_{17} range[7]. The results of these calculations are given in Appendix A. Based on these predictions and the criteria from the REACH Guidance, an estimate of the potential persistence of each structure (in relation to the REACH Annex XIII criteria) is provided in .

Table 19.

Table 19

SUMMARY OF PREDICTED PERSISTENCE FOR CHLORINATED PARAFFINS					
Carbon chain length	**Chlorine content (% wt.)**	**BIOWIN Prediction**			**Assignment based on prediction**
		BIOWIN2	**BIOWIN3**	**BIOWIN6**	
C_{13}	28.1	0.0795	2.5915	0.0863	Further data needed
	37.0	0.0013	2.0438	0.0108	P
	44.1	0.0001	1.7945*	0.0012	P (not all predictions considered to be reliable)
	49.8	0	1.5452*	0.0001	P (not all predictions considered to be reliable)
	54.5	0	1.2959*	0	P (not all predictions considered to be reliable)
	61.7	0*	0.7973*	0	P (not all predictions considered to be reliable)
C_{14}	26.6	0.0661	2.5605	0.0883	Further data needed
	35.3	0.0068	2.3112	0.011	Further data needed
	42.3	0.0001	1.7635*	0.0013	P (not all predictions considered to be reliable)

[7] Although this evaluation concerns MCCPs (C_{14-17}), it is also relevant to consider C_{13} structures as they are potential constituents of the commercial MCCP products above 0.1% w/w (see Section 6.3).

SUMMARY OF PREDICTED PERSISTENCE FOR CHLORINATED PARAFFINS					
Carbon chain length	**Chlorine content (% wt.)**	**BIOWIN Prediction**			**Assignment based on prediction**
		BIOWIN2	**BIOWIN3**	**BIOWIN6**	
C_{14}	47.9	0	1.5142*	0.0001	P (not all predictions considered to be reliable)
	52.6	0	1.2649*	0	P (not all predictions considered to be reliable)
	62.8	0*	0.5171*	0	P (not all predictions considered to be reliable)
C_{15}	33.8	0.0055	2.2802	0.0113	Further data needed
	40.6	0.0005	2.0309*	0.0013	P (not all predictions considered to be reliable)
	46.2	0	1.4832*	0.0002	P (not all predictions considered to be reliable)
	50.8	0	1.234*	0	P (not all predictions considered to be reliable)
	54.8	0*	0.9847*	0	P (not all predictions considered to be reliable)
	61.1	0*	0.4861*	0	P (not all predictions considered to be reliable)
C_{16}	32.3	0.0007	1.9508	0.0116	P
	39.0	0.0001	1.7016*	0.0013	P (not all predictions considered to be reliable)
	44.5	0	1.4523*	0.0002	P (not all predictions considered to be reliable)
C_{16}	49.2	0	1.203*	0	P (not all predictions considered to be reliable)
	53.2	0*	0.9537*	0	P (not all predictions considered to be reliable)
	62.2	0*	0.2058*	0	P (not all predictions considered to be reliable)
C_{17}	31.0	0.0006	1.9199	0.0118	P
	37.6	0.0001	1.6706*	0.0014	P (not all predictions considered to be reliable)
	43.0	0	1.4213*	0.0002	P (not all predictions considered to be reliable)
	47.7	0	1.172*	0	P (not all predictions considered to be reliable)
	51.6	0*	0.9227*	0	P (not all predictions considered to be reliable)
	60.7	0*	0.1748*	0	P (not all predictions considered to be reliable)

*The number of chlorine atoms contained in this molecule is greater than the maximum number of instances of the fragment in any training set compound for the BIOWIN model.

Almost all of the structures are predicted to be persistent, although the predictions may not all be reliable. The REACH Guidance interpretation of the BIOWIN predictions is conservative when compared to the results of the available modified screening tests for chlorinated paraffins (Section 6.7.2.3). This may partly be due to the fact that the guidance is based on the results of standard ready biodegradation tests rather than tests that have been modified to ensure appropriate dosing of the test substance.

When considering these predictions, it is important to note that several of the constituents contain more chlorine atoms than the maximum number of instances of the fragment in any training set compound for the BIOWIN 2 and 3 models. Therefore, these constituents are outside the applicability domain of the model and the predictions may not be accurate (see the REACH Guidance, Chapter R.6: QSARs and grouping of chemicals).

The eMSCA attempted to predict the biotransformation pathways of several congeners of MCCPs using enviPath (the Environmental Contaminant Biotransformation Pathway Resource) (Wicker *et al.*, 2015). However, no pathways were returned by the model. This may be due to the high chlorine content of the MCCP constituents.

6.7.2.3 Screening tests

EC (2005) did not describe any standard ready or inherent biodegradation tests or simulation studies. Based on non-standard test data from biological oxygen demand (BOD) studies (cited in the REACH registrations as Madeley and Birtley, 1980), MCCPs was not expected to be readily or inherently biodegradable within the definition of standard screening tests. There was evidence that some microorganisms may be capable of degrading MCCPs in the environment in acclimated or cometabolic systems, but it was not possible to estimate a realistic environmental half-life. The potential for biodegradation appears to decrease with increasing chlorine content, which implies that more highly chlorinated MCCPs may be more persistent than products with low chlorine content. The most common types of MCCPs in commercial use have chlorine contents of around 45 - 52% by weight. Of these, the 52% Cl wt. product types would be expected to be more persistent than the 45% wt. product types (EC, 2005).

Since EC (2005) was published, the Registrants have performed a series of non-standard screening studies (OECD TG 301D and 302A) using a single laboratory. The studies have all been enhanced or modified through the use of solubilising agents to allow stable dispersion of the test substances through the test systems and/or by increasing the incubation period beyond 28 days. All available data are summarised below and have been reviewed in detail by the eMSCA as part of this evaluation. Unless explicitly stated, RSS have been provided for all screening tests by the Registrants in the registration dossier. Full study reports were also provided for this evaluation.

1) *Test Substance - C_{14} chlorinated n-alkane, 45% Cl wt. (Unpublished 2010a; Registrants' Validity Rating – 2; reliable with restrictions)*

A GLP-certified enhanced OECD TG 301D (closed bottle test) study was performed using C_{14} chlorinated n-alkane, 45% Cl wt. (Unpublished, 2010a). Test substance purity was reported as 99% and the average formula was $C_{14}H_{25.4}Cl_{4.6}$. No study specific purity measurements were documented and therefore this could not be verified. Secondary activated sludge from a sewage treatment plant treating predominantly domestic waste water was used to prepare the inoculum. The test substance was administered as a suspension to the test vessels. A 1 g/L stock suspension was prepared by mixing 80 mg of the test substance, 90 mg of alkylphenol polyalkoxylate (PAAP) and 0.08 L of deionised water, followed by ultrasonification for 10 minutes. The final concentration of the test substance in the test bottles was 2.0 mg/L. Both non-amended and PAAP controls were included in the experiment and sodium acetate was used as a positive control (concentration of 6.7 mg/L). The bottles were incubated at 24 °C, the exposure period was 42 days and the dissolved oxygen concentration was analysed in duplicate bottles on day

7, 14, 21, 28 and 42 of the study. The theoretical oxygen demand (ThOD) of the test substance was calculated to be 1.75 mg O_2/mg. The results are summarised in Table 20.

Table 20

RESULTS OF THE CBT WITH A C_{14} CHLORINATED N-ALKANE, 45% CL WT. SUBSTANCE						
Time (days)	**Mean dissolved oxygen concentration (mg/L)**				**Percentage degradation**	
	Control	**Control with PAAP**	**Chlorinated paraffin with PAAP**	**Positive control (sodium acetate)**	**Chlorinated paraffin**	**Positive control (sodium acetate)**
0	8.9	8.9	8.9	8.9	0%	0%
7	8.3	8.3	8.2	5.1	3%	62%
14	8.0	8.0	7.5	4.3	14%	71%
21	8.0	8.0	6.9	-	32%	-
28	7.8	7.7	5.5	-	64%	-
42	-	7.6	5.3	-	67%	-

A mean biodegradation level of 64% had occurred by day 28. Only a further 3% degradation took place over the following two weeks.

2) Test Substance - Commercial C_{14-17}, 45.6% Cl wt. (Unpublished, 2010b; Registrants' Validity Rating – 2; reliable with restrictions)

A GLP-certified enhanced OECD TG 301D study was performed using a commercial 45.6% Cl wt. MCCP product (Unpublished, 2010b). The inoculum was prepared from pre-conditioned secondary activated sludge from a sewage treatment plant treating predominantly domestic waste water. The substance was tested as a suspension. A 1 g/L stock suspension was prepared by mixing 320 mg of the test substance and 310 mg of PAAP in 0.310 L of deionised water, followed by ultrasonification for 5 minutes. The stock solution was diluted in nutrient medium in the test flasks to give a final concentration of test substance of 2.0 mg/L. The concentration of the inoculum was not reported (the test substance should be in great excess to the microbial density). A blank control, a PAAP control and a positive control (sodium acetate at a concentration of 6.7 mg/L) were also included. The bottles were incubated at 22 – 24 °C for up to 42 days and dissolved oxygen concentration analysed in duplicate bottles at intervals during the study. The ThOD of the test substance was calculated to be 1.75 mg O_2/mg [8]. The results are summarised in

Table 21.

A mean biodegradation level of 51% had occurred by day 28 and some further degradation occurred with prolonged incubation (60% at day 35 and 63% at day 42). The results show that oxygen began to be consumed in the test substance system after 14 days. This appears to be an extended lag phase, which might be explained by either an increasing bioavailability of the test substance or adaptation of the test system.

[8] For a C_{14-17}, 45.6% wt. Cl substance the actual ThOD should be around 1.73 mg O_2/mg. This is similar to, but slightly lower than the value used in the test report (the lower value will lead to a slightly higher percentage degradation for a given oxygen consumption).

Table 21

RESULTS OF THE CBT WITH A COMMERCIAL C_{14-17}, 45.6% CL WT. SUBSTANCE						
Time (days)	Mean dissolved oxygen concentration (mg/L)				Percentage degradation	
	Control	Control with PAAP	Chlorinated paraffin with PAAP	Positive control (sodium acetate)	Chlorinated paraffin	Positive control (sodium acetate)
0	8.8	8.8	8.8	8.8	0%	0%
7	8.3	8.3	8.3	4.4	0%	72%
14	7.8	7.9	7.6	3.7	9%	76%
21	7.8	7.9	6.8	-	31%	-
28	7.7	7.6	5.8	-	51%	-
35	-	7.7	5.6	-	60%	-

3) Test Substance - Commercial C_{14-17}, 63.2% Cl wt.(Unpublished, 2010c; Registrants' Validity Rating – 2; reliable with restrictions)

A GLP-certified OECD TG 301D study was performed using a commercial 63.2% Cl wt. MCCP product (Unpublished, 2010c). The same methodology was used as for the study with the 45.6% Cl wt. product (Unpublished, 2010b), with the test duration extended to 60 days, and so the concerns raised by the eMSCA are identical. The ThOD of the test substance was calculated to be 1.05 mg O_2/mg. The results are summarised in Table 22

Table 22.

Table 22

RESULTS OF THE CBT WITH A COMMERCIAL C_{14-17}, 63.2% CL WT. SUBSTANCE						
Time (days)	Mean dissolved oxygen concentration (mg/L)				Percentage degradation	
	Control	Control with solubilising agent	Chlorinated paraffin with solubilising agent	Positive control (sodium acetate)	Chlorinated paraffin	Positive control (sodium acetate)
0	8.8	8.8	8.8	8.8	0%	0%
7	8.3	8.3	8.3	4.4	0%	72%
14	7.8	7.9	7.8	3.7	5%	76%
21	7.8	7.9	7.6	-	14%	-
28	7.7	7.6	7.5	-	5%	-
42	-	7.5	7.4	-	5%	-
60	-	7.2	7.0	-	10%	-

Data from the dosed study vessels did not demonstrate a cumulative increase in the biological oxygen demand, and the degradation level appeared to fluctuate. Control vessels met the validity criteria and so the test system vessels were handled correctly. It is possible that an error was made in application of the test substance to the test vessels or a data handling error might have occurred. Nevertheless, from the results presented in Table 22, a mean biodegradation level of only 5% and 10% had occurred by days 28 and 60, respectively.

4) Test Substance - Commercial C_{14-17}, 51.7% Cl wt. (Unpublished, 2010d; Registrants' Validity Rating – 1; reliable without restrictions)

A GLP-certified enhanced OECD TG 301D study was performed using a commercial 51.7% Cl wt. MCCP product (Unpublished, 2010d). The same methodology was used as for the study with the 45.6% Cl wt. product (Unpublished, 2010c), and so the concerns raised by the eMSCA are identical. The ThOD for the test substance was 1.5 mg O_2/mg. The results of the test are summarised in Table 23.

Table 23

RESULTS OF THE CBT WITH A COMMERCIAL C_{14-17}, 51.7% CL WT. SUBSTANCE

Time (days)	Mean dissolved oxygen concentration (mg/L)				Percentage degradation	
	Control	Control with solubilising agent	Chlorinated paraffin with solubilising agent	Positive control (sodium acetate)	Chlorinated paraffin	Positive control (sodium acetate)
0	8.5	8.5	8.5	8.8	0%	0%
7	8.0	8.0	7.8	4.0	7%	74%
14	7.8	7.8	7.5	3.7	10%	76%
21	7.6	7.5	7.0	-	17%	-
28	7.6	7.5	6.7	-	27%	-
42	-	7.3	5.9	-	47%	-
60	-	7.0	5.3	-	57%	-

The degradation of the test substance did not exceed the 60% pass mark by day 28 or day 60 (although it was almost achieved by the end of the test).

5) Biodegradation tests using inocula derived from activated sludge or river water (Unpublished, 2010e; Registrants' Validity Rating – 1; reliable without restrictions)

Unpublished (2010e) reports the non-GLP assessment of biodegradability of chlorinated tetradecane (C_{14}) using enhanced ready tests. The five test substances had a chlorine content of 41.3, 45.5, 50.0, 55.0 and 60.2% by weight. A certificate of analysis was included, but there are no details of how these values were obtained. Two tests methods were used: 1) Closed Bottle Test, which was equivalent to an enhanced OECD TG 301D, using activated sludge and river water as inocula; and 2) Modified Sturm Test (batch culture), which was equivalent to OECD TG 301B. Closed bottle test systems were prepared in 300 mL test vessels. The activated sludge inoculum was prepared from secondary activated sludge from a sewage treatment plant treating predominantly domestic waste water. The river water inoculum was prepared by aeration for seven days after collection and removal of particulate matter through sedimentation. The final

concentration of activated sludge in the test vessels was 2 mg/L dry weight (dw). The river water was used undiluted. The test substance was administered as a suspension to the test vessels using single stock solutions of 1 g/L prepared in PAAP. The stock solution was diluted in nutrient medium in the test flasks to give a final concentration of test substance of 2.0 mg/L. A blank control, a PAAP control and a positive control (sodium acetate at a concentration of 6.7 mg/L) were also included. The dissolved oxygen concentration was measured at intervals throughout the study. The closed bottle test was performed in two series for the activated sludge inocula. For the first series, oxygen measurements were made on day 0, 7, 14, 21, 28, 42 and 56. For test systems dosed with C_{14} 50% Cl w/w and C_{14} 60.2% Cl w/w an additional sampling interval was performed on day 84. For the second series and the river water inoculated vessels, the sampling intervals were day 0, 7, 14, 21, 28, 42 and 56. Test vessels for the Sturm (batch culture assessment) were prepared using 20 mg dw/L of activated sludge (washed to remove chloride ions) and 40 mg/L of C_{14} (45.5%). The mineral salt medium used in this test was also free from chloride. No further details were presented.

Results were only reported for the closed bottle tests and are presented in Table 24. No explanation is provided about the omission of the Sturm test results.

Table 24

CBTs WITH C_{14} CHLORINATED N-ALKANES WITH VARYING CHLORINE CONTENT USING ACTIVATED SLUDGE OR RIVER WATER INOCULA

Substance	Inoculum	Percentage degradation on day						
		7	14	21	28	42	56	84
C_{14}, 41.3% Cl wt.	Activated sludge – series 1	18	44	54	66	71	74	-
	Activated sludge – series 2	3	34	56	62	74	83	-
	River water	13	31	48	61	62	65	-
C_{14}, 45.5% Cl wt.	Activated sludge – series 1	9	25	34	49	73	74	-
	Activated sludge – series 2	5	28	64	73	75	73	-
	River water	2	19	34	43	54	70	-
C_{14}, 50.0% Cl wt.	Activated sludge – series 1	4	13	22	29	60	63	-
	Activated sludge – series 2	1	13	46	54	71	78	-
	River water	2	6	23	43	48	63	-
C_{14}, 55.0% Cl wt.	Activated sludge – series 1	5	6	12	19	40	44	58
	Activated sludge – series 2	0	4	18	30	50	57	-
	River water	-14	-11	-4	2	21	39	-
C_{14}, 60.2% Cl wt.	Activated sludge – series 1	3	6	11	13	19	21	40
	Activated sludge – series 2	4	11	22	28	39	49	-
	River water	-11	-15	-8	-11	-11	4	-

The eMSCA concludes that C_{14} constituents with chlorine contents of 41.3% Cl wt. are readily biodegradable under the conditions of this enhanced test. The rate of biodegradation of C_{14} constituents with ≥50% Cl wt. decreases as the percentage chlorination increases.

Unpublished (2010e) states that the results for the C_{14} chlorinated n-alkane, 55.0% Cl wt. and the C_{14} chlorinated n-alkane, 60.2% Cl wt. substances using the river water inoculum showed that the endogenous respiration of the microorganisms present was inhibited by these substances, as evidenced by the negative biodegradation percentage. Whilst toxicity is a possible explanation for the lack of degradation seen in these studies, this could not be verified as no toxicity controls were performed. The OECD 301 guidance also recommends repeating such studies with either a lower concentration of the test substance or an increased concentration of inoculum solids, up to a maximum of 30 mg solids/L. The eMSCA notes that for negative biodegradation percentages to have occurred, the dissolved oxygen concentration in the test solutions must have been higher than in the solubilising agent control solution. It is difficult to assess this as these data were not reported. Therefore, it has not been possible to establish a) what the likely variability in the measured oxygen concentration would be between replicates and b) whether there was a difference in the BOD between the control and the solubilising agent control. This is important because the ThOD for the chlorinated paraffins decreases with increasing chlorine content (the ThOD of the C_{14} chlorinated n-alkane, 55.0% Cl wt. is 1.36 mg O_2/mg and the ThOD of the C_{14} chlorinated n-alkane, 60.2% Cl wt. is 1.15 mg O_2/mg). A 0.1 mg/L difference in the measured dissolved oxygen concentration between solubilising agent control and the test solution results in a calculated percentage degradation of 3.7% for the C_{14} chlorinated n-alkane, 55.0% Cl wt. substance and 4.3% for the C_{14} chlorinated n-alkane, 60.2% Cl wt. substance). Relatively small fluctuations in dissolved oxygen concentration between the solubilising agent control and the test solution can therefore result in a relatively large calculated percentage degradation (or inhibition). This will increase as the chlorine content increases.

6) Biodegradation assessment using a Sequencing Batch Reactor (Unpublished, 2010f; Registrants' Validity Rating – 2; reliable with restrictions)

Three C_{14} chlorinated n-alkanes (chlorine contents of 41.3% Cl wt., 45.5% Cl wt. and 50.0% Cl wt.) have been assessed for biodegradability in sequencing batch reactors (Unpublished, 2010f). The tests were carried out according to GLP, using an inoculum derived from secondary activated sludge from a waste water treatment plant treating predominantly domestic waste (2 g dry weight of suspended solids/L were used as the inoculum) and a chloride-free mineral salts medium was used to feed the batch reactors. As an excess of carbon is present in the test vessels in the form of the inocula solids (compared to the concentration of the test substance or the solubilising agent), the eMSCA considers these studies to be comparable to inherent biodegradation OECD TG 302A (Inherent Biodegradability: Modified SCAS Test) studies. Data generated from studies performed to this guideline cannot be used for persistence assessment because the test conditions are too favourable to the selection and/or adaptation of micro-organisms (REACH Guidance R.7b and R.11 (ECHA, 2017)).

At the start of the test the reactors were filled with 150 mL of activated sludge and aerated for 23 hours. Sampling was performed after settling for one hour, 15 mL of supernatant liquor was removed and 15 mL of mineral salts medium containing the test substance (75 mg/L of the chlorinated paraffin) and emulsifier (TWEEN® 80 also at 75 mg/L) were added as required. The units were aerated for 23 hours and the above sampling repeated daily throughout the test. Under these conditions, the units would reach an approximate steady state for a non- or slowly- degradable substance whereby the amount of substance added each day was balanced by the amount of substance or degradation product removed. It is documented that this should occur within approximately 30 days (effectively one volume replacement would occur every 10 days).

At each sampling point the supernatant was withdrawn from the reactor was analysed for non-purgeable organic carbon (NPOC) and chloride ion concentration. The NPOC was determined after filtering of the supernatant with a 0.45 µm filter and effectively represents the organic carbon remaining in solution in the test chamber (i.e. not including that lost from the test system through volatilisation or that adsorbed to particulates/not in solution). The carbon load was very high in both the solubilisation controls and the test substance exposure vessels and therefore

measurement of dissolved organic carbon and determination of inorganic carbon may have been increasingly difficult considering the very low solubility of MCCPs.

The extent of carbon removal in the reactors was determined based on the difference between the NPOC measurements in the test reactor with that in a control reactor that was fed with the emulsifier only. The data showed that essentially all of the carbon arising from MCCPs was removed, either by degradation, by filtration, by volatilisation or a combination of these processes. The omission of a true control vessel that was not being treated with either the solubilising agent or solubilising agent plus test substance would have improved confidence in the study results.

Chloride ion and carbon removal measurements are summarised in Table 25. According to the results, C_{14} chlorinated n-alkane, 41.3% Cl wt. was almost completely de-chlorinated, evolving free chloride ions. It is not possible to interpret the carbon removal results as degradation for the reasons given above.

For C_{14} chlorinated n-alkane, 45.5% Cl wt. and C_{14} chlorinated n-alkane, 60.2% Cl wt. complete liberation of chloride ions was not observed. This indicates that these substances were only partially degraded under the conditions of this test. It should be noted that the chloride ion recovery itself does not preclude that more extensive degradation of these substances could have been occurring in these tests. For example, metabolites other than chloride ion that contain chlorine may have been formed but would not have been detectable by the methods used.

Table 25

SUMMARY OF THE RESULTS OF BIODEGRADATION TESTS USING SEQUENCING BATCH REACTORS

Day	C_{14}, 41.3% Cl wt.		C_{14}, 45.5% Cl wt.		C_{14}, 50.0% Cl wt.	
	Carbon removal (%)	Chloride ion recovery (%)	Carbon removal (%)	Chloride ion recovery (%)	Carbon removal (%)	Chloride ion recovery (%)
21	101	79	104	36	107	14
27	101	81	97	37	104	16
36	101	81	102	38	105	14
41	100	83	101	31	100	12
49	97	88	101	22	106	10
76	-	101	-	57	-	9
77	-	97	-	51	-	9
78	-	92	-	51	-	7
79	98	90	100	52	103	6
80	92	91	93	54	95	5
98	-	95	-	56	-	-
105	94	94	92	63	-	-

7) Test Substance - C_{15} chlorinated n-alkane, 51% Cl wt. (Unpublished, 2014a; Registrants' Validity Rating – 1; reliable without restrictions)

A GLP-certified enhanced OECD TG 301D study was performed using C_{15} chlorinated n-alkane, 51% Cl wt. (Unpublished, 2014a). The inoculum was prepared from secondary activated sludge from a sewage treatment plant treating predominantly domestic waste water. The inoculum concentration was 2 mg dry weight/L and was not pre-adapted. The substance was tested as a suspension using PAAP and the final concentration of test substance was 2.0 mg/L. Blank controls, PAAP controls and a positive control (sodium acetate) were also included. The bottles were incubated at 22 – 24 °C for up to 60 days and dissolved oxygen concentration analysed in duplicate bottles at intervals during the study. The ThOD of the test substance was calculated to be 1.52 mg O_2/mg. The results are summarised in Table 26.

Table 26

RESULTS OF THE CBT WITH C_{15} CHLORINATED N-ALKANE, 51% CL WT. SUBSTANCE USING ACTIVATED SLUDGE AS INOCULUM		
Time (days)	**Percentage degradation (%)**	
	Chlorinated paraffin (based on O_2 consumption)	**Positive control (sodium acetate)**
14	17	87
21	23	-
28	43	-
42	50	-
60	63	-

The degradation of the test substance did not exceed the 60% pass mark by day 28, but had by day 60.

8) *Test Substance - C_{15} chlorinated n-alkane, 51% Cl wt. (Unpublished, 2014b; Registrants' Validity Rating – 1, reliable without restriction)*

A GLP-certified enhanced OECD TG 301D study was performed using C_{15} chlorinated n-alkane, 51% Cl wt. (Unpublished, 2014b). The inoculum was river water, and the test substance suspension was prepared using an unspecified solubilising agent. The test conditions were otherwise the same as for Unpublished (2014a). The results are summarised in Table 27.

Table 27

RESULTS OF THE CBT WITH C_{15} CHLORINATED N-ALKANE, 51% CL WT. SUBSTANCE USING RIVER WATER AS INOCULUM		
Time (days)	**Percentage degradation (%)**	
	Chlorinated paraffin (based on O_2 consumption)	**Positive control (sodium acetate)**
14	13	81
21	20	-
28	37	-
42	47	-
60	57	-

The degradation of the test substance did not exceed the 60% pass mark by day 60.

9) Test Substance - C_{14} chlorinated n-alkane, 50% Cl wt. (Unpublished 2018a, Registrants' Validity Rating – 1, reliable without restriction)

A GLP-certified enhanced OECD TG 301D study was performed using C_{14} chlorinated n-alkane, 50.07% Cl wt. (Unpublished, 2018a). The test substance purity was stated to be 100%, with compositional details presented in an analytical report (although no certificate of analysis was provided). The inoculum was secondary activated sludge from a sewage treatment plant treating predominantly domestic waste water. The activated sludge was pre-conditioned (aerating 0.4 g dw/L activated sludge solids) to reduce the endogenous respiration rates. This non-adapted sludge was diluted to a final concentration of 2.0 mg/L in each test vessel. Blank controls, PAAP controls and a positive control (sodium acetate) were also included. Concentrations of test substance, emulsifier (PAAP) and sodium acetate were 2.0, 2.0 and 6.7 mg/L, respectively. The temperature range measured during the exposure period was 22.1 to 23.2 °C (within the desired range detailed in the test guidelines). Dissolved oxygen concentrations were measured in duplicate bottles for each exposure scenario. Sampling intervals for inoculum plus emulsifier and inoculum, emulsifier plus test substance exposure vessels were 0 d, 7 d, 14 d, 21 d, 28 d, 42 d, 60 d and 120 d. Sampling intervals for the inoculum only vessels were 0 d, 7 d, 14 d, 21 d and 28 d. Sampling for the emulsifier and sodium acetate exposure vessels were 0 d, 7 d and 14 d. The ThOD of the test substance was calculated to be 1.54 mg O_2/mg.

In addition to determination of dissolved oxygen, isomeric specific analyses were performed, and samples were prepared for dissolved and non-dissolved fractions. These samples were subjected to two-dimensional gas chromatography electron capture detection (GCxGC-ECD) and atmospheric-pressure chemical ionization time-of-flight mass spectrometry (APCI-TOF-MS) for quantification of C_{14} congeners (40 - 65% Cl wt.). No extraction efficiencies or method development details were reported. The results are summarised in Table 28.

Table 28

RESULTS OF THE CBT WITH C_{14} CHLORINATED N-ALKANE, 50% CL WT. SUBSTANCE			
Time (days)	**Percentage degradation (%)**		
	Chlorinated paraffin (based on O_2 consumption)	**Chlorinated paraffin (based on test material)**	**Positive control (sodium acetate)**
7	3	-	73
14	13	-	83
21	29	-	-
28	45	-	-
42	51	-	-
60	61	88	-
120	61	85	-

Based on oxygen consumption, 45% biodegradation of the test substance had occurred by day 28 which continued with prolonged incubation (51%, 61% and 61% at days 42, 60 and 120, respectively). Therefore, although the test substance cannot be considered to meet the criteria for ready biodegradation in this test, the results show that degradation was occurring throughout, up to around 60 days, after which it appears to have stopped.

The final report presents the following data with regards to the additional analyses:

- 92.2% and 97.8% of C_{14} chlorinated n-alkane, 50% Cl wt. was bound to particles at day 0 and day 120, respectively.
- The dissolved fraction contained 7.6% and 1.9% of the test substance at days 0 and 120, respectively.
- The total removal of the test substance was 88% at day 60, and 85% at day 120.

From the information presented in the final study report and the CSR (2018), the eMSCA has not been able to verify these statements. No details were presented for extraction recoveries or method development for suspended solid extraction, liquid-liquid extraction, or acknowledgement of adherence to test vessels and processing glassware. The eMSCA therefore considers the results based on oxygen consumption to be the most reliable.

10) Test Item - C_{14} chlorinated n-alkane, 55% Cl wt. (Unpublished 2018b, Registrants' Validity Rating – 1, reliable without restriction)

A GLP-certified OECD TG 301D study was performed using C_{14} chlorinated n-alkane, 55.34% Cl wt. (Unpublished, 2018b). The test substance purity was stated to be 100%, with compositional details presented in an analytical report (although no certificate of analysis was provided). The same method and analyses were carried out as for Unpublished (2018a). The ThOD of the test substance was calculated to be 1.36 mg O_2/mg. The results are summarised in Table 29.

Table 29

RESULTS OF THE CBT WITH C_{14} CHLORINATED N-ALKANE, 55% CL WT. SUBSTANCE

Time (days)	Percentage degradation (%)		
	Chlorinated paraffin (based on O_2 consumption)	Chlorinated paraffin (based on test material)	Positive control (sodium acetate)
7	0	-	73
14	0	-	83
21	0	-	-
28	4	-	-
42	11	-	-
60	15	46	-
120	22	51	-

Based on oxygen consumption, 4% biodegradation had occurred by day 28 and further degradation occurred with prolonged incubation (reaching 22% at 120 days).

The final report presents the following data with regards to the additional analyses:

- 88.0% and 91.4% of C_{14} chlorinated n-alkane, 55% Cl wt. was bound to particles at day 0 and day 120, respectively.
- The dissolved fraction contained 11.6% and 7.7% of the test substance at days 0 and 120, respectively.
- The total removal of the test substance was 46% at day 60, and 51% at day 120.

For the same reasons as Unpublished (2018a), the eMSCA considers the results based on oxygen consumption to be the most reliable.

11) Test Substance - C_{14} chlorinated n-alkane, 60% Cl wt. (Unpublished 2018c, Registrants' Validity Rating – 1, reliable without restriction)

A GLP-certified OECD TG 301D study was performed using C_{14} chlorinated n-alkane, 60.14% Cl wt. (Unpublished, 2018c). The test substance purity was stated to be 100%, with compositional details presented in an analytical report (although no certificate of analysis was provided). The same method and analyses were carried out as for Unpublished (2018a). The ThOD of the test substance was calculated to be 1.17 mg O_2/mg. The results are summarised in Table 30.

Table 30

RESULTS OF THE CBT WITH C_{14} CHLORINATED N-ALKANE, 60% CL WT. SUBSTANCE			
Time (days)	**Percentage degradation (%)**		
	Chlorinated paraffin (based on O_2 consumption)	**Chlorinated paraffin (based on test material)**	**Positive control (sodium acetate)**
7	0	-	73
14	0	-	83
21	0	-	-
28	8	-	-
42	13	-	-
60	8	39	-
120	13	77	-

Based on oxygen consumption, 8% biodegradation had occurred by day 28, reaching 13% after 120 days, although due to fluctuations it appears that there may have been very little degradation over the final three months.

The final report presents the following data with regards to the additional analyses:

- 97.6% and 93.3% of C_{14} chlorinated n-alkane, 60% Cl wt. was bound to particles at day 0 and day 120, respectively.
- The dissolved fraction contained 2.0% and 6.2% of the test substance at days 0 and 120, respectively.
- The total removal of the test substance was 39% at day 60, and 77% at day 120.

For the same reasons as Unpublished (2018a), the eMSCA considers the results based on oxygen consumption to be the most reliable.

12) Test Substance - C_{15} chlorinated n-alkane, 51% Cl wt. (Unpublished 2018d; Registrants' Validity Rating – 1, reliable without restrictions)

A GLP-certified OECD TG 301D study was performed using C_{15} chlorinated n-alkane, 51.12% Cl wt. (Unpublished, 2018d). The test substance purity was stated to be 100%, with compositional details presented in an analytical report (although no certificate of analysis was provided). The same method and analyses were carried out as for Unpublished (2018a). The ThOD of the test substance was calculated to be 1.75 mg O_2/mg. The results are summarised in Table 31.

Table 31

RESULTS OF THE CBT WITH C_{15} CHLORINATED N-ALKANE, 51% CL WT. SUBSTANCE			
Time (days)	**Percentage degradation (%)**		
	Chlorinated paraffin (based on O_2 consumption)	**Chlorinated paraffin (based on test material)**	**Positive control (sodium acetate)**
7	3	-	73
14	3	-	83
21	10	-	-
28	20	-	-
42	30	-	-
60	40	-	-
120	50	86	-

Based on oxygen consumption, 20% biodegradation had occurred by day 28 and further degradation occurred with prolonged incubation (reaching 50% after 120 days). Unpublished (2018d) concludes that this level of degradation means that the test substance should be classed as inherently biodegradable. However, since the study was not performed using OECD TG 302B or OECD TG 302C, the eMSCA considers that no conclusion can be made concerning inherent biodegradability.

The final report presents the following data with regards to the additional analyses:

- 91.3% and 98.9% of C_{15} chlorinated n-alkane, 51% Cl wt. was bound to particles at day 0 and day 120, respectively.
- The dissolved fraction contained 8.2% and 0.3% of the test substance at days 0 and 120, respectively.
- The total removal of the test substance was 86% at day 120.

For the same reasons as Unpublished (2018a), the eMSCA considers the results based on oxygen consumption to be the most reliable.

Discussion

The REACH Guidance R7.9.4 clearly states that the validity criterion of achieving the pass level within a 10-day window for OECD TG 301D studies is not relevant for a substance that is composed of a homologous series of constituents, such as MCCPs. The reason is that the various constituents may not necessarily be degraded by a single microorganism, nor at the same rate. Therefore, as the test generates a single biodegradation curve (effectively the sum of the individual biodegradation curves) it is possible that the 10-day window criterion is met for some of the constituents making up the curve. However, the REACH Guidance also states that enhanced biodegradation screening tests that do not reach the pass criteria for a ready biodegradation study without amendment to the study design cannot be used to reach a conclusion of ready biodegradabability.

Comparison of data from different studies that use the same test substance should also be undertaken with caution, because inocula composition will always be variable, even when sampled from the same sewage treatment works or river. Impurities may also add to biological oxygen demand, positively biasing the results.

The studies deviate from the OECD 301D test guideline in some respects:

i) Ammonium chloride was omitted from the mineral medium prescribed in the test guideline to prevent oxygen consumption resulting from nitrification. It was reported that this omission did not result in nitrogen limitation as shown by the biodegradation of the reference compound. However, the degradation of the reference compound occurred over the first 14 days and so this comparison does not provide any information on potential nitrogen limitation during prolonged incubation.

ii) The inoculum used in some of the tests was secondary activated sludge from a sewage treatment plant treating predominantly domestic waste water. Although full details are not available for all studies, it appears that the initial activated sludge (400 mg dry weight/L) was aerated for one week prior to use, and this was diluted to a concentration of 2 mg dry weight/L for use in the test. The introductory section to the OECD Test Guidelines on ready biodegradability indicates that the preferred inoculum source for the closed bottle test method is a coarsely filtered (or settled) secondary effluent from a domestic waste water treatment plant or laboratory-scale unit as a more dilute inoculum without sludge flocs is needed. The concentration of such an effluent-derived inoculum to be used is ≤5 mL/L (giving an approximate cell count of 10^4 - 10^6 cells/L). Based on the reported concentrations of activated sludge used it appears that around 5 mL/L of the activated sludge was added as the inoculum in most of the studies. However, it is not clear if the cell counts present in the activated sludge test medium were analogous to that of the preferred secondary effluent medium. It is likely that the use of the activated sludge will have meant that the cell concentration was exceeded. However, during preparation the activated sludge was kept for longer than a week before being used in the test. It is not specified if the sludge was fed. There are also no details about the storage temperature or pH adjustments that are needed to keep a sludge healthy over a period of time.

iii) Due to inconsistent information presented in the various reports, it has not always been possible to assess individual studies against the validity criteria of OECD TG 301D. These include – but are not necessarily limited to – a lack of data or graphical representations of biodegradation of the test chemical/reference substances that would allow verification of lag and biodegradation phases; omission of positive controls in a few studies; and no toxicity controls were included in any of the study designs.

Despite these deviations, the tests appear to have been performed well. The use of results from enhanced ready biodegradation tests in assessments of persistence in relation to the Annex XIII criteria is discussed in detail in the REACH Guidance. The main points are summarised below:

- Very high test substance concentrations increase the probability of mass transfer issues for test substances with a low water solubility. In this case, the studies were all conducted with a test concentration of 2 mg/L, which appears to be at least two orders of magnitude higher than the water solubility limit (≤0.027 mg/L) (Chapter R.7b, p. 209).

- Low test concentrations (2-5 mg/L) used for the closed bottle test can sometimes lead to an overestimate of the degradation owing to the poor signal-to-noise ratio (theoretical versus background) in the test (Chapter R.7b, p. 209).

- Poorly soluble substances present difficulties in carrying out standard ready biodegradation tests, so modifications are permitted to improve bioavailability (for example by use of a solubiliser (see Appendix 7.9 - 3 of Chapter R.7b of the REACH Guidance); this is also allowable in the OECD Test Guideline itself). This creates a suspension, potentially limiting adherence to any residual particulate matter or the glass walls of the test vessels.

- If sufficient degradation is shown in an enhanced biodegradation screening test, i.e. the pass level as given in the test guidelines for ready biodegradation is reached (60% of ThOD within 28 days for respirometric methods), the substance can be considered "not

persistent" within the meaning of the Annex XIII criteria. In this case, the 10-day window does not need to be fulfilled (Chapter R.11, p. 51 (ECHA, 2017)).

- Enhanced screening studies that involve an extended timescale to allow time for adaptation to occur should be carried out using a natural medium as the source of inoculum (i.e. marine or freshwater). Extended studies using inocula derived from sewage treatment works cannot be used in PBT/vPvB assessments (Chapter R.7b, p. 198 & 217). This is particularly important to note because a number of the MCCP studies involving timescales above 28 days used inocula derived from sewage treatment works.
- The REACH Guidance recommends the use of a poorly soluble positive reference compound rather than the normal positive reference substance in tests with poorly soluble substances (Appendix 7.9 - 3 of Chapter R.7b of the REACH Guidance (p. 273)). Most of the studies for MCCPs used sodium acetate as the reference compound, which is easily degradable under the conditions of these tests. This offers little support in the assessment of poorly soluble substances other than to demonstrate that the inoculum is active.

Taking account of these considerations, the overall results of the various screening tests are presented in Table 32. Studies that more closely resemble inherent biodegradability assessments have not been included.

Table 32

SUMMARY OF MODIFIED AND ENHANCED READY BIODEGRADATION TEST RESULTS						
Substance tested	**Inoculum**	**Administration method**		**Pass/fail**		**Reference**
				Modified	**Modified & Enhanced**	
C_{14}, 41.3% Cl wt.	Activated sludge	Suspension using alkylphenol polyalkoxylate (PAAP)	Series 1	Pass	Pass	Unpublished (2010e)
			Series 2	Pass	Pass	Unpublished (2010e)
	River water	Suspension using PAAP		Pass	Pass	Unpublished (2010e)
C_{14}, 45.5% Cl wt.	Activated sludge	Suspension using PAAP	Series 1	Fail	Pass	Unpublished (2010e)
			Series 2	Pass	Pass	Unpublished (2010e)
	Activated sludge	Suspension using PAAP		Pass	Pass	Unpublished (2010a)
	River water	Suspension using PAAP		Fail	Pass	Unpublished (2010e)
C_{14}, 50% Cl wt.	Activated sludge	Suspension using PAAP	Series 1	Fail	Pass	Unpublished (2010e)
			Series 2	Fail	Pass	Unpublished (2010e)
	Activated sludge	Suspension using PAAP		Fail	Pass	Unpublished (2018a)
	River water	Suspension using PAAP		Fail	Pass	Unpublished (2010e)

SUMMARY OF MODIFIED AND ENHANCED READY BIODEGRADATION TEST RESULTS						
Substance tested	**Inoculum**	**Administration method**		**Pass/fail**		**Reference**
				Modified Ready Test	**Modified & Enhanced Ready Test**	
C_{14}, 55% Cl wt.	Activated sludge	Suspension using PAAP	Series 1	Fail	Fail	Unpublished (2010e)
			Series 2	Fail	Fail	Unpublished (2010e)
	Activated sludge	Suspension using PAAP		Fail	Fail	Unpublished (2018b)
	River water	Suspension using PAAP		Fail	Fail	Unpublished (2010e)
C_{14}, 60% Cl wt.	Activated sludge	Suspension using PAAP	Series 1	Fail	Fail	Unpublished (2010e)
			Series 2	Fail	Fail	Unpublished (2010e)
	Activated sludge	Suspension using PAAP		Fail	Fail	Unpublished (2018c)
	River water	Suspension using PAAP		Fail	Fail	Unpublished (2010e)
C_{15}, 51% Cl wt.	Activated sludge	Suspension using PAAP		Fail	Fail	Unpublished (2018d)
	Activated sludge	Suspension using PAAP		Fail	Pass	Unpublished (2014a)
	River water	Unspecified solubilising agent		Fail	Fail	Unpublished (2014b)
C_{14-17}, 45.6% Cl wt.	Activated sludge	Suspension using PAAP		Fail	Pass	Unpublished (2010b)
C_{14-17}, 51.7% Cl	Activated sludge	Suspension using PAAP		Fail	Fail	Unpublished (2010d)
C_{14-17}, 63.2% Cl wt.	Activated sludge	Suspension using PAAP		Fail	Fail	Unpublished (2010c)

Note: 'Modified' means use of solubiliser. 'Enhanced' means extended timescale. Light brown shading indicates that although the pass level was achieved after 28 days, the inoculum was not appropriate for a conclusion relating to the Annex XIII criteria.

It can be concluded from Table 32 that C_{14} chlorinated n-alkane, 41.3% and 45.5% Cl wt. meet the criteria for ready biodegradation in a modified ready test using alkylphenol polyalkoxylate to increase availability. Although C_{14} chlorinated n-alkane, 50% Cl wt. failed to meet the criteria for ready biodegradation, it met the 60% pass threshold after 56 days when river water was

used as the inoculum.[9] The alkane chains would typically have around four to five chlorine atoms per molecule on average.

The overall level of degradation appears to decline with increasing numbers of chlorine atoms. Both the 55% and 60% Cl wt. C_{14} chlorinated n-alkane failed to meet the pass threshold even after extended timescales using inocula derived from activated sludge. The alkane chains would typically have around six to nine chlorine atoms per molecule on average. Similarly, C_{15} chlorinated n-alkane, 51% Cl wt. failed to meet the pass threshold after an extended timescale in river water (although it achieved up to 63% degradation after 60 days using inocula derived from activated sludge). The alkane chains would typically have around six to seven chlorine atoms per molecule on average.

The interpretation of the results for test substances containing a mixture of alkane chain lengths is complicated, because no details about the proportion of different chain lengths are available. $C_{14\text{-}17}$ chlorinated n-alkane, 45.5% Cl wt. is not readily biodegradable, but more than 60% degradation was seen after extended timescales (i.e. after 28 days) using inocula derived from activated sludge (no data are available using river water as the inoculum, although the degradation rate would be expected to be slower). Although it may contain a significant proportion of constituents (e.g. C_{14}) that are readily biodegradable, some constituents with longer chain lengths and/or a greater number of chlorine atoms are clearly less degradable.

Both the 51.7% and 63.2% Cl wt. $C_{14\text{-}17}$ chlorinated n-alkane failed to meet the pass threshold after extended timescales using inocula derived from activated sludge (no data are available using river water as the inoculum, although the degradation rate would be expected to be slower), although the former substance only narrowly failed (57% degradation was achieved after 60 days).

Longer chain lengths would be expected to be less water soluble and more adsorptive than the C_{14} and C_{15} substances, but there are no degradation data for specific C_{16} or C_{17} substances, so the actual influence of chain length is unknown. However, both C_{10} chlorinated n-alkane, 65% Cl wt. (~ 6 - 7 chlorine atoms per molecule) and C_{13} chlorinated n-alkane, 65% Cl wt. (~ 7 - 9 chlorine atoms per molecule) have long degradation half-lives in sediment (e.g. 335 and 680 days, respectively, in marine sediments) (see Section 6.7.2.4).[10] This suggests that chlorine content is a key factor in degradation behaviour regardless of chain length. It can tentatively be concluded that n-alkanes in MCCPs that contain six or more chlorine atoms per molecule are potentially persistent.

6.7.2.4 Simulation tests (water and sediments)

The ECHA decision letter requested a tiered testing approach to assess concerns about the persistence of MCCPs (ECHA, 2014). The first stage was an OECD TG 308 study on a C_{14} chlorinated n-alkane with a chlorine content of 50 – 52% by weight. If this substance was found not to be persistent, the tiered approach required an additional OECD TG 308 study on a C_{14}

[9] Some additional Closed Bottle tests were reported previously for a C_{14}, 45% wt Cl substance, and briefly summarised in EA (2010). Few test details are available, but they appear to have used the same general methodology as those reported here, but using different administration methods (dichloromethane, silicon oil, 'silicon oil plus surfactant' or 'surfactant' alone) and/or a slightly lower test concentration (1 mg/L). Of four tests using activated sludge as the inoculum, one met the ready biodegradation criterion (66% after 28 days). All four passed the threshold after 42 days. Three studies used river water as the inoculum, and one of those met the ready biodegradation criterion (64% after 28 days). All three passed the threshold after 42 days. These results are consistent with the result of the study reported by the Registrants.

[10] Appendix E summarises the findings of a Closed Bottle test performed with $C_{10\text{-}13}$, chlorinated n-alkane, 49.8% Cl wt. (Unpublished, 2010g). This substance was found to be readily biodegradable when surfactant was used to enhance bioavailability.

chlorinated n-alkane with a chlorine content of 55 - 60% by weight. If this substance was also found not to be persistent, a third OECD TG 308 study using a C_{15} chlorinated n-alkane with a chlorine content of 51% by weight was required. The Registrants were given the option of reading across the results of any of the tests if persistence was confirmed.

An OECD TG 308 study conducted at 12 °C in the dark using non-radiolabelled C_{14} chlorinated n-alkane, 50% Cl wt. has been performed in accordance with GLP (Unpublished, 2019d). The Registrants rate it as 'reliable without restriction'. The original test report was provided to the eMSCA for review in 2019. The study was conducted under aerobic conditions using two types of natural sediment and their associated overlying waters: a high organic carbon sediment (4.65%) with a fine texture (Brandywine Creek) and a low organic carbon content (0.55%) with a coarse texture (Choptank River). The samples were taken from the entire 5 – 10 cm of the upper sediment layers, covered by approximately 10 - 15 cm of water at the time of collection. The sediments were analysed for chlorinated paraffin content and none was found. The test report does not describe storage conditions between collection and preparation of the test vessels. Sediment was separated and wet sieved using a 2 mm sieve. Prior to filling the test vessels, it was determined that the moisture content of the Brandywine sediment was too high to achieve the required layer depth and dry weight of sediment for testing, so the moisture content was reduced by centrifugation of a portion of the sediment. The test vessels were 50 mL plastic centrifuge tubes with conical bases. The set-up of the test vessels deviated significantly from the test guideline requirements (paragraph 32) that state '*the test should be performed in incubation apparatus with a water/sediment volume ratio between 3:1 and 4:1, and a sediment layer of 2.5 cm (±0.5 cm). A minimum amount of 50 g of sediment (dry weight basis) per incubation vessel is recommended*.' It has not been possible to calculate the actual water: sediment ratio as the test vessels had conical bases and no measurements have been provided of depth or density of the sediments. The test vessels were very small and unusually shaped for a simulation study. Test vessels were acclimated for 12 days prior to dosing. The test substance was dissolved in a solvent and mixed with fine quartz sand before the solvent was removed via rotary evaporation. The treated sand was then applied to each test vessel to give a nominal test substance concentration of 5 µg/g dw in sediment. The treated sand was noted to disperse quickly from the overlying water to the sediment layer. Test vessels were gently shaken to stimulate aeration without visible disturbance of the sediment layer. The vessels were covered with surgical tape to allow air transfer to the water layers during incubation. Volatile losses were not expected – the eMSCA notes that humidified air is usually used to prevent and reduce evaporation, but the test report does not mention whether this was the case in this study.

Test sub-groups consisted of treated live vessels, treated inactivated vessels (inactivated by freezing immediately after dosing), and untreated (blank) control vessels. The inactivated vessels were included to provide a reference for non-biological losses and/or changing extraction efficiencies and analytical quantification with time. However, no details of how each of these were addressed has been included in the study protocol or the study report. Additional vessels were set up for characterization measurements (without addition of test substance), and were maintained under the same test conditions as vessels used to monitor transformation.

Parameter measurements consisted of pH, total organic carbon (TOC), dissolved oxygen (DO), redox, and microbial biomass measurements for both the water and sediment made at the start of acclimation, and day 0, 60 and 120. The measurement of pH (in overlying water), dissolved oxygen concentration (in overlying water) and redox (in overlying water, upper sediment and lower sediment) throughout the acclimation and exposure period are necessary to demonstrate that equilibrium had been achieved in the test system prior to application of the test item, and that the test system was at a steady state throughout the exposure period. However, no assessment of this appears to have been performed in this study. The eMSCA notes that the equilibration requirements of OECD TG 308 were not met for the sediment compartment in this study. Twelve days is a very short time period for these test systems to equilibrate into the different redox layers in the sediment; macroscopic separation of phases (i.e. the establishment of aerobic and anaerobic/anoxic layers) should be visible to the naked eye. From the pH and DO measurements, the overlying water can be concluded to be aerobic. Oxidising conditions were established in the sediments. However, further to this, oxidising conditions need to be

established in the upper sediment (E_h > - 80 mV) and reducing conditions (E_h -80 to 190 mV; but can be a lot lower) in the lower portions. The characterization measurements made during the study indicated that aerobic conditions were maintained for the duration of incubation. However, test guideline requirements for test system parameters to be at a steady state were not met.

Test vessels were sacrificed on days 0, 15, 30, 45, 60, 91 and 120 (the test guideline specifies that the test should not be run for longer than 100 days). Samples were freeze-dried and kept frozen until termination of the incubation period, when they were transferred to an academic laboratory specialising in the analysis of MCCPs. The eMSCA notes that total removal of water can increase encapsulation of the substance in the sediment structure and reduce its availability during extraction processes. At the academic laboratory, exposure samples were transferred in their entirety to Accelerated Solvent Extraction (ASE) cells. The test vessels were rinsed with hexane, and the rinse transferred to the extraction cells. In addition Dechlorane Plus™ was added as an internal standard. Three extraction cycles of hexane:acetone (3:1, *v/v*) at elevated temperature and pressure were performed. After extraction was completed isooctane was added and the total extract was evaporated to ~1 mL. The concentrated evaporates were then cleaned using apolar solvents and silica gel columns. Additional cleaning steps were required to remove impurities that were causing signal suppression in the detector. These extracts were evaporated to dryness and dissolved in acetonitrile before analyses using APCI-TOF-HRMS. Quantification was performed against external standards. This is a recently developed congener-specific method, and the eMSCA believes it is reliable (although a radiolabelled study could have produced better data in terms of mass balance and compartment association). The results were presented in an Excel™ spreadsheet attached to the RSS. The study report states that the measured concentrations are in µg/L but the graphs state that the concentrations are in ng/L. It is assumed that the concentrations are in µg/g as the nominal dosed concentration was 5 µg/g dw. Results of the analyses of the spiked sand extracts (essentially the application solution) indicated that the nominal concentration of 100 µg/g was marginally exceeded and measured to be 105 µg/g. Congener analysis indicated that the observed distribution and signal intensities were practically identical to that of the test substance. No data were presented by the performing laboratory about the use of Dechlorane Plus™ as a control in the extraction process.

For both high and low organic carbon sediment systems the mean measured concentrations from all sampling intervals did not deviate by greater than 8% (calculated relative standard deviation; RSD) of the applied nominal concentration (5 µg/g), with the exception of one sampling interval (an RSD of 19% was reported for the low organic carbon test system at 91 days). Desired recoveries of material for non-labelled analysis are between 70 and 110% of nominal. Values measured in this study indicated that no material is unaccounted for. Acceptable variations around these values will likely have been incurred through the extraction process and general handling. The Registrants conclude that chemical analysis showed no observable biotransformation, and so the sediment half-life was >120 days at 12 °C under the conditions of this study. Congener-specific analyses were presented for the extracted samples and no significant variation was observed between these extracts, the extracted spiked sand and the original test substance. The eMSCA notes that the lack of degradation seen in this study may be due to a reduction in bioavailability due to sediment sorption processes.

Further OECD TG 308 studies to assess a C_{14} chlorinated n-alkane, 55-60% Cl wt. and C_{15} chlorinated n-alkane, 51% Cl wt. were waived by the Registrants with the following justifications: "*The C_{14} chlorinated n-alkane, 55-60% Cl wt. study is not needed because the congener analysis of the C_{14} chlorinated n-alkane, 50% Cl test material will include the same congener groups as in this test material*" and "*The C_{15} chlorinated n-alkane, 51% Cl wt. test material was shown to be inherently biodegradable in closed bottle tests with 63% biodegradation at Day 60. This test material also has similar results to the C_{14} chlorinated n-alkane, 50% Cl wt. test material in CBT studies*". The eMSCA does not agree that it can be concluded that C_{15} chlorinated n-alkane, 51% Cl wt. is inherently biodegradable from the evidence included in the dossier (see Section 6.7.2.3). Based on the results of the water-sediment simulation study with C_{14} chlorinated n-alkane, 50% Cl wt., the eMSCA considers that these other two substances are unlikely to undergo

biodegradation under the conditions of this test, and so their sediment half-lives will also be longer than 120 days at 12 °C.

Other simulation studies

Relatively short half-lives of 12 days and 58 days have been reported in aerobic sediment for two MCCPs (^{14}C-labelled $C_{16}H_{30.7}Cl_{3.3}$ (35% Cl wt., labelled in the 1-position) and $C_{16}H_{20.6}Cl_{13.4}$ (69% Cl wt., uniformly labelled)) at 11.6 °C (Fisk *et al.*, 1998a). This study is included in the registration dossier as 'reliable with restrictions'. However, the eMSCA considers that the analytical method was not sufficient to draw any conclusion about transformation rates. These data were collected as part of a study investigating the accumulation of MCCPs in oligochaetes (*Lumbriculus variegatus*), and are summarised in EC (2005). The reported degradation was based on the difference between toluene-extractable ^{14}C-measurements (taken to represent unchanged chlorinated paraffins) and total ^{14}C-measurements in the sediment. Therefore the quoted half-lives depend on the assumption that the non-extractable ^{14}C represented total degraded chlorinated paraffins. It should also be noted that the report does not differentiate between dissipation half-life and transformation half-life. The performing laboratory should have calculated both. It is not known if the authors tried to examine non-extractable residues (NER). As no elevated temperature/pressure or acidic extraction conditions were examined, it must be assumed that all bound residues are parent substance. In addition, if no degradation was observed in chromatographic profiling of the solvent extracts then it is highly unlikely that degradation to more strongly bound moieties occurred to a significant level. It is also worth noting that, based on the available screening data in Section 6.7.2.3, the 35% Cl wt. substance would be expected to be readily biodegradable but the 69% Cl wt. would not.

Biodegradation simulation studies using the OECD TG 308 were performed for SCCPs and the results were summarised in ECHA (2008). A C_{10} chlorinated n-alkane, 65% Cl wt. (~ 7 chlorine atoms per molecule) and a C_{13} chlorinated n-alkane, 65% Cl wt. (~ 9 chlorine atoms per molecule) had degradation half-lives of 335 and 680 days, respectively, in marine sediments and 1 340 and 1 790 days, respectively, in freshwater sediments. The half-lives have been extrapolated beyond the 100-d exposure period and therefore should be treated with caution.

6.7.2.5 Other information

Iozza *et al.* (2008) investigated the levels of chlorinated paraffins, including MCCPs, in a dated sediment core from Lake Thun, Switzerland. These data were not considered directly in the registration dossiers. The lake is located in a rural, densely populated alpine catchment area without any known point sources (e.g. metal or polymer industries). The sediment core was collected in May 2004 at a depth of 60 m and was sectioned into 1 cm slices. The core was dated using ^{137}Cs and ^{210}Pb analysis and the average sedimentation rate was determined to be 0.45 cm/year. The level of MCCPs in the sediment core showed an increasing trend from 1965 onwards reaching a level of 26 µg/kg dry weight in the surface layer (corresponding to 2004). Concentrations between 15 and 20 µg/kg dry weight were evident in the samples from the 1980s. The C_{14} carbon chain length was the most abundant constituent of MCCPs present (accounting for 41 to 64% of the total MCCPs). Analysis of the chlorine contents present indicated that there was a continuous increase in the chlorine contents of the MCCPs present in those parts of the sediment cores representing the last 20 years. The chlorine contents were generally between 53.3% and 56.6% by weight and a similar pattern of increase in the chlorine content was also seen with the short-chain chlorinated paraffins. Three possible explanations were given for this trend in chlorine content:

a) As a consequence of increased usage of chlorinated paraffins with higher chlorine contents; and/or

b) As a result of dechlorination/biotransformation of the higher chlorinated paraffins to lower chlorinated paraffins in the older sediment layers[11].

c) Biodegradation of lower chlorinated congeners ultimately led to the accumulation of the less bioavailable longer chain congeners.

It was not possible to distinguish between these three possibilities.

Overall, although the data provide some possible evidence for dechlorination of chlorinated paraffins in the sediment core, the fact that measurable levels of MCCPs were present in the layers from the 1980s at concentrations of 15 to 20 µg/kg dry weight, when compared with the level of 26 µg/kg dry weight present in the surface layer, suggests that if degradation occurs it is likely to be very slow. This provides some strong, though indirect, evidence that the substance may be persistent (in terms of the REACH Annex XIII criteria) in these cores. It should be noted, however, that the conditions in sediment cores may vary with depth (e.g. aerobic versus anaerobic, redox environments etc.) and degradation mechanisms may also change accordingly. In addition, the levels found in the sediment layers will depend on the emissions to the environment occurring at the time the sediment layer was deposited. These factors therefore introduce uncertainties into the interpretation of the data. Additionally, the analytical method used was ECNI-MS. Given recent analytical developments, the accuracy of this technique in terms of quantitation may be uncertain. However, it is likely that the qualitative detection of MCCPs can still be considered to be reliable even if the quantification may not be so.

A further sediment core was analysed for MCCPs by Chen *et al.* (2011). For this study the sediment core was taken from the Dongjiang River within Dongguan in the Pearl River Delta area of South China. The sediment core was collected to a depth of approximately 68 cm. The core was not dated but it was known that the sedimentation rate in the area was 4 - 6 cm/year and so it was thought that the sediment core contained about 15 years of deposition (the core was collected at some point between July 2009 and October 2010).

The concentrations of MCCPs were higher in the upper layers of the core than in the deeper layers of the core, with the concentration determined to be 1 400 - 3 800 µg/kg dry weight between 0 and 32 cm depth compared with 1 100 - 1 400 µg/kg dry weight between 36 and 68 cm depth. The increasing concentrations in the upper layers were thought to be a result of increasing use of MCCPs in the area. The MCCP concentrations in the lower layers were relatively constant.

The carbon chain length and chlorine content distribution of MCCPs present in the sediment core were also investigated. It was noted that there was a higher relative abundance of C_{16} and C_{17} substances in the upper layers (from 0 cm to around 44 cm depth) than in the lower layers, with the relative proportion of C_{14} substances being higher in the lower layers than the upper layers. Chen *et al.* (2011) suggested that this may reflect changes in the composition of MCCPs used in the area over time.

Chen *et al.* (2011) also found that the chlorine content of MCCPs showed a decreasing trend with increasing depth (for example the relative abundance of congeners with 9 and 10 chlorine atoms per molecule decreased with increasing depth whilst the relative abundance of congeners with less than 8 chlorine atoms per molecule increased with increasing depth. Chen *et al.* (2011) concluded that this provided evidence that the higher chlorinated substances were undergoing de-halogenation to the lower chlorinated substances in the sediment core. However, as is the case with the Iozza *et al.* (2008) sediment core data above, the same pattern could be explained if there was an increased usage of chlorinated paraffins with higher chlorine contents in recent

[11] This would not be consistent with the results of the biodegradation screening studies which suggest that the lower chlorinated substances may be more degradable than the higher chlorinated substances. However, the conditions in the sediment layers are likely to be different to those in the screening studies (anaerobic versus aerobic).

years compared with the earlier years and so it is not possible to distinguish between these two possibilities here.

Overall, although the Chen *et al.* (2011) data also provide some possible evidence for dechlorination of chlorinated paraffins in the sediment core, similar to the Iozza *et al.* (2008) data, the fact that measurable levels of MCCPs were present in the deeper layers at concentrations of 1 100 - 1 400 µg/kg dry weight µg/kg dry weight, when compared with the level of 3 800 µg/kg dry weight present in the surface layer, suggests that if degradation occurs it is likely to be very slow. However, as with the data from the Iozza *et al.* (2008) study, the accuracy of this technique in terms of quantitation may be uncertain. However, it is likely that the qualitative detection of MCCPs can still be considered to be reliable even if the quantification may be less so.

Sediment cores from Lake St. Francis, downstream of Cornwall, Ontario, were found to contain total MCCPs concentrations ranging from 0.75 to 1.2 mg/kg dw, with the highest concentrations estimated to have been deposited in 1972 (Muir *et al.* 2002). A back-calculation method using standard first order decay equations was used to determine that MCCPs have a half-life in sediments longer than 1 year (Environment Canada 2008). The detection of MCCPs in a sediment core from 1972 suggests that MCCPs can persist for more than 30 years in subsurface anaerobic sediments.

Sediment cores obtained from a range of environments in Sweden were analysed using APCI-QTOF-MS by Yuan *et al.* (2017). A sediment core from an area with wood-related industry was found to contain MCCPs at concentrations of < 6.5–93 ng/g dw. The maximum concentration of MCCPs occurred in 2015. However, MCCPs were measured above the LOQ in the oldest sediment section representing the year 1954. A further sediment core from an area receiving sewage treatment plant discharge was found to contain between < 6.5–15 ng/g dw of MCCPs. The oldest sediment section in which they were detected was from 1960. A sediment core taken near a steel factory was found to contain MCCPs at concentrations of < 6.5–1200 ng/g dw. In this core, MCCPs reached their maximum concentration in the top layer.

Brandsma *et al.* (2017) found that MCCPs were the dominant chloroparaffins in sludge samples collected from 15 different WWTPs in Australia. MCCPs were detected in all sludge samples with concentrations ranging from 542 to 3 645 ng/g dw, using APCI-QTOF-MS.

There is some evidence that adapted microbes can degrade chloroparaffins to chloro-olefins. For example, Heeb *et al.* (2019) investigated the degradation of $C_{11\text{-}13}$ chloroparaffins with between 4 and 10 chlorine atoms using the bacterium *Sphingobium indicum* B90A. Levels of chloro-olefins were found to increase up to 96 hours' exposure. Levels decreased after this time suggesting further conversion by the bacteria. Higher chlorinated paraffins were converted more rapidly to olefins than lower chlorinated paraffins. The ability of this species to degrade longer or more heavily chlorinated molecules is unknown. EC (2005) also cites studies providing evidence that some microorganisms may be capable of degrading MCCPs in the environment in acclimated or cometabolic systems

6.7.2.6 Summary and discussion of biodegradation in water and sediment

Constituents of MCCPs that contain up to around five chlorine atoms per molecule can be extensively degraded by micro-organisms under conditions of enhanced bioavailability. Data available from ready biodegradation tests (OECD TG 301) using a surfactant lead to the conclusion that C_{14} chlorinated n-alkanes with a chlorine content of 41.3 – 45.5% are readily biodegradable. Although C_{14} chlorinated n-alkane, 50% Cl wt. failed to meet the criteria for ready biodegradation, it met the 60% pass threshold after 56 days when river water was used as the inoculum.

Degradability reduces as the number of chlorine atoms per molecule increases. Both a 55% and 60% Cl wt. C_{14} chlorinated n-alkane failed to meet the pass threshold of 60% degradation even with a surfactant and after extended timescales using inocula derived from activated sludge.

Similarly, C_{15} chlorinated n-alkane, 51% Cl wt. failed to meet the pass threshold after an extended timescale in river water (although it achieved up to 63% degradation after 60 days with a surfactant using inocula derived from activated sludge).

Longer chain lengths are expected to be less water soluble and more adsorptive than the C_{14} and C_{15} substances, but there are no degradation data for specific C_{16} or C_{17} substances, so the actual influence of chain length is unknown. Although $C_{14\text{-}17}$ chlorinated n-alkane, 45.5% Cl wt. is not readily biodegradable, more than 60% degradation was seen after extended timescales with a surfactant using inocula derived from activated sludge (no data are available using river water as the inoculum, although the degradation rate would be expected to be slower).

$C_{14\text{-}17}$ chlorinated n-alkane, 51.7% Cl wt. was also extensively degraded over an extended period by activated sludge micro-organisms when bioavailability was enhanced, although it narrowly failed to meet the pass threshold (57% degradation was achieved after 60 days). In contrast, $C_{14\text{-}17}$ chlorinated n-alkane, 63.2% Cl wt. only achieved 10% degradation under the same conditions.

This complexity led to the ECHA request for measured environmental half-life data for up to three representative test substances. The Registrants subsequently investigated one of these substances (likely to be the least persistent based on chain length and chlorine content). No transformation of C_{14} chlorinated n-alkane, 50% Cl. wt. was observed over 120 days at 12 °C in an OECD TG 308 study (Unpublished, 2019c). Although it is possible that there is a long lag period, the fact that there was no significant measurable degradation over 120 days suggests that it is unlikely that ≥50% mineralisation would occur over a subsequent 60-day period. Therefore, the eMSCA considers that the sediment half-life of C_{14} chlorinated n-alkane, 50% Cl wt. is likely to exceed 180 days, although there is no empirical evidence to confirm this.

The same test substance was found to degrade by 60% after 56 days in a ready test using surfactant and a river water inoculum. The negligible degradation rate in aerobic sediment may reflect a reduction in bioavailability caused by adsorption. Since the water-sediment simulation test is more environmentally relevant than the ready biodegradation test, it must be given more weight in the assessment of persistence.

All of the substances that were less degradable than C_{14} chlorinated n-alkane, 50% Cl. wt. in modified and enhanced ready tests are likely to have similar or longer sediment half-lives. It is possible that adsorption could cause substances that were found to be readily biodegradable in modified tests (C_{14} chlorinated n-alkanes, 41.3 – 45.5% Cl wt.) to have longer sediment half-lives than expected, but no data are available to allow a conclusion to be drawn.

Given the predicted and observed trends in physico-chemical properties, it is likely that $C_{15\text{-}17}$ constituents with similar or higher chlorine contents to C_{14} chlorinated n-alkane, 50% Cl. wt. will be equally or more adsorptive to sediment. They are therefore likely to be equally or more persistent in sediment.

The exact composition of the registered substance is claimed as confidential business information. However, commercial MCCPs contain a large proportion of C_{14} chlorinated n-alkanes (see Section 6.3). The eMSCA's conclusion is therefore that a significant proportion of the constituents of most current commercial MCCP products will have sediment half-lives that exceed 120 days at 12 °C. Some constituents with lower chlorine content (≤45% Cl wt.) are readily biodegradable. However, given the remaining uncertainties about the role of adsorption and the fact that $C_{14\text{-}17}$ chlorinated n-alkane, 45.5% Cl wt. is not readily biodegradable, the eMSCA believes that a firm conclusion cannot be drawn about whether all relevant constituents of such substances would have sediment half-lives below 120 days. Further simulation data would be needed to confirm this. The eMSCA recommends the use of radiolabel and congener analysis to clearly identify which constituents of the substance (if any) have a sediment half-life below 120 days. Since such data are not essential for a risk management decision, the Substance Evaluation can be concluded without a further formal information request.

The available monitoring data, particularly from sediment core studies, provide some evidence for dechlorination of chlorinated paraffins with high chlorine contents in sediment cores, but they also suggest that degradation in the environment for at least some product types may be slow and provide indirect evidence that MCCPs with chlorine contents of ~ 55% by weight may persist for a long time in sediments.

Information on $C_{<14}$ constituents

The eMSCA notes that both C_{10} chlorinated n-alkane, 65% Cl wt. and C_{13} chlorinated n-alkane, 65% Cl wt. have long degradation half-lives in sediment (e.g. 335 and 680 days, respectively, in marine sediments). In contrast, $C_{10\text{-}13}$ chlorinated n-alkane, 49.8% Cl wt. was found to be readily biodegradable when surfactant was used to enhance bioavailability. Such chain lengths are relevant for the persistence assessment as they are present in commercial MCCPs above 0.1% w/w.

6.7.2.7 Biodegradation in soil

No data are available on the biodegradation of MCCPs in soil.

6.7.3 Summary and discussion on degradation

MCCPs is not expected to hydrolyse significantly. The estimated atmospheric half-life is estimated to be 1 - 2 days for MCCPs with chlorine contents between around 40 and 56% Cl wt. However, MCCPs with >65% chlorine by weight have estimated half-lives which are longer than 2 days. No information is available on phototransformation potential in water or soil. It is noted that stabilizers are often added to commercial product types to improve light (and thermal) stability.

Several biodegradation screening studies under conditions of enhanced bioavailability have been performed with commercial SCCP and MCCP product types (and some of their constituents) to investigate the influence of chain length and chlorination level on biodegradation potential. Constituents of MCCPs that contain up to around five chlorine atoms per molecule can be extensively degraded by micro-organisms. Nevertheless, a more environmentally realistic OECD TG 308 study indicates that the sediment half-life of C_{14} chlorinated n-alkane, 50% Cl wt. is greater than 120 days, and likely exceeds 180 days at 12 °C. The negligible degradation rate in aerobic sediment may reflect a reduction in bioavailability caused by adsorption.

All of the substances that were less degradable than C_{14} chlorinated n-alkane, 50% Cl. wt. in modified and enhanced ready tests are likely to have similar or longer sediment half-lives. It is possible that adsorption could cause substances that were found to be readily biodegradable in modified tests (C_{14} chlorinated n-alkanes, 41.3 – 45.5% Cl wt.) to have longer sediment half-lives than expected, but no data are available to allow a conclusion to be drawn.

The eMSCA's conclusion is that a significant proportion of the constituents of many commercial MCCP products will have sediment half-lives that exceed 120 days at 12 °C. Some constituents with lower chlorine content (≤45% Cl wt.) are readily biodegradable. However, given the remaining uncertainties about the role of adsorption and the fact that $C_{14\text{-}17}$ chlorinated n-alkane, 45.5% Cl wt. is not readily biodegradable, the eMSCA believes that a firm conclusion cannot be drawn about whether all relevant constituents of such low chlorine content MCCPs would have sediment half-lives below 120 days.

6.7.4 Environmental distribution

6.7.4.1 Adsorption/desorption

No experimental data from an OECD TG 106 or equivalent guideline study are presented in the registrations. The substance has a high log K_{ow}, with values for many constituents likely to be ≥ 6.5, depending on the chlorine content and carbon chain length. The Registrants choose a representative value of 7 (see Section 6.4.3). The log K_{ow} can be used to estimate the organic carbon-water partition coefficient (K_{oc}). EC (2005) derived a K_{oc} value of 588 844 L/kg based on a log K_{ow} of 7. In addition the substance has a low solubility in water (maximum 0.027 mg/L – see Section 6.4.2). These properties in combination indicate that MCCPs is likely to partition to suspended matter and sediment in aquatic environments. Therefore, persistence in the sediment compartment is more relevant than persistence in the water compartment.

6.7.4.2 Volatilisation

The potential for long-range transport via the atmosphere is not considered in the registration dossiers. The REACH Guidance (Chapter R.7B, Section R.7.9.4.3) indicates that long-range transport can be considered on a case-by-case basis, but there is no guidance about how to use the information in the overall assessment.

The potential for long-range atmospheric transport has been considered briefly in EC (2005 and 2007). SCCPs is a Persistent Organic Pollutant (POP) under the UN Stockholm Convention. EC (2005 and 2007) concluded that the potential for long-range transport (and subsequent accumulation) of MCCPs appears to be lower than SCCPs. This is because MCCPs generally have lower vapour pressures and are likely to adsorb more strongly to soil and sediment than SCCPs. However, MCCPs is a UVCB substance with constituents exhibiting a range of physico-chemical properties. Some constituents of the commercial products may have properties that mean that long-range transport via the atmosphere is a possibility.

The long-range atmospheric transport potential for MCCPs has been considered by Environment Canada (2008). This concluded that the atmospheric half-lives for vapour phase MCCPs ranged from 2.7 to 7.1 days, with the longest half-lives for MCCPs with the highest chlorine contents and also with the shorter chain lengths (for comparison, EC (2005) estimated that the atmospheric half-life was of the order of 1 - 2 days for MCCPs with chlorine contents between 40 and 56% Cl wt.; see Section 6.7.1.3). Environment Canada (2008) concluded that MCCPs have estimated vapour pressures (around 4.5×10^{-8} to 2.27×10^{-3} Pa at 20 – 25 °C) and Henry's law constants (around 0.014 to 51.3 $Pa.m^3/mol$) that are in the range of values for some POPs that are known to undergo long-range atmospheric transport, such as lindane, heptachlor and mirex. The predicted vapour pressures and Henry's law constants can be found in

Table 33. The eMSCA has not considered the reliability of the predictions, but notes that the data could suggest that long-range atmospheric transport is a possibility for some constituents of MCCPs.

Table 33

ESTIMATES OF VOLATILITY OF MCCPs AND POPs DERIVED USING EPI SUITE™ (US EPA, 2012)		
Substance	**Vapour pressure (mm Hg at 25 °C)**	**Henry's law constant ($atm.m^3/mol$)**
MCCPs	1.44×10^{-10} – 2.25×10^{-2}	1.81×10^{-16} – 4.12×10^{-2}
Lindane	4.2×10^{-5}	4.25×10^{-11} - 2.56×10^{-4}
Heptachlor	4×10^{-4}	1.76×10^{-4}
Mirex	8×10^{-7}	1.28×10^{-6}

The OECD has produced a decision support tool[12] for estimating the long-range transport potential (LRTP) of organic chemicals at a screening level. It is a steady state non-equilibrium model in a standardised evaluative environment, and predicts three characteristics that can be used to provide an indication of the LRTP of a substance: Characteristic Travel Distance, Transfer Efficiency and overall persistence (P_{OV}). To estimate the LRTP of MCCPs, the eMSCA has performed calculations using input parameters for two example constituents of MCCPs, as indicated in Table 34.

Table 34

VALUES USED TO PREDICT THE LONG RANGE TRANSPORT POTENTIAL OF TWO EXAMPLE MCCP CONSTITUENTS (DERIVED USING EPI SUITE™ (US EPA, 2012))		
Required parameters	**Long chain, high chlorine content MCCP constituent**	**Short chain, low chlorine content MCCP constituent**
SMILES	C(CL)CC(CL)CC(CL)CC(CL)CC(CL)C(CL)CC(CL)C(CL)C(CL)CC(CL)C(CL)C	CC(CL)CC(CL)CCC(CL)CCC
Molecular mass	633.40	245.62
Log K_{AW}	-2.414	0.226
Log K_{OW}	11.24	5.79
Half-life in air (h)	39.19	43.78
Half-life in water (h)	4 320	1 440
Half-life in soil (h)	8 640	12 960

As noted in Section 6.4, EPI Suite™ might not be the most appropriate model for chlorinated paraffins. In addition, the predicted half-life in water (and soil) for the low chlorine short chain constituent is not consistent with its status as readily biodegradable (see Annex E). These values are therefore used for illustration only. The OECD screening tool results for MCCPs based on these input values are provided in

Table 35.

Table 35

LRTP POTENTIAL PREDICTIONS FROM THE OECD SCREENING TOOL		
Predictions	**Long chain, high chlorine content MCCP constituent**	**Short chain, low chlorine content MCCP constituent**
Characteristic Travel Distance (km)	2 840	909
Transfer Efficiency (%)	12.5	0.001
P_{OV} (days)	519	225

The OECD LRTP screening tool allows comparisons of these three characteristics for a range of substances, provided in Figures 1 – 2.

[12] http://www.oecd.org/chemicalsafety/risk-assessment/oecdpovandlrtpscreeningtool.htm

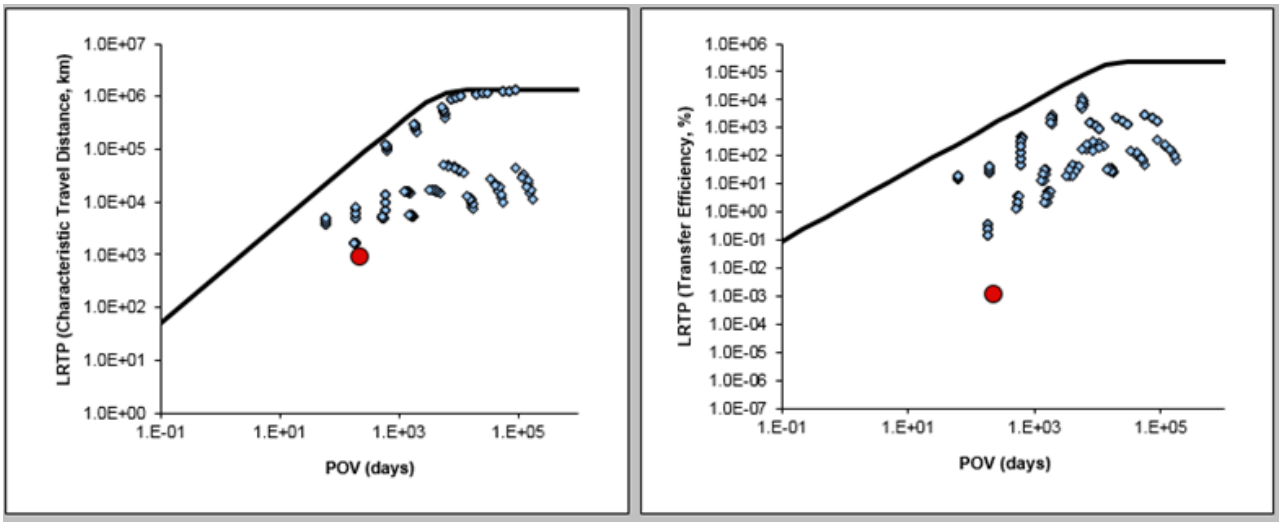


Figure 1 – The red dot represents the example short chain, low chlorine content MCCP constituent compared to substances that meet the POPs criteria

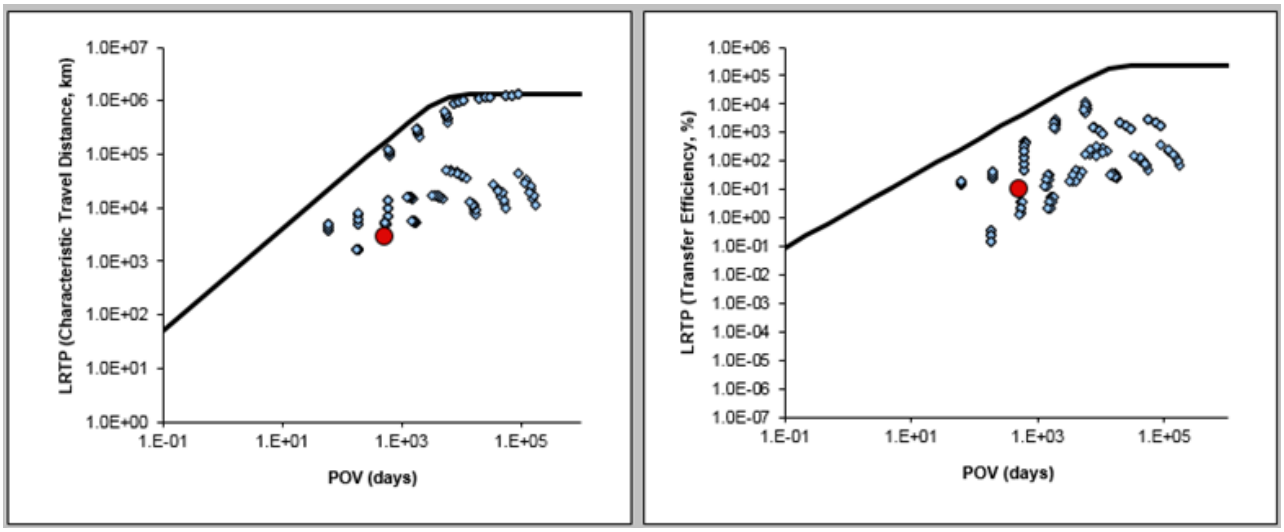


Figure 2 – The red dot represents the example long chain, high chlorine content MCCP constituent compared to substances that meet the POPs criteria

It appears that longer chain, higher chlorine content MCCP constituents may be capable of long range transport. However, a more comprehensive review of properties would be needed to draw a definitive conclusion. For example, Glüge *et al.* (2013) calculated Henry's law constants for 29 constituents of MCCPs using COSMO*therm*, SPARC and EPI Suite™, and provided recommended values. These have not been evaluated by the eMSCA, nor compared with the log K_{AW} values estimated in Table 34. In addition, evidence of occurrence (or not) of MCCPs in the Arctic and other remote regions also needs to be taken into account (noting the proximity of industrial activity and population centres). This is beyond the scope of this evaluation.

6.7.4.3 Distribution modelling

The registration dossiers all assume the following distribution behaviour during waste water treatment:

Percentage to sludge	97.1%
Percentage to air	0%
Percentage degraded	0%
Percentage to surface water	2.9%

The eMSCA draws the same conclusion using SimpleTreat 4.0 and the parameters listed in Table 53. The eMSCA agrees with the Registrants that MCCPs will be mainly removed to sludge in a wastewater treatment plant given its high K_{OC} and limited biodegradation potential.

A different approach was taken in EC (2005), based on an equilibrium removal percentage of 93% for adsorption of SCCPs onto sludge from a Coupled Units test (assuming that MCCPs will adsorb onto sludge to at least the same extent as SCCPs). The influence of this slight difference in removal rate is considered in Section 6.12.2.1.

6.7.4.4 Summary and discussion of environmental distribution

Removal during waste water treatment processes is estimated to be around 97% mainly by adsorption onto sludge. EC (2005) concluded that MCCPs is likely to be associated mainly with the sediment and soil compartments when released to the environment, but would also occur in the water phase if released to water. Long-range atmospheric transport would appear to be a possibility for some constituents of MCCPs but this aspect has not been investigated by the Registrants, and only a preliminary analysis has been performed by the eMSCA.

6.7.5 Bioaccumulation

6.7.5.1 Aquatic bioaccumulation

6.7.5.1.1 Screening data

As described in Section 6.4, constituents of MCCPs generally have a low water solubility and log K_{OW} values in the range 6-8, with a "typical" value around 7. MCCPs is therefore potentially bioaccumulative.

6.7.5.1.2 Measured bioaccumulation data

6.7.5.2 Aqueous exposure studies

A fish bioconcentration factor (BCF) was measured in Rainbow Trout (*Oncorhynchus mykiss*) for a C_{15} chlorinated n-alkane, 51% Cl wt. (Thompson *et al*., 2000, summarised in EC, 2005). This is a key study in the registration dossiers, rated as 'reliable with restrictions'. The test substance would have had approximately six to seven chlorine atoms per molecule. A kinetic BCF of 1 087 L/kg was derived, based on total radioactivity measurements (so may represent accumulation of metabolites as well as the chlorinated paraffin). No lipid data were presented in the original study report, so it was not possible to lipid normalise the BCF (the REACH Guidance recommends normalization to a 5% lipid content if the data allow). A significant contributing factor to the apparent depuration during this study was growth dilution. Subsequent further analysis of the data by the eMSCA indicates that the growth-corrected kinetic BCF would be

around 1 833 – 2 072 L/kg (see Appendix B, previously presented in EA, 2010)[13]. This change has not been reflected in the RSS produced by the Registrants.

An additional fish bioconcentration study was requested for MCCPs under Commission Regulation (EC) No. 466/2008, with a deadline of 30 November 2008. The resulting study (Unpublished, 2010h) is a key study in the registration dossiers, rated as 'reliable with restrictions'. It was discussed in detail in EA (2010), and the eMSCA's analysis is repeated here. It was performed in accordance with OECD TG 305 and GLP using Rainbow Trout (*Oncorhynchus mykiss*). The test substance was a ^{14}C-labelled[14] C_{14} chlorinated n-alkane, 45% Cl wt. and would have had 4 – 5 chlorine atoms per molecule (it was the same substance that was tested in the modified ready biodegradation tests described in Section 6.7.2.3). Dechlorinated tap water was used as the dilution water, with a pH in the range 7.33 to 7.75 and mean total hardness of 44.3 mg/L as $CaCO_3$. A flow-through test system was used with a flow rate sufficient to provide 13.7 volume additions per 24 hours. A single test concentration was used (nominally 0.5 µg/L). The substance was added to the test vessels as a solution in dimethyl formamide (the solvent concentration in the vessel was 0.004 mL/L). The exposure concentration was maintained over the duration of the uptake phase and the mean measured concentration was 0.34 µg/L (range was 0.26 to 0.44 µg/L), which was well below the expected water solubility for this substance. A solvent control was also included.

At the start of the test the fish were in the weight range 0.75 to 1.79 g (mean weight 1.21 g). The fish were exposed to the substance for 35 days followed by a 42-day depuration period. The test was carried out at 15 °C and the concentrations in fish (and water) were determined at intervals by total ^{14}C-analysis. A plot showing the uptake and depuration data is in Figure 3. The resulting BCFs (based on the mean whole body concentration measured at day 35 and the kinetic data) are summarised in Table 36.

The lipid contents of the fish were determined on day 0 and at the end of the depuration phase as 7.5 and 12.2% respectively. The mean lipid content was 10.3%. The REACH Guidance recommends that where possible the BCF data should be normalised to a 5% lipid content. The results of this normalisation (based on the mean lipid content) are shown in.

The fish were found to grow significantly during this test and the rate constant for growth dilution was determined from the slope of a plot of the natural logarithm of the fish weight against time. The growth rate constants determined in the exposure group and solvent control group were 0.033 day^{-1} and 0.026 day^{-1} and the mean growth rate was 0.030 day^{-1}. These rate constants are significant compared with the overall depuration rate constant determined for the substance (0.0432 day^{-1}), implying that a major portion of the depuration seen resulted from growth dilution. The effect of growth correction on the resulting BCF values is shown in Table 36.

The lipid-normalised steady state BCF is 3 230 L/kg (based on the day 35 concentration) and the lipid-normalised kinetic BCF is 4 460 L/kg. Growth dilution appears to account for a significant proportion of the depuration seen, and correcting for this results in BCFs of around 10 500 – 14 600 L/kg. This is important, because although the estimation method introduces some additional uncertainty, the resulting value is more likely to be appropriate for a fish that is not growing rapidly. As stated in the OECD guidance, this correction allows comparison between studies where feeding rates may differ and subsequently growth rate and lipid content vary (OECD, 2013).

[13] Given the low water solubility of MCCPs and their potential to adsorb to suspended and dissolved organic matter, it is possible that reported concentrations in water in BCF studies may over-estimate the truly dissolved concentration, which in turn would under-estimate steady state BCFs. Appendix C contains further discussion on this issue.

[14] The radio-label was in the 1-position on the carbon chain.

Table 36

SUMMARY OF BCF DATA FOR C_{14} CHLORINATED N-ALKANE, 45% CL WT. (Unpublished, 2010h)	
Endpoint	**Value**
Mean exposure concentration	0.34 µg/L
Mean measured concentration in fish at day 35 (wet weight)	2 265 µg/kg
Uptake rate constant (k_1)	397 day^{-1}
Overall depuration rate constant (k_2)	0.0432 day^{-1}
Rate constant for growth dilution	0.030 day^{-1}
"Steady-state" BCF[a] at day 35 (as reported)	6 660 L/kg
"Steady-state" BCF at day 35 (normalised to 5% lipid)	3 230 L/kg
"Steady-state" BCF at day 35 (normalised to 5% lipid and corrected for growth)	~ 10 600 L/kg
Kinetic BCF at day 35 (as reported)	9 190 L/kg
Kinetic BCF at day 35 (normalised to 5% lipid)	4 460 L/kg
Kinetic BCF at day 35 (normalised to 5% lipid and corrected for growth)	~ 14 600 L/kg

[a] The "steady state" BCF was determined as the concentration in fish at day 35 divided by the concentration in water.

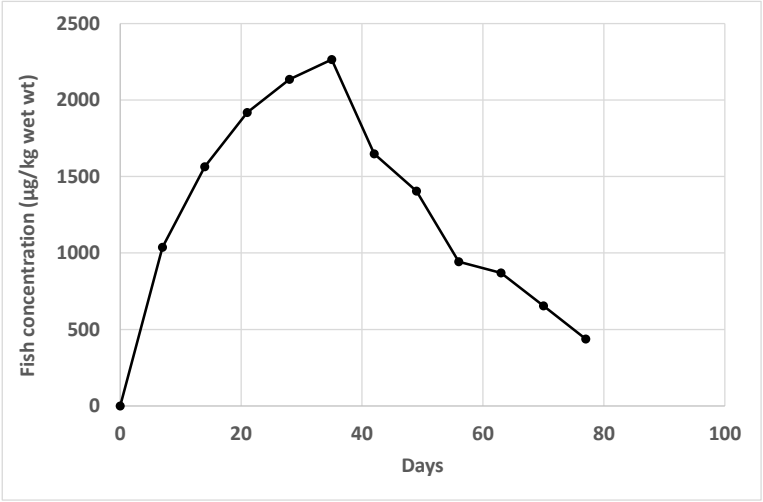


Figure 3: Uptake and depuration curve for a C_{14} chlorinated n-alkane, 45% Cl wt. in Rainbow Trout (redrawn from the data reported in Unpublished, 2010h)

It should be noted that this study is based on total ^{14}C measurements and so represents both the parent compound and metabolites. Further analytical work was carried out to investigate the extent of metabolism that occurred in the fish (Unpublished, 2010i). A method for extraction and separation of the chlorinated paraffin from polar metabolites in the fish was developed and validated. The fish used for the analysis were from the end of the depuration phase (day 77 of the study; a total of ten fish were available). The analysis showed that the ^{14}C-activity in the fish was associated mainly with the parent compound and little or no evidence of the presence of polar extractable metabolites was found. A minor part (around 21%) of the radioactivity present was, however, found to be associated with non-extractable metabolites. Thus, the results of this analysis suggest that the majority of the radiolabel present in the fish was parent compound. It should be noted that this analysis was carried out on fish at the end of the depuration phase and it is not clear if the same ratio between parent compound and metabolites

would have been present during the uptake phase. Therefore it is possible that a higher (or indeed lower) percentage of metabolites could have been present at other times during the study, but it is not possible to infer from the available data whether or not this was the case[15]. Assuming that the parent substance was present in the fish samples at around 79% of the total radioactivity at the end of the uptake phase, the *minimum* lipid-normalised BCFs from this study would be in the range 2 500 – 3 500 L/kg (growth-corrected values would still be above 5 000 L/kg, i.e. approximately 8 300 – 11 530 L/kg).

Given that the identity of the metabolites from this study are not known (and hence it cannot be ruled out whether or not they themselves may be toxic or accumulative) the eMSCA considers that the BCFs based on total ^{14}C represent a conservative estimate of the bioaccumulation potential of the chlorinated paraffin tested. Therefore the eMSCA believes that the most appropriate values for MCCPs derived from this study are a non-growth-corrected BCF of 3 230 – 4 460 L/kg and a growth-corrected BCF of 10 500 – 14 600 L/kg. The REACH registrations only refer to the non-growth-corrected values.

Some additional reported fish BCFs (e.g. from Bengtsson *et al.*, 1979) are summarised in EC (2005), but are either not reliable or difficult to interpret (for example, owing to use of concentrations in excess of the water solubility or short exposure durations). They may underestimate the true BCF and so the eMSCA has not considered them further.

Information on $C_{<14}$ constituents

As MCCPs contain constituents with carbon chain lengths shorter than C_{14} it is also relevant to consider the available data for SCCPs. These were evaluated in ECHA (2008), and a brief summary of the key data is given in Table 37.

Table 37

SUMMARY OF FISH BCF DATA FOR SCCPs, FROM ECHA (2008)

Substance	Species	BCF (L/kg)	Comment
C_{11}, ~ 58% Cl wt.	Rainbow Trout (*Oncorhynchus mykiss*)	5 300 - 7 816	Steady state value, not lipid normalised or growth corrected.
$C_{10\text{-}13}$, 49% Cl wt. $C_{10\text{-}13}$, 59% Cl wt. $C_{10\text{-}13}$, 71% Cl wt.	Common Bleak (*Alburnus alburnus*)	~800 – 1 000 ~800 – 1 000 ~200	Value estimated after 14 days exposure. Not lipid normalised or growth corrected.
C_{10}, 63.7% Cl wt. C_{12}, 58.5% Cl wt.	Japanese Medaka (*Oryzias latipes*)	690 – 2 700 740 – 1 700	Estimated as part of a 20-day embryo-larval study. Values relate to 3 days post-hatch. No indication as to whether steady-state was reached. Not lipid normalised or growth corrected.

The life stages of the organisms, short exposure duration, and/or lack of growth-corrected and lipid-normalised kinetic BCFs means that these data cannot be directly compared with the data for MCCPs described above.

[15] Theoretically the amounts of metabolites present in the fish at any one time will be a balance between their rate of formation from MCCPs and the rate of elimination of the metabolites from the fish (or binding in the case of non-extractable metabolites). The effects of this will depend on the kinetics of the various processes.

A further bioconcentration study has been carried out with a C_{13} chlorinated paraffin. The full study report is available in Japanese only (Mitsubishi, 2009) but an English summary is available (UNEP, 2009). These data were discussed in detail in EA (2010), and the eMSCA's analysis is repeated here. The study was conducted in accordance with the test method prescribed under the Chemical Substances Control Law of Japan for testing new substances[16] and in compliance with GLP. The substance tested was a C_{13} chlorinated n-alkane, 48.7% Cl wt. The average chemical formula was $C_{13}H_{23.2}Cl_{4.8}$ and the substance contained soya bean oil epoxide as an additive/stabiliser. Three main constituents of the test substance could be determined/distinguished during the test[17]. These were $C_{13}H_{23}Cl_5$ (49.8% Cl wt.), $C_{13}H_{22}Cl_6$ (54.5% Cl wt.) and $C_{13}H_{21}Cl_7$ (58.4% Cl wt.) and the water solubilities of these constituents were determined as 0.05, 0.07 and 0.09 mg/L, respectively.

The test was carried out using two nominal concentrations, 0.01 mg/L and 0.001 mg/L. The test system was a flow-through system and acetone (at 25 ppm by volume) was also present in the exposure solutions. The fish used in the test were Common Carp (*Cyprinus carpio*) which had an average lipid content of 3.9% at the start of the test. The test was carried out at 24 °C and the exposure period was for 62 days. Samples of water and fish were collected at various times during the test and analysed for the presence of the C_{13} chlorinated paraffins (by parent compound analysis). Steady state was found to be reached after approximately 28 days and the steady state BCF was determined based on the mean concentrations measured in fish over day 28 to 62 divided by the mean concentration in the water over the same time period. The steady state BCFs obtained are summarised in

Table 38.

No kinetic evaluation of the data was carried out in the UNEP (2009) report and only data for the concentration in fish at various time points during the uptake phase were given. However, the Mitsubishi (2009) report contains some information on depuration (it appears that a 21 day depuration period was also included in the study), and elimination half-lives of 5.4 - 6.9 days (depuration rate constants (k_2) of 0.10 - 0.13 day^{-1}) for the $C_{13}H_{23}Cl_5$ constituent, 9.0 - 9.9 days (k_2 of 0.070 - 0.077 day^{-1}) for the $C_{13}H_{22}Cl_6$ constituent and 13.7 - 11.4 days (k_2 of 0.051 - 0.061 day^{-1}) for the $C_{13}H_{21}Cl_7$ constituent are given.

Some fish weight data are presented in UNEP (2009) but these data are few in number and showed large variability. However, they did indicate that only limited growth of fish occurred during the 62 day uptake period (a rate constant for growth dilutions of approximately 0.008 day^{-1} can be estimated from the data). Therefore growth correction does not appear to be so important in this study.

It is relevant to consider normalizing the data to the "standard" lipid content of 5% as recommended in the REACH Guidance. As the fish did not grow significantly during the test, it seems reasonable to assume that the lipid content remained relatively constant during the exposure phase. The effect of normalization using the lipid content of 3.9% measured at the start of the exposure period is shown in

Table 38

[16] Bioconcentration test of chemical substances in fish and shellfish. Yakushokuhatsu No1121002, Heisei 15.11.3 Seikyoky No.2, Kanpokihatsu No.031121002, November 21, 2003; latest revision November 20, 2006.

[17] As the mean chlorine content of the substance tested was reported to be 48.7% there would be other lower chlorine constituents in the substance that could not be determined.

Table 38

SUMMARY OF BCF DATA AVAILABLE FOR C_{13} CHLORINATED PARAFFINS				
Constituent	**Mean exposure concentration (day 28 - 62) (mg/L)**	**Mean concentration in fish (day 28 - 62) (mg/kg)**	**Steady state BCF (L/kg)**	
			As reported	**Normalised to 5% lipid content**
$C_{13}H_{23}Cl_5$ (49.8% Cl)	0.000699	1.070	1 530	2 150
	0.00764	12.84	1 680	1 962
$C_{13}H_{22}Cl_6$ (54.5% Cl)	0.000764	1.256	1 640	2 100
	0.00799	15.72	1 970	2 530
$C_{13}H_{21}Cl_7$ (58.4% Cl)	0.000816	1.907	2 340	3 630
	0.00842	23.86	2 830	3 000

In summary, the Mitsubishi (2009) study indicates that C_{13} chlorinated paraffins with 5 to 7 chlorine atoms (49.8% - 58.4% Cl wt.) have fish BCFs of 2 000 L/kg or higher.

6.7.5.2.1 Dietary studies

The ECHA decision letter requested a tiered testing approach for bioaccumulation assessment of MCCPs. A fish bioaccumulation test was required using a C_{14} chlorinated n-alkane, 50-52% Cl wt., the choice of aqueous or dietary exposure being left to the Registrants' discretion. A subsequent test using C_{14} chlorinated n-alkane, 55-60% Cl wt. was also required, although the Registrants could read-across the result from the lower chlorine content substance if it was found to be significantly bioaccumulative. In response, the Registrants have performed a GLP-certified OECD TG 305 dietary study using a C_{14} chlorinated n-alkane, 50% Cl wt. (Unpublished, 2019d).

The Registrants provided the study report for the eMSCA to review. The RSS in the registration dossiers also includes attachments with details of the analytical work conducted by a sub-contracted laboratory. The eMSCA does not know whether these spreadsheets have been checked as part of the Quality Assurance process of the lead laboratory. The Registrants assign the study a reliability rating of 1 (reliable without restriction).

Dietary exposure was chosen by the Registrants due to the insoluble nature of MCCPs. The test species was Rainbow Trout (*Oncorhynchus mykiss*). Fish were exposed to the test substance in their diet for 14 days in a flow-through system. All physico-chemical parameter measurements were within that required by OECD TG 305. No mortalities were observed in the control or dosed groups of fish throughout the study. Three exposure scenarios were performed in parallel: a control group fed solely on fish food modified with cod liver oil; a dosed group that were fed food containing a nominal 15 µg/g of test substance; and a positive control group that were fed food dosed with a nominal 15 µg/g of test substance plus 3 µg/g of hexachlorobenzene (HCB) (the mean measured concentrations were 15.5 µg/g and 2.64 µg/g, respectively). The test and reference substances were incorporated into the fish feed as a solution using apolar solvents. Residual solvents were removed under a gentle stream of nitrogen, after which the aliquot was recombined with a known mass of fish feed, to which cod liver oil was then added (0.5 mL per 100g) and the feeds homogenised. The exposure (uptake) period of 14 days was followed by 56 days of depuration during which the fish were fed non-dosed food. Sampling during the uptake phase took place on days 1, 7 and 14. During the depuration phase, samples were taken on days 1, 3, 7, 14, 28 and 56. On each of the sampling days, five samples were taken with two fish per sample from each of the exposure groups. Feeding rates for all groups were maintained

at approximately 1.5% of body weight (wet weight). Initial rates were determined from weight measurements of a sample of the stock population at day 0. Adjustment to the food quantity was made according to weight measurements that were taken at each sampling interval to account for growth during the test.

Concentrations of total C_{14} chlorinated n-alkane, 50% Cl wt. and HCB were measured in fish food and tissues throughout the study. The performing laboratory analysed samples from the non-dosed control and positive control group using a GCMS method. Samples from the fish group dosed with the test substance were pooled, homogenised, lyophilised and stored at -80 °C prior to shipping to a sub-contractor for extraction and specific analyses using an APCI-QToF-HRMS method. (Congener-specific analysis was also conducted using APCI-QToF-MS, but the data were not used in the calculation of depuration rate constants as they were not considered sufficiently reliable because the mass balance and true extraction efficiency could not be calculated for the individual components.)

The eMSCA considers that the analyses appear to be well performed, but without additional information about the efficiency of sample extraction it is unclear whether all material relating to the test substance was recovered. The data may therefore underestimate the 'true' concentrations in fish tissues, which could affect the depuration rate constant. The report also states that internal standards (Dechlorane Plus™ (anti- isomer) and hexabromocyclododecane) were applied to samples, but no results or conclusions relating to their use have been presented. The eMSCA also notes that the effect of lyophilisation on the availability of the substance for extraction does not seem to have been considered.

At day 14 of the uptake phase, mean measured concentrations of C_{14} chlorinated n-alkane, 50% Cl wt. and HCB in fish were 0.235 µg/g and 0.32 µg/g, respectively. After 56 days of depuration, the mean measured concentrations of C_{14} chlorinated n-alkane, 50% Cl wt. and HCB were less than the limit of detection (LOD) (<0.071 µg/g) and 0.027 µg/g, respectively.

Mean lipid fractions in both the diet (L_{food}) and fish tissues (L_{fish}) of the positive control group were 0.164 (standard deviation: ±0.389) and 0.0606 (standard deviation: ±0.0120), respectively. These values were calculated from the mean lipid fraction in food on days -3 and 14 of uptake and mean percentage lipid fraction in the whole fish from each sampling interval. The lipid correction factor (L_c) was calculated to be 0.371 ($L_c = L_{fish}/L_{food}$).

Depuration rate constants and dietary biomagnification factors for total C_{14} chlorinated n-alkane, 50% Cl wt. and HCB are presented in Table 39. These values are those presented in the final study report and have been checked by the eMSCA. The growth-corrected depuration half-life was 108.9 days. The growth-corrected and lipid-normalised BMF derived for C_{14} chlorinated n-alkane, 50% Cl wt. was 0.448.

Interpretation of the analytical data was not performed by the contracted laboratory. Instead, an appendix to the final report was produced by the Registrant's representative in consultation with other specialists. Data from analyses were also reported in Unpublished (2019f). A large number of results were below the limit of detection of the analytical technique (0.071 µg/g wet weight of fish). At each depuration sampling interval (n=6), five replicate fish were sampled. No measurements below the LOD were noted on day 1 and 28; one measurement below the LOD was noted on day 7; two measurements below the LOD were noted on day 3 and 14; and four measurements below the LOD were noted on day 56. It is not unusual to see such measurements at later sampling intervals of a depuration period. However, the occurrence at the earlier sampling intervals has not been explained. All values below the LOD were replaced with LOD and/or ½LOD. The influence of these replacements on the depuration rate constant (k_2; days^{-1}) and statistical fit (R^2; unit less) were assessed. The eMSCA agrees with this approach.

The eMSCA has also had access to the spread sheets produced, and is satisfied that the handling of the data has been performed correctly, although these sheets cannot be considered to be GLP-certified. The results presented in Table 39 are acceptable for assessing the bioaccumulation of C_{14} chlorinated n-alkane, 50% Cl wt.

Table 39

SUBSTANCE DEPURATION RATE CONSTANTS AND BIOMAGNIFICATION FACTORS FOR TOTAL C_{14} CHLORINATED N-ALKANE, 50% CL WT. AND HEXACHLOROBENZENE (UNPUBLISHED, 2019d)			
Parameter	**Total C_{14} 50% Cl. wt.**	**HCB**	**Units**
k_g growth rate constant	0.0199	0.0199	day^{-1}
k_2 overall depuration rate constant	0.0262	0.0462	day^{-1}
k_{2L} lipid corrected rate constant	0.0285	0.0488	day^{-1}
k_{2g} growth corrected depuration rate constant	0.006362	0.0264	day^{-1}
$C_{0,m}$ measured time 0 concentration, concentration in fish at the end of the uptake phase	0.235	0.324	µg/g
$C_{0,d}$ derived time 0 concentration of depuration phase	0.184	0.337	µg/g
$C_{0,d}$ (lipid corrected)	3.1227	6.0832	µg/g lipid wt.
I feed ingestion rate, adjusted for growth	0.0150	0.0150	g food/g fish/day
I_g effective feeding rate, adjusted for growth	0.0104	0.0104	g food/g fish/day
C_{food} concentration of substance in food	15.5	2.6	µg/g
C_{food} lipid basis	94.83	16.154	µg/g
a substance assimilation efficiency	0.0677	0.825	unit less
$a_{lipid\ corrected}$ substance assimilation efficiency	0.2735	3.561	unit less
BMF_K kinetic dietary BMF	0.0387	0.267	unit less
BMF_{Kg} growth corrected kinetic dietary BMF	0.160	0.469	unit less
BMF_{KL} lipid corrected kinetic dietary BMF	0.1002	0.760	unit less
BMF_{KgL} lipid corrected growth corrected kinetic dietary BMF	0.448	1.408	unit less
$t_{½}$ half-life	26.4	15.0	days
$t_{½g}$ (growth corrected half-life; days)	108.9	26.0	days
t_{ss} 95%	472	114	days
L_c lipid correction factor	0.371	0.371	fish/food lipid ratio
L_{fish}	0.0606	0.0606	mean lipid fraction in fish
L_{food}	0.164	0.164	mean lipid fraction in fish food

The eMSCA has calculated fish BCFs for the test substance and HCB using the 15 models within the OECD TG 305 BCF estimation tool (Excel® spread sheet, downloaded September 2019). The mean fish lipid at the uptake end or depuration start (fraction) and the mean fish lipid at depuration end (fraction) were calculated using the percentage lipid in five fish. Values calculated by the eMSCA were 0.0581 and 0.0652 for the depuration start and the depuration end, respectively. The mean weight of the fish at day 0 of the study was calculated using k_1 and the intercept value of the trend line. A summary of the inputs/outputs are presented in Table 40 (the models by Brooke and Crookes (2012) and Inoue *et al.* (2012) do not include a step in which a k_1 value is calculated).

Table 40

INPUT VALUES USED TO ESTIMATE BCF FOR TOTAL C_{14} CHLORINATED N-ALKANE, 50% CL WT. AND HCB USING DATA FROM UNPUBLISHED (2019d) OR CALCULATED BY THE eMSCA FROM DATA PROVIDED BY THE REGISTRANT			
Variable	**Total C_{14} chlorinated n-alkane, 50% Cl wt.**	**HCB**	**Source**
Mean weight at test start (g)	2.02	2.02	Unpublished, 2019d
Uptake phase duration (days)	14	14	Unpublished, 2019d
Growth rate, k_2 (day^{-1})	0.0199	0.0199	Unpublished, 2019d
Log K_{OW}	6.58 Unpublished, 2019b	5.5 OECD GD 191	-
$k_{2\,g}$ (k_2 - k_g)	0.0264	0.0264	Unpublished, 2019d
Mean fish lipid uptake end or depuration start (fraction)	0.0581	0.581	eMSCA
Mean fish lipid depuration end (fraction)	0.0652	0.0652	eMSCA
Depuration phase duration (days)	56	56	Unpublished, 2019d
BMF $_{KgL}$	0.448	-	Unpublished, 2019d

Inputs and outputs from the OECD TG 305 BCF estimation using growth and lipid-corrected values are presented in Figure 4 for the test substance and Figure 5 for HCB. The BCF estimations for HCB correlate well with those that were generated during the OECD-sponsored ring testing of the dietary study method (see OECD Guidance Document 191: ENV/JM/MONO(2013)15). The results indicate a BCF for the test substance well above 5 000 L/kg for all of the models.

The eMSCA notes that this study was not performed with a radiolabel (which would have allowed a total radioactive residue associated with ingested/biomass related test substance to be calculated). Therefore the assimilation efficiency and bioaccumulation factors may be significantly greater that the values presented. There is no way of assessing how much of the test material was metabolised or retained in the tissues during exposure or after extraction. Therefore, the eMSCA believes that the results of this study should be treated with caution.

Figure 4 - Inputs and Outputs from the OECD TG 305 BCF Estimation Tool for C_{14} chlorinated n-alkane, 50% Cl. wt.

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0.0199
Log K_{OW}	6.58
$K_{2\,g}$ (K_2 - K_g)	0.006362
Mean fish lipid uptake end or depuration start (fraction)	0.0581
Mean fish lipid depuration end (fraction)	0.0652
Depuration phase duration (days)	56
$BMF_{g\,l}$	0.448

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.100
Mean lipid content midpoint depuration phase	0.062
$K_{2\,g\,l}$	0.008

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	435.55	55523.7	Hayton and Barron (1990)
weight	598.56	76305.2	Erickson and McKim (1990a)
weight	594.66	75807.4	Barber et al. (1991)
weight	384.50	49015.8	Barber (2003) - observed
weight	614.97	78396.1	Barber (2001)
weight	116.47	14847.1	Streit and Sire (1993)
weight	481.00	61317.9	Erickson and McKim (1990b)
weight	410.12	52282.0	Sijm et al. (1995)
weight	496.39	63280.2	Barber (2003) - calibrated
log Kow	988.01	125951.5	Tolls and Sijm (1995)
log Kow	885.65	112902.4	Spacie and Hamelink (1982)
weight, log Kow	106.26	13546.0	Hendriks et al. (2001)
weight, log Kow	81.48	10386.6	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
$K_{2\,g\,l}$	725.95	92544.7	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
$BMF_{g\,l}$	53.19	6780.4	Inoue et al (2012)

Figure 5 - Inputs and Outputs from the OECD TG 305 BCF Estimation Tool for HCB

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0.0199
Log K_{OW}	5.5
$K_{2\,g}$ (K_2 - K_g)	0.0264
Mean fish lipid uptake end or depuration start (fraction)	0.0581
Mean fish lipid depuration end (fraction)	0.0652
Depuration phase duration (days)	56
$BMF_{g\,l}$	1.408

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.100
Mean lipid content midpoint depuration phase	0.062
$K_{2\,g\,l}$	0.033

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	435.55	13380.4	Hayton and Barron (1990)
weight	598.56	18388.4	Erickson and McKim (1990a)
weight	594.66	18268.4	Barber et al. (1991)
weight	384.50	11812.1	Barber (2003) - observed
weight	614.97	18892.3	Barber (2001)
weight	116.47	3577.9	Streit and Sire (1993)
weight	481.00	14776.7	Erickson and McKim (1990b)
weight	410.12	12599.2	Sijm et al. (1995)
weight	496.24	15245.0	Barber (2003) - calibrated
log Kow	729.46	22409.5	Tolls and Sijm (1995)
log Kow	614.47	18877.0	Spacie and Hamelink (1982)
weight, log Kow	103.65	3184.1	Hendriks et al. (2001)
weight, log Kow	160.00	4915.3	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
$K_{2\,g\,l}$	529.31	16260.8	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
$BMF_{g\,l}$	569.65	17500.2	Inoue et al (2012)

Other studies

A series of other dietary accumulation studies have been carried out with Rainbow Trout (*Oncorhynchus mykiss*), i.e. Fisk *et al.*, 1996; Fisk *et al.*, 1998b; and Fisk *et al.*, 2000 (summarised in EC, 2005). These studies are included in the registration dossiers as supporting or "other" information, and are rated as 'reliable with restrictions'.

Dietary BMFs (defined as the growth-corrected concentration in fish on a lipid weight basis divided by the concentration in food on a lipid weight basis) in the range 1 - 3 were determined for several MCCPs of specific carbon chain lengths, although there is some uncertainty over the relevant basis on which to express these BMFs (for further details, see EC, 2005). It should also be noted that the majority of the food uptake studies were based on ^{14}C-measurements. This means that although radioactivity was found in the organisms, the concentrations do not necessarily represent the parent compound. In addition, the series of studies carried out by Fisk *et al.* (1998b) involved non-radiolabelled test substances with chlorine substituted on the terminal and adjacent carbon atoms. These particular terminal-substituted substances may not be representative of the constituents likely to be present in MCCPs (the method of manufacture of MCCPs means that it is very unlikely that a chlorine atom will be present on both the terminal and adjacent carbon atoms).

In response to an earlier draft version of this Substance Evaluation Report, the Registrants provided an independent commentary (Unpublished, 2013), which reviewed the Fisk *et al.* series of studies and estimated the metabolism rate constant for the substances tested. Nevertheless, "no clear differences" in the estimated metabolism rate constant were found for the terminal Cl-substituted substances compared with the non-terminal Cl-substituted substances (although there was evidence for a slightly higher assimilation efficiency for the terminal Cl-substituted substances compared with the non-terminal Cl-substituted substances). Unpublished (2013) speculated that this could be due to some slow but relevant degradation of the non-terminal Cl-substituted substances in the gastro-intestinal tract by microorganisms and/or some first pass effects in the gastro-intestinal tissues and liver that do not occur as quickly for terminal Cl-substituted substance[18].

There was some evidence that metabolism may have been occurring in the organisms. The Fisk *et al.* (1996 and 2000) studies concluded that the potential for metabolism decreases with increasing carbon chain length and chlorine content. Based on an analysis of all the available data, Fisk *et al.* (2000) estimated that chlorinated paraffins with more than 14 carbon atoms, nine chlorine atoms and a total number of carbon and chlorine atoms of around 22 to 30 are metabolised only very slowly, if at all. It was recognised that this conclusion should be treated with caution as it was based on relatively few data.

Since the EC (2005) risk assessment was completed further guidance on how to carry out and interpret the results of dietary exposure studies with fish has become available. The OECD TG 305 was revised in 2012, and now provides internationally-agreed methodology for carrying out such tests. In particular, the test guideline recommends that the BMFs from feeding studies are both growth-corrected and lipid-normalised. The relevant growth-corrected and lipid-normalised data from the available studies with MCCPs is summarised in Table 41 (see EC (2005) for further details of these studies). When considering these data, it is important to note that the method used by Fisk *et al.* (1996, 1998b and 2000) for estimating the assimilation efficiency is different to those recommended in the test guideline. The Fisk *et al.* papers corrected the concentrations measured in the fish for growth dilution during the uptake phase, whereas the revised OECD TG 305 estimates the

[18] Although this is a possible explanation, it needs to be considered alongside the overall uncertainty of the assimilation efficiencies reported for this study, in particular how the data from the uptake phase of the study were analysed and reported (as discussed on the next page of this report).

assimilation efficiency from the fish concentrations without this correction and then subtracts the effects of growth from the depuration rate constant. The Fisk *et al.* papers may therefore overestimate the assimilation efficiency (which could be the reason why the assimilation efficiency for one substance is reported to be above 100%). However, the estimation of the growth-corrected depuration rate constant/half-life is consistent with OECD TG 305. The study report for Unpublished (2019d) provides a growth-corrected and lipid-normalised BMF value directly.

Table 41

SUMMARY OF DIETARY ACCUMULATION DATA FOR MCCPs

Substance	Concentration in food (µg/kg)	Feeding rate (% body weight)	Assimilation efficiency - α[c] (%)	Growth corrected depuration half-life (days)	Kinetic dietary BMF[d]	Reference
^{14}C - $C_{14}H_{26}Cl_4$ (42.3% Cl)	92	Not given	33	39	1.7	Fisk *et al.* (1998b)
^{14}C - $C_{14}H_{25}Cl_5$ (a) (47.9% C)	66	Not given	51	53	3.6	Fisk *et al.* (1998b)
^{14}C - $C_{14}H_{25}Cl_5$ (b) (47.9% Cl)	54	Not given	46	46	2.9	Fisk *et al.* (1998b)
^{14}C - $C_{14}H_{24}Cl_6$ (a) (52.6% Cl)	63	Not given	130	29	5.0[e]	Fisk *et al.* (1998b)
^{14}C - $C_{14}H_{24}Cl_6$ (b) (52.6% Cl)	40	Not given	27	43	1.6	Fisk *et al.* (1998b)
^{14}C - $C_{14}H_{23.3}Cl_{6.7}$ (55.4% Cl)	1 300	1.5	10	58	0.43	Fisk *et al.* (2000)
^{14}C - $C_{14}H_{23.3}Cl_{6.7}$ (55.4% Cl)	13 000	1.5	11	41	0.27	Fisk *et al.* (2000)
C_{14} chlorinated n-alkane 50% Cl wt.	15 000	1.5	6.77	108.9	0.448	Unpublished (2019d)
^{14}C - $C_{16}H_{31}Cl_3$ (32.3% Cl)	29	1.5	33	50	1.07	Fisk *et al.* (1996)
^{14}C - $C_{16}H_{31}Cl_3$ (32.3% Cl)	296	1.5	35	37	0.90	Fisk *et al.* (1996)
^{14}C - $C_{16}H_{21}Cl_{13}$ (68.4% Cl)	21	1.5	30	58	0.72	Fisk *et al.* (1996)
^{14}C - $C_{16}H_{21}Cl_{13}$ (68.4% Cl)	198	1.5	9.4	63	0.44	Fisk *et al.* (1996)
^{14}C - $C_{16}H_{21}Cl_{13}$ (68.4% Cl)	2 000	1.5	11.4	77	0.50	Fisk *et al.* (1996)

Notes: a) and b) denote different isomers.
c) As reported in the paper; the method used to estimate these values is not entirely consistent with that in OECD TG 305.
d) Kinetic BMF is estimated on a lipid normalised and growth corrected basis.
e) This value can be questioned as the assimilation efficiency used in the calculation is >100%.

The available dietary BMF data strongly suggest that C_{14} chlorinated paraffins are taken up from food but that the potential for uptake (as measured by assimilation efficiency) decreases with increasing carbon chain length and increasing chlorine content. Depuration

from fish is relatively slow and BMFs above one are estimated for C_{14} chlorinated paraffins with 4 and 6 chlorine atoms per molecule (corresponding to chlorine contents of approximately 42 - 53% by weight). In contrast, the most recent OECD TG 305 study for C_{14} chlorinated n-alkane, 50% Cl wt. reports a growth-corrected and lipid-normalised BMF value of 0.448 (Unpublished, 2019d). BMFs are estimated to be close to one for C_{16} chlorinated paraffins with three chlorine atoms per molecule (chlorine content approximately 32% by weight). At higher chlorine contents than these the BMF is below one for both the C_{14} and C_{16} substances. The C_{14} and C_{16} chlorinated paraffins for which the BMF is close to or above 1 cover broadly the same chlorine content range as those for which the BCF is expected to be above 2 000 L/kg. It is important to note, however, that the method used for calculating the assimilation efficiencies in these studies is not comparable with the method currently recommended in OECD TG 305, and this introduces some uncertainty over the values reported. Furthermore, for five of the six substances resulting in a BMF above 1 (i.e. the Fisk *et al.* 1998b study) the structure of the substance tested had terminal and adjacent chlorine atoms and so may not be representative of the structures present in commercial MCCPs.

As well as BMF data, these feeding studies provide information on the growth-corrected depuration half-life of MCCPs (and other chlorinated paraffins). This can be used to estimate an equivalent BCF value using the 15 models within the OECD TG 305 BCF estimation tool (Excel® spread sheet). Further information can be found in Brooke *et al*. (2012). The eMSCA has calculated fish BCFs using this tool based on relevant data from the Fisk *et al.* (1996), Fisk *et al.* (1998b), Fisk *et al.* (2000) and Unpublished (2019d) studies as shown in Appendix F. These studies only give the starting weights of the fish (as a range) and the rate constant for growth dilution. The weights of fish at the end of the uptake/start of depuration have been estimated for the purposes of this substance evaluation using the mid-point of the starting weight range and applying the growth dilution rate constant to calculate the equivalent weight at day 40 of the study (the end of the uptake phase). As well as information on substances with chain lengths within the MCCPs range (i.e. C_{14} to C_{17}), other chlorinated paraffins have been included for comparison. Based on this analysis, very high growth-corrected BCF values of the order of 10 000 to 126 000 L/kg and 13 000 to 140 000 L/kg can be estimated for C_{14} and C_{16} chlorinated paraffins, respectively. An analysis has also been carried out by estimating the non-growth-corrected BCF (using the overall depuration rate constants that can be derived from the studies and the predicted uptake rate constants). In this case, the non-growth-corrected BCF is estimated to be of the order of 6 000 to 45 000 L/kg for the C_{14} chlorinated paraffins, 8 000 to 62 000 L/kg for the C_{16} chlorinated paraffins, and a maximum 30 584 L/kg for C_{14} chlorinated n-alkane, 50% Cl wt. (setting the growth rate to 0, using k_2, k_{2g} and BMF_L). Whilst indicating a very high level of bioaccumulation, the reliability of all these estimates is uncertain.

It is worth noting that the growth-corrected depuration rate constant determined in the Fisk *et al.* series of studies, and hence depuration half-life, is similar for all MCCPs considered (the general range for the depuration rate constant is 0.009 to 0.024 day^{-1}, which is equivalent to a growth-corrected depuration half-life of 29 to 77 days). This is also similar to the growth-corrected depuration rate constant determined in the Thompson *et al.* (2000) BCF study (0.0194 - 0.0251 day^{-1}, corresponding to a half-life of 28 to 36 days) and the Unpublished (2010h) BCF study (0.0132 day^{-1}, corresponding to a half-life of 53 days). The new OECD TG 305 study found a growth corrected depuration constant of 0.006362 day^{-1}, corresponding to a half-life of 108.9 days (Unpublished, 2019d). Work by Brooke and Crookes (2012) suggests that a depuration rate constant around 0.178 day^{-1} or less, and around 0.085 day^{-1} or less, would indicate a BCF above 2 000 and 5 000 L/kg, respectively. All of the tested substances would therefore be expected to have a BCF above 5 000 L/kg.

A further study of the uptake of MCCPs by Rainbow Trout (*Oncorhynchus mykiss*) was carried out by Cooley *et al.* (2001) as part of a toxicity investigation. The study is included

in the registration dossiers but disregarded as part of the bioaccumulation assessment. It was discussed in detail in EC (2005). Juvenile fish were exposed daily to food containing one of two MCCPs ($C_{14}H_{24.9}Cl_{5.1}$ (48.4% Cl wt.) or ^{14}C - $C_{14}H_{23.3}Cl_{6.7}$ (55.4% Cl wt.)) for either 21 or 85 days. At the end of the exposure period the concentration in the fish was determined either by parent compound analysis (for the 48.4% Cl wt. substance) or ^{14}C analysis (for the 55.4% Cl wt. substance). The BMF was estimated as the ratio of fish and food concentrations. The BMFs at day 85 were 0.22 for the 48.4% Cl wt. substance and 0.10 for the 55.4% Cl wt. substance (lower BMFs were reported in the 21 day studies). It is important to note that these values are not growth-corrected or lipid-normalised (the food used in the test had a lipid content of 14%) and so are not directly comparable with the data reported in Appendix F (lipid normalization and growth correction would tend to increase the BMF values). In addition, Cooley *et al.* (2001) reported that fish from some of the higher exposure concentrations fed erratically during the test, which might confound the results (although the 85 day studies used lower test concentrations than the 21 day studies). The exposure concentrations are not consistent between tables and text, and some concentrations with the same numerical value have differing units (ng/g or µg/g). The Registrants assign this study a reliability rating of 3 ("unreliable"), and the eMSCA agrees.

6.7.5.2.2 Field bioaccumulation data

As discussed in Section 6.3.1, there are considerable analytical challenges associated with the detection and quantification of MCCPs. Therefore, detections of MCCPs in biota and the environment are considered valid but qualitative indicators only in the following discussion.

The Swedish Environmental Protection Agency (1998) found no evidence for biomagnification in the herring to seal food chain for chlorinated paraffins based on the results of Jansson *et al.* (1993) (the levels found in herring were higher than in seals by an order of magnitude on a lipid weight basis). The actual chlorinated paraffins determined in the Jansson *et al.* (1993) study were of unspecified carbon chain length, with between 6 and 16 chlorine atoms per molecule, and so may contain chlorinated paraffins other than MCCPs.

Muir *et al.* (2002) (summarised in detail in EC, 2005) found no indications of biomagnification in three Lake Trout-fish food chains, but did suggest biomagnification factors (BMFs) above one for MCCPs in a fish-invertebrate food chain. Furthermore, there were some indications that the actual bioaccumulation seen in fish was higher than would be expected by bioconcentration processes alone (although it should be noted that there is considerable uncertainty in these data).

A similar study (possibly including some of the same information as Muir *et al.*, 2002) was published by Houde *et al.* (2008). In this study MCCP levels were determined in samples of biota collected in Lake Ontario and northern Lake Michigan between 1999 and 2004. These were compared with the mean level of MCCPs determined in water samples from 2004 (0.9 pg/L). Based on these results, lipid normalised bioaccumulation factors (BAFs, expressed as log BAF_{lipid}) for C_{14} and C_{15} chlorinated paraffins were determined as 6.2 and 6.6 in plankton, 7.0 and 6.8 in Alewife (*Alosa pseudoharengus*), 7.4 and 7.2 in Slimy Sculpin (*Cottus cognatus*), 7.4 and 7.1 in Rainbow Smelt (*Osmerus mordax*) and 6.8 and 6.5 in Lake Trout (*Salvelinus namaycush*), respectively. Again the lipid-normalised BMF values for total MCCPs were below one in food chains consisting of Lake Trout–Alewife (BMF 0.22 - 0.25), Lake Trout–Rainbow Smelt (BMF 0.14), Lake Trout–Slimy Sculpin (BMF 0.11 - 0.94). The lipid-normalised BMF was above one for the Slimy Sculpin–*Diporeia* food chain in Lake Ontario (BMF 8.7), but below one in the same food chain from Lake Michigan (BMF 0.88). It was noted that the BMF for Slimy Sculpin–*Diporeia* in Lake Ontario was based on the detectable concentration in one sample only. Trophic magnification factors were determined to be in the range 0.06 to 0.36 for fourteen individual constituents in the C_{14} to C_{16} chain length range for the Lake Ontario food chain (a similar analysis could not

be carried out for Lake Michigan samples), suggesting trophic dilution was occurring overall. When considering these data it should be noted that the water concentrations relate to samples collected in 2004 whereas the biota samples were taken between 1999 and 2004. There is no information reported on how the dissolved concentration in water varied over the period 1999 and 2004 and so this means that the reported BAFs in particular are highly uncertain.

6.7.5.2.3 Monitoring data

The available monitoring data for MCCPs in biota are summarised in Appendix D. When considering these data, it is important to recognise that the analysis of MCCPs in environmental samples is challenging (see Section 6.3.1). In particular, some commonly used low resolution mass spectrometry methods may be subject to interferences from both the matrix and other contaminants (such as chlordanes, polychlorobiphenyls and toxaphenes) unless highly efficient sample clean-up procedures are used. In addition, quantification often requires the use of commercial products as standards due to the lack of certified reference standards. The sensitivity of the detection method can depend significantly on the chlorine content of these. This means that the reported concentrations are uncertain in many cases. Nevertheless, many of the more recent studies (e.g. Reth *et al.*, 2006) took precautions to minimise these problems.

The following studies provide an indication of the findings:

- Bennie *et al.* (2000) reported levels of MCCPs up to around 80 mg/kg wet weight (ww.) in blubber samples from stranded Beluga Whales *(Delphinapterus leucas)* from the St. Lawrence River, Canada, although the analytical method may have been affected by the possible presence of co-eluting interfering organochlorine substances[19].

- Reth *et al.* (2006) found MCCPs to be present in samples of Arctic Char (*Salvelinus alpinus*) liver and muscle, Little Auk (*Alle alle*) liver and muscle and Black-legged Kittiwake (*Rissa tridactyla*) liver and muscle from the Arctic (Bear Island). The highest concentration was 0.37 mg/kg (in Little Auk liver tissue). The relative abundance of C_{14} substances was between 55 and 82% (mean 65.8%) and the ratio of C_{14}/C_{15} substances was around two (higher ratios up to around 4 - 5 were found in some Cod samples). This C_{14}/C_{15} ratio was reported to be similar to that found in commercially supplied products. The MCCPs had between 6 and 9 chlorine atoms per molecule, and the mean chlorine content of the MCCPs found was estimated to be 55.85% (range 54.5 - 57.4%).

- Houde *et al.* (2008) measured the levels of C_{14}, C_{15}, C_{16} and C_{17} chlorinated paraffins in biota samples from Lake Michigan and Lake Ontario, North America. The data are presented as mean concentrations over the period 1999 – 2004. The highest average concentrations were found in Slimy Sculpin and Rainbow Smelt (0.11 mg/kg). When MCCPs was detected, C_{14} chlorinated paraffins were the predominant constituents found in samples from Lake Michigan. However, samples from Lake Ontario generally showed that C_{15} constituents were present at similar, and in several cases higher, concentrations than the C_{14} constituents in those samples. An indication of potential variability is that the mean concentration of MCCPs in Lake Trout from Lake Ontario reported by two different papers was

[19] A gas-chromatography-low resolution negative ion mass spectrometry method was used. Although no comparison was carried out for MCCPs, Bennie *et al.* (2000) compared their results for SCCPs with those obtained on Beluga Whale samples using a gas-chromatography-high resolution negative ion mass spectrometry method from another study. They found that the concentrations were one to two orders of magnitude lower using the high resolution method than the low resolution method.

25 µg/kg in 1998, 15 µg/kg in 2001 and 8 µg/kg in 2004 (Muir *et al.*, 2002; Ismail *et al*., 2009).

- Du *et al.* (2018) investigated the occurrence of chlorinated paraffins in wildlife from paddy fields in the Yangtze River Delta, China. Nine species (2 fish, 3 reptiles, 1 mammal and 3 birds) were sampled: Pond Loach *(Misgurnus anguillicaudatus),* Rice Field Eel *(Monopterus albus),* Red-backed Rat-snake *(Elaphe rufodorsata),* Short-tailed Mamushi Snake *(Gloydius brevicaudus),* Red-banded Snake *(Dinodon rufozonatum),* Yellow Weasel *(Mustela sibirica),* Peregrine Falcon *(Falco peregrinus),* Collared Scops-owl *(Otus lettia)* and Common Cuckoo *(Cuculus canorus)*. Numerical values are provided in Appendix D. The highest values were found in snakes, the weasel and predatory birds (up to 33 mg/kg lw or 4.7 mg/kg dw). The authors found that the average concentrations were in the order MCCPs > SCCPs > LCCPs, except in birds where SCCPs were found to be more abundant. The eMSCA has not evaluated this study, but notes that MCCPs appears to be widely dispersed in wildlife at the sampling locations. The sampled species were not necessarily part of the same food web (e.g. some are terrestrial rather than aquatic feeders), so it is not possible to draw firm conclusions about trophic magnification from this study.
- Yuan and de Wit (2018) and Yuan *et al*. (2019) analysed for chlorinated paraffins with a chain length up to C_{30} in the Swedish environment using APCI-QTOF-MS. Numerical values are provided in Appendix D. In the marine food web, concentrations of MCCPs in White-tailed Sea-eagles, Grey Seal, Harbour Seal and Harbour Porpoise (around 0.2 – 0.5 mg/kg lipid) were generally similar to or higher than those in Herring (around 0.03-0.44 mg/kg lipid). The eMSCA has not evaluated this study.
- Several studies have indicated that MCCPs can undergo maternal transfer to birds' eggs, the highest reported concentration being 0.135 mg/kg ww (e.g. Heimstad *et al*., 2017; Ruus *et al*., 2018; Green *et al*., 2018; Yuan *et al*., 2019).

Despite the general uncertainty in available data, MCCPs is present in a wide range of organisms living and feeding in locations that are close to input sources (industrial areas, urban areas). Whilst more limited in number, MCCPs have also been detected in samples from remote regions, including the Arctic, and also in top predators. Only limited information is available on the actual carbon chain length distribution and chlorine contents of MCCPs detected in environmental samples, although advances in analytical methodologies have meant that this has been possible in some of the more recent studies. C_{14} chain lengths are frequently the predominant constituents of MCCPs present in commercial product types (see Section 6.3) and environmental media such as sediment (Hüttig and Oehme, 2006).

6.7.5.2.1 Other supporting data

Castro *et al*. (2019) investigated bioaccumulation potential in the cladoceran water flea *Daphnia magna*. This study is not included in the REACH registrations. Five commercially available chlorinated paraffin products were used, including one MCCP product: a C_{13}-C_{18} 45% Cl wt. product from the UK (Cereclor S45)[20]. Daphnids were cultured in M7 media with a stock density of approximately 10 individuals per litre, and fed a mixture of the green algae *Pseudokirchneriella subcapitata* and *Scenedesmus spicatus* three times per week. A passive dosing device was created to generate stable solutions in water, by

[20] The others were a C_9-C_{14} 50% Cl wt. product from the UK; a C_9-C_{14} 70% Cl wt. product from Germany; a "C_{10}-C_{14}, C_{21}-C_{31}" 42% Cl wt. product from the UK [the text also says this was a "C_{10}-C_{17}, C_{21}-C_{31}" substance but later describes it as containing short and long chains, so this may be a typographical error); and a C_9-C_{30} 52% Cl wt. product from China.

loading medical grade silicone with 1.0 or 2.5 g (±1%) of the chlorinated paraffin (to give a final concentration of each technical substance of 1 mg per g silicone). The dosed silicone was added to water in test vessels and equilibrated for 48 h to create the test solutions. The experiments were conducted under static conditions, at a constant temperature of 22 °C and a 16:8 h light/dark cycle. Blank controls were also prepared (no silicone or substance, n = 10).

Daphnia neonates (<24 h old) were exposed to dosed water alone (aqueous exposure) or dosed water with food (dietary exposure) for a 48-hour period, followed by a depuration period of 24 hours (using clean water and food). The density of animals in the tests was 2 mL per neonate in accordance with OECD TG 202. The food concentration (when added) was 4 µC/mL. Five replicates per treatment were used. At the end of the exposure period, 20 mL water samples were collected into screw capped glass tubes and spiked with 20 ng of $^{13}C_{10}H_6Cl_6$ (hexachlorodecane) as the internal standard. In addition, the test vessels were emptied, cleaned and then fresh medium added (without organisms), and allowed to equilibrate for 24 h with the loaded silicone, to measure the freely dissolved concentration (avoiding sorption to organic matter). Liquid−liquid extraction was performed twice with iso-hexane in glass tubes, the solvent evaporated, and 20 ng of dechlorane-603 added prior to analysis as a volumetric standard. Juvenile daphnids (3 and 4 days old after the uptake or depuration phase, respectively) were collected, and dead animals discarded. The samples were freeze-dried. Exoskeletons shed by unexposed adult daphnids were also collected and left to equilibrate in the passive dosing vials for 1 week. Before extraction, 20 ng of the internal standard was added to each daphnid sample, which was then homogenized in a mixture of Milli-Q water and iso-hexane (1:1 v/v). After a centrifugation step, the iso-hexane phase was collected. The extract volume was reduced with a gentle nitrogen flow and transferred into 300 µL dark glass vials. The samples were stored at −18 °C until analysis. Prior to injection, 20 ng of dechlorane-603 was added to the vials as a volumetric standard. Quantification of chlorinated paraffins was by APCI-QTOF-MS. The recovery of the internal standard was determined using GC-ECNI-LRMS. The limit of detection (LOD) in the water and daphnid samples was 0.39 µg/L and 0.13 ng/µg dry weight, respectively, based on the amount measured in the blank plus three times the standard deviation (SD). The limit of quantification in the water and daphnid samples was 0.47 µg/L and 0.25 ng/µg dry weight, respectively, based on the amount measured in the blank plus ten times the SD. Recoveries were on average 130 ± 0.2 and 101 ± 0.1% for daphnid and water samples, respectively. The high average recoveries for *Daphnia* were thought to be caused by interferences in either the internal or the volumetric standard, due to the high number of congeners present in the technical substance and their overlapping isotopic mass patterns.

The average lipid content of the daphnids was determined by extraction followed by gravimetric analysis. The lipid content was 5 and 7% of the dry weight (w/w) for starved and fed daphnid juveniles, respectively. The ratio between lipid content and dry weight determined in control individuals was used to estimate the lipid content for the remaining samples, where only the dry weight was known. Lipid content was not expected to change much over the short duration of the experiment.

Mortality did not exceed 10% in any of the controls (no information is provided for the treatment groups). BCF and BAF values were calculated using the freely dissolved water concentration (1.2 µg/L). Kinetic data were also derived using the concentration at the end of the uptake phase and at the end of the depuration phase, assuming first-order kinetics. The results for the MCCP product are provided in

Table 42. The BCF and BAF for MCCPs were around 500 000 L/kg dw.

Table 42

MCCPs BIOACCUMULATION DATA FOR *DAPHNIA MAGNA* (CASTRO *ET AL.*, 2019)	
Parameter	**Result**
Log BAF	5.6 ± 0.1 L/kg dw 6.7 ± 0.1 L/kg lipid
Log BCF	5.7 ± 0.2 L/kg dw 7.0 ± 0.2 L/kg lipid
Uptake rate constant for fed daphnids, k_u	1.1×10^5
Uptake rate constant for unfed daphnids, k_1	1.8×10^5
Depuration rate constant, k_d	0.31 (fed) 0.33 (unfed)
Depuration half-life ($t_{1/2}$)[a]	2 h
Time to 95% to steady state (t_{95})	9 h

Note: a - After the depuration phase, levels in daphnids were below the LOD, and so the LOD value was used to calculate the depuration rate (using 0.13 ng/µg dw).

After 1 week's exposure, the amount of MCCPs adsorbed to the exoskeleton represented less than 5% (w/w) of the body burden. This suggests that approximately 95% of the body burden can be explained by passive diffusion through the respiratory area and body surface (and moulting is not a major depuration process for this species).

Concentrations in daphnids were generally higher after aqueous exposure than after simultaneous aqueous and dietary exposure, again indicating that passive diffusion is the dominant uptake process. It is possible that when food is available during the uptake phase, elimination processes such as growth, metabolism and faecal egestion might be increased, although this was not indicated by the depuration rates. The eMSCA also notes that bioavailability might be reduced by adsorption to uneaten food or ingestion by uneaten food.

The highest log BCF and log BAF values were observed for the C_9-C_{14} 70% Cl wt. product (SCCPs) (e.g. log BAF = 5.9 ± 0.2 L/kg dw or 7.0 ± 0.1 L/kg lipid). The lowest values were obtained for the LCCP product, although they were still in the same order of magnitude as MCCPs (e.g. log BAF = 5.4 ± 0.1 L/kg dw or 6.5 ± 0.1 L/kg lipid). MCCPs had the shortest depuration half-life of the five products tested; the LCCP product had a half-life of 7 days. The authors noted that there was an increase in depuration rate of approximately 35% when food was added for the "C_{10}-C_{14}, C_{21}-C_{31}" 42% Cl wt. product. It was speculated that this could have been explained by metabolism of low chlorine content congeners. Increasing levels of chlorination appear to increase both BCF and BAF values, whereas changes in carbon chain length did not appear to affect uptake significantly.

The eMSCA notes the following points:

- There is no standard internationally recognised test guideline for *Daphnia* bioaccumulation. The study appears to have been performed well, but in the absence of a ring-test, the reliability and reproducibility of the method is unknown.

- The data are based on analysis of non-radiolabelled test substance in tissues with no measure of the efficiency or effectiveness of the extraction method. Therefore the calculated bioaccumulation factors might not provide a true indication of the actual level of bioaccumulation. It would have been preferable to have used a radiolabel allowing the total radioactive residue associated with ingested/biomass-related test substance to be calculated.

- The dissolved concentration of MCCPs was below the water solubility limit (27 µg/L). It is not known whether 48 hours gave sufficient time for all soluble congeners to fully dissolve. Only a single water concentration value is presented in the paper, which was derived in the absence of test organisms. It is not clear how this differs from the actual

exposure concentration, or how variable this might have been over the duration of the test.

- It is likely that some daphnids died (at least in the vessels without food) as the dissolved concentration is only a factor of 5 below the 48-h EC_{50} of 5.9 µg/L. Although the paper mentions that dead daphnids were discarded, there is no further information about the number. Bioaccumulation tests are normally carried out at a concentration that avoids adverse effects, and causes less than 10% mortality in the treatment groups.

- *Daphnia* are very small organisms, and the amount of sample collected for each measurement is not stated. This could affect the reliability of concentration measurements, which would also have been affected by the analytical recovery rate exceeding 100%. Only two measurements were used to derive the kinetics and hence the BCF and BAFs. The sensitivity of the results to variations in the measured concentrations is unclear. In addition, the depuration kinetics are based on an LOD value, and since the actual concentration in the organisms may have been lower, the depuration rate constant could have been higher. The depuration rate is used directly to estimate the uptake rate, so influences the final result. As noted by the authors, since static conditions were used, the concentration of MCCPs in water after 24 h depuration would not have been zero, which complicates the interpretation of depuration.

- The results are expressed in terms of dry weight, but for fish studies they are wet weight. Wet weight concentrations would be lower.

- Steady-state was claimed to have been achieved after 48 hours[21]. The OECD TG 305 states that "*steady-state is reached when the curve in the plot of test substance concentration in the organisms against time becomes parallel to the time axis and three successive analyses of organism concentrations made on samples taken at intervals of at least two days are within ± 20% of each other, and there is no significant increase between the first and last successive analysis. When pooled samples are analysed, at least four successive analyses are required. For test substances which are taken up slowly the intervals would more appropriately be seven days*." Daphnia are very small organisms, so it is likely that a steady state can be achieved more quickly than in fish, especially if passive diffusion is the dominant process (as suggested by the data). However, the eMSCA cannot be certain that the organisms had reached steady state because only the concentration at the end of uptake was measured. However, if steady state had not been reached, the final concentration may have been higher. The supporting information shows the equilibration time for three sampling intervals for the CP-52 product in *Daphnia magna*. In order to have confidence in the 48 h value, further detailed information should have been provided for a minimum of five intervals.

- The eMSCA questions the use of the terms 'equilibration' and 'steady-state' by the authors relating to the use of solid-state passive dosing methods. It is not known whether the chlorinated paraffins were evenly distributed in the test systems prior to addition of food and the neonates within the time-frame of the exposure periods. Data presented in an earlier paper (Castro *et al*., 2018) show that a good number of variables had been assessed, but that a longer time period was probably required for the longer

[21] The duration of the uptake and depuration phase was based on a pilot screening study that lasted 72 h, but the data are not provided in the paper. In a previous study (Castro *et al*., 2018), chlorinated paraffins were observed to equilibrate within 24 h in a passive dosing system. The authors also noted that studies with polychlorobiphenyls (PCBs) have also used 2−4 day uptake and depuration phases for this species.

chain length substances. This might also have influenced the distribution of congeners observed in the analysis.

Overall, the eMSCA considers that the results of this study suggest very high BCF/BAFs for *Daphnia*, but there are major uncertainties in the numerical values.

Two bioaccumulation studies are available for Common (Blue) Mussel (*Mytilus edulis*), with BCFs reported as the ratio of concentrations in mussel tissue (mg/kg wet wt) and in water:

- Bioaccumulation was assessed as part of a 60-day GLP-certified toxicity study (Madeley and Thompson, 1983). The test substance was a commercial $C_{14\text{-}17}$ chlorinated n-alkane, 52% Cl wt. product that was mixed with a small amount of radiolabelled chlorinated paraffin (n-pentadecane-8-^{14}C, 51% wt. Cl). Further details are provided in EC (2005). The mean measured concentrations were 0.22 and 3.8 mg/L in the two exposure groups based on radiochemical analysis (significantly higher than the reported water solubility of up to 0.027 mg/L). No mortality occurred in the test, but a reduction in filter feeding activity was seen at the higher test concentration. Higher BCFs were determined at the lower exposure concentration. This is probably the result of incomplete dissolution of the test substance at the higher concentration (the solution was cloudy in appearance), although the feeding rate may also have been a factor. The BCF at the lower concentration was 2 182 L/kg (based on parent compound analysis) or 2 856 L/kg (based on ^{14}C-measurements). The similarity between the values obtained by the two analytical methods suggests that the majority of the ^{14}C present in the organisms must have been as parent compound rather than metabolites.

- Renberg *et al.* (1986) tested a ^{14}C-labelled C_{16} chlorinated n-alkane, 34% Cl wt. (the average formula was given as $C_{16}H_{30.7}Cl_{3.3}$). Further details are provided in EC (2007). The radiolabel was in the 1-position of the carbon chain but no information on the purity of the radiolabelled substance was given (the paper indicates that the purity was checked but gives no further details). The test substance, along with a control substance (2,4',5-trichlorobiphenyl) was delivered to the exposure vessel as a solution in acetone, under flow-through conditions. The exposure consisted of a 28-day uptake phase (depuration was not studied). The measured concentration of the chlorinated paraffin in water was between 0.080 and 0.172 µg/L. The mean measured concentration was not given in the paper, but it can be calculated as 0.11 µg/L (standard deviation: ±0.04 µg/L) from the data reported. The concentration of the chlorinated paraffin in the mussel was found to reach a relatively constant value after 14 days exposure and the authors concluded that the BCF for the C_{16} chlorinated paraffin was 7 090 L/kg with a standard error of 1 100 L/kg and confidence limits[22] of 4 620-9 570 L/kg. The BCF for the control substance was around 13 800 L/kg.

It should be noted that the chlorine content of the substance tested in the Renberg *et al*. (1986) study was lower than that of the main MCCP products in commercial use, although similar substances could still be present as constituents. These studies may have underestimated the true BCF, because they were performed at MCCP concentrations above the water solubility limit (and so the bioavailable dissolved fraction may have been lower than suggested by the reported water concentrations). However, interpretation is not straightforward as there is a possibility that at least some of the exposure of the organisms resulted from direct ingestion of undissolved substance or the substance adsorbed to food

[22] The actual confidence level was not given. The values probably refer to the 90% or 95% confidence limits.

particles. These data are therefore BAFs, and are not directly comparable to the fish BCF value used in the registration dossiers.

A biota-sediment accumulation factor (BSAF) of 4.4 on a lipid normalised basis (defined as the concentration in organism (mg/kg lipid (wet weight)) divided by the concentration in sediment (mg/kg organic carbon (dry weight)) was determined for a C_{16} chlorinated n-alkane, 35% Cl wt. in a study using *Lumbriculus variegatus*; the BSAF for a C_{16} chlorinated n-alkane, 69% Cl wt. substance was lower at 0.6 (for further details, see EC, 2005). The registration dossiers have a RSS for this study and rate it as 'reliable with restrictions'.

6.7.5.3 Terrestrial bioaccumulation

Given the findings for aquatic bioaccumulation, only a very brief summary of available terrestrial bioaccumulation data is presented here:

- An earthworm-soil accumulation factor of 2.4 for adults and 2.3 for juveniles was determined for a C_{15} chlorinated n-alkane, 51% Cl wt. in a 56-day study using *Eisenia fetida*.

- An accumulation factor for uptake from soil into carrots (*Daucus carota*) of 0.045 has been determined for a C_{15} chlorinated n-alkane, 52.5% Cl wt.

The registration dossiers include a RSS for both studies, and rate them 'reliable with restrictions'. Further details can be found in EC (2005 and 2007).

Nicholls *et al.* (2001) reported the concentrations of SCCPs and MCCPs in earthworms residing in fields on which sludge had been applied ranging from <0.1 to 0.7 mg/kg dry wt. in the United Kingdom in the summer of 1998.

Iozza *et al.* (2009a and 2009b) showed that MCCPs were present in samples of spruce needles from the European Alps. MCCPs was detected at concentrations of 0.0052 – 0.095 mg/kg in 8 samples collected in October 2004. C_{14} substances with 6 - 8 chlorine atoms per molecule predominated, although 5, 9 and 10 chlorine atom substances and substances with longer chain lengths were also detectable at a few percent relative abundance. The findings may reflect atmospheric deposition rather than plant uptake.

Wang *et al.* (2016) measured MCCP concentrations in Masson Pine (*Pinus massoniana L.*) needles from Shanghai, China. The measured concentrations were 0.012 to 33.5 mg/kg dw with a geometric mean value of 0.7 mg/kg dw. The details of the analytical method were not available. The findings may reflect atmospheric deposition rather than plant uptake.

Yuan and de Wit (2018) and Yuan *et al*. (2019) analysed for chlorinated paraffins with a chain length up to C_{30} in the Swedish environment using APCI-QTOF-MS. Numerical values are provided in Appendix D. In the terrestrial food web, Bank Voles were found to contain the lowest amounts of MCCPs. The detected concentrations of MCCPs in muscle were comparable in Eurasian Lynx and Grey Wolf (0.75 – 0.83 mg/kg lipid), whilst Moose muscle contained the highest concentrations (1.6 mg/kg lipid). MCCPs were also detected in muscle or eggs of terrestrial birds of prey (Tawny Owl, Eagle Owl, Marsh Harrier, Golden Eagle and Peregrine Falcon) up to 0.72 mg/kg lipid. The authors conclude that this may indicate that MCCPs has the potential to bioaccumulate. The eMSCA has not evaluated this study.

6.7.5.4 Mammalian data

Available mammalian toxicokinetic data have not been reviewed as part of this evaluation, but are relevant to the assessment of bioaccumulation potential. A consideration of the main data for mammals in a laboratory environment was given in EC (2007) and the conclusions are repeated here for completeness. Mammalian studies using radiolabelled MCCPs have shown that absorption following oral exposure is significant (probably at least 50% of the administered dose; however the concentration reached in the organism is generally lower than that in food). Following absorption in mammals there is an initial preferential distribution of the radiolabel to tissues of high metabolic turnover/cellular proliferation. Subsequently there is a re-distribution of radiolabel to fatty tissues where half-lives of up to 8 weeks have been determined for abdominal fat. Of special interest is the study by CXR Biosciences Ltd (2005a) that found that a steady state concentration in white adipose tissue was reached after approximately 13 weeks' exposure via the diet. The elimination from this tissue was found to be biphasic with an initial half-life of 4 weeks followed by a much slower elimination.

Greenpeace (1995) analysed human breast milk for MCCP content using pooled samples from six fish-eaters (who ate fish a minimum of once per week) and two non-fish-eaters (who ate fish a maximum of once a month). Similar results were obtained for both groups (the total chlorinated paraffin content of the fish-eating group was 50.4 µg/kg lipid, compared to 40.5 µg/kg lipid in the non-fish-eaters; the low sample size meant that it was not possible to determine if any significant differences were apparent between the two groups).

Thomas and Jones (2002) detected MCCPs in one out of 22 samples of human breast milk from the UK, at 61 µg/kg lipid. The analytical detection limit was relatively high (in the range 16-740 µg/kg lipid depending on the sample size). A follow-up study (Thomas *et al*., 2003) detected MCCPs in twenty-five samples of human breast milk at 6.2-320 µg/kg lipid. The median and 95th percentile levels were 21 and 127.5 µg/kg lipid, respectively.

C_{14} chlorinated paraffins were found to be the predominant constituents of MCCPs present in samples of human breast milk from Bavaria (Hilger *et al.* 2011b).

Li *et al.* (2017) determined the concentration of SCCPs, MCCPs and LCCPs in 50 human blood samples taken from the general population in Shanghai, China. The SCCP, MCCP, and LCCP concentrations were reported as 370−35 000, 130−3 200, and 22−530 ng/g lipid weight, respectively. The relative exposure of the participants to each substance is unknown. MCCPs were also detected in human breast milk, human blood and human placenta samples in additional studies from China (Xia *et al.* 2017; Wang *et al.* 2018b).

6.7.6 Summary and discussion of bioaccumulation

Two reliable aquatic fish BCF studies are available for MCCPs. The eMSCA has calculated a growth-corrected and lipid-normalised kinetic BCF of 10 500 – 14 600 L/kg for a C_{14} chlorinated n-alkane, 45% Cl wt. product using the data reported by Unpublished (2010h & 2010i) (without growth correction, the BCF is 3 230 – 4 460 L/kg). The highest growth-corrected kinetic BCF for a C_{15} chlorinated n-alkane, 51% Cl wt. substance reported in Thompson *et al*. (2000) is 2 164 L/kg (lipid normalisation is not possible).

It is not ethical to collect measured fish BCF data for all of the potential constituents of MCCPs. However, chloroalkanes are neutral organohalogen compounds, so bioaccumulation is likely to involve simple partitioning to lipid storage tissues. The degree of bioaccumulation of the constituents will depend on their hydrophobicity (which is reflected by their octanol-water partition coefficients, K_{OW}) and metabolism potential. As described in Section 6.4.3, log K_{OW} value is relatively independent of the chlorine content for a given carbon chain length between approximately 45 and 55% Cl wt. For higher chlorine contents (up to 70% Cl wt.), the log K_{OW} increases with increasing chlorine

content in a non-linear fashion. It is therefore likely that many C_{14} constituents of MCCPs will have a similar BCF to that reported by Unpublished (2010h). This is a major congener group in the commercial products. Evidence from enhanced ready biodegradation studies suggest that some constituents (particularly those with low chlorine contents) are susceptible to microbial transformation under the conditions of those tests. However, there is no information about metabolic rate constants in fish for different constituents. Given the large number of constituents, their low water solubility, and difficulties associated with accurate chemical analysis, it is likely to be very difficult to generate more data on fish metabolism.

There are no definitive fish BCF data for C_{14} chlorinated n-alkanes with chlorine contents above 50% Cl wt., C_{15} chlorinated n-alkanes below 50% or ≥55% Cl wt., or longer chain length substances. Steady state fish BCFs (normalised to a 5% lipid content) are available for three C_{13} chlorinated n-alkanes (49 to 58% Cl wt.) as follows: 1 962 - 2 150 L/kg for a $C_{13}H_{23}Cl_5$ substance; 2 100 - 2 530 L/kg for a $C_{13}H_{22}Cl_6$ substance; and 3 000 – 3 630 L/kg for a $C_{13}H_{21}Cl_7$ substance. A C_{11} chlorinated n-alkane, ~58% Cl wt. had a steady state fish BCF of 5 300 - 7 816 (not lipid normalised or growth corrected).

A new fish dietary bioaccumulation test with C_{14} chlorinated n-alkane, 50% Cl wt. gave a growth-corrected depuration half-life of 108.9 days and growth-corrected and lipid-normalised BMF of 0.448 (Unpublished, 2019d). The eMSCA used these values in combination with additional study information to calculate BCFs using the 15 models within the OECD TG 305 BCF estimation tool. All 15 models predict that the BCF significantly exceeds 5 000 L/kg. This is consistent with the findings of the aqueous tests. The evidence from this study suggests that metabolism is not sufficiently quick to prevent high levels of bioaccumulation.

The ECHA decision letter requested that the Registrants conduct a further OECD TG 305 on a C_{14} chlorinated n-alkane, 55-60% Cl wt. substance. This study has not been performed, and no waiver has been provided. However, the OECD TG 308 study on C_{14} chlorinated n-alkane, 55-60% Cl wt. has been waived on the basis that it "*is not needed because the congener analysis of the C_{14}, 50% Cl test material will include the same congener groups as in this test material*". Therefore, the eMSCA concludes that C_{14} chlorinated n-alkane, 55-60% Cl wt. also has a BCF above 5 000 L/kg.

The available fish dietary bioaccumulation data from a series of studies by Fisk *et al*. show a generally similar pattern of accumulation, with the potential for uptake (as measured by assimilation efficiency) decreasing with increasing carbon chain length and increasing chlorine content. Depuration from the fish is relatively slow and dietary BMFs above one are estimated for C_{14} chlorinated paraffins with 4 to 6 chlorine atoms per molecule (corresponding to chlorine contents of approximately 42 - 53% by weight). The eMSCA has calculated BCFs from these studies using the 15 models within the OECD TG 305 BCF estimation tool, and they significantly exceed 5 000 L/kg for C_{14} (42 – 55% Cl wt.), C_{16} (32 – 68% Cl wt.) and C_{18} (49% Cl wt.) substances. However, the structure of the substance tested had terminal and adjacent chlorine atoms and so may not be representative of the structures present in commercial MCCPs. Therefore the relevance of these data is unclear. BMFs are estimated to be close to one for C_{16} chlorinated paraffins with three chlorine atoms per molecule (chlorine content approximately 32% by weight). At higher chlorine contents than these, the BMF is below one for both the C_{14} and C_{16} substances. It is important to note, however, that the method used for calculating the assimilation efficiencies in these studies is not comparable with the method currently recommended in OECD TG 305, and this introduces some uncertainty over the values reported.

A high degree of accumulation has been observed in aquatic invertebrates in laboratory studies using $C_{14\text{-}17}$ chlorinated n-alkane, 52% Cl wt., C_{13}-C_{18} chlorinated n-alkane, 45% Cl wt. and C_{16} chlorinated n-alkane, 34% Cl wt. products, with BCFs and BAFs exceeding 2 000 L/kg, although there are significant uncertainties and there may be some under-

estimation in two studies due to the nominal exposure concentrations exceeding the water solubility limit.

A BSAF of 4.4 on a lipid normalised basis was determined for a C_{16} chlorinated n-alkane, 35% Cl wt. in a study using *Lumbriculus variegatus*; the BSAF for a C_{16} chlorinated n-alkane, 69% Cl wt. substance was 0.6. An earthworm-soil accumulation factor of 2.4 for adults and 2.3 for juveniles was determined for a C_{15} chlorinated n-alkane, 51% Cl wt. in a 56-day study using *Eisenia fetida*.

MCCPs appear to have a low bioaccumulation potential in terrestrial plants.

The limited monitoring data show that MCCPs is present in biota, including predatory species, particularly near to sources of release but also in more remote areas such as the Arctic. These data provide supporting evidence that MCCPs is taken up by organisms in the environment. However, they cannot be used on their own to determine whether the substance is bioaccumulative within the meaning of the PBT assessment, since the related exposures are unknown. The available (limited) field bioaccumulation studies for MCCPs are equivocal: trophic magnification factors below and above 1 have been derived, and although most BMFs are below 1, some individual BMF values above 1 have been derived.

MCCPs have been demonstrated to have relatively long elimination or depuration half-lives in fish and mammals. This long elimination half-life means that significant concentrations of the substance may remain within an organism for several months, possibly years, after cessation of emission. A long elimination half-life is a characteristic of a bioaccumulative substance providing sufficient uptake has occurred.

6.8 Environmental hazard assessment

6.8.1 Aquatic compartment (including sediment)

Aquatic toxicity testing is hampered by the low water solubility, complex nature of the test substance and the potential inaccuracy of the analytical methods (see Section 6.3.1). This needs to be taken into account when considering the available data. In the following discussion, the most detail has been provided for studies that drive the hazard and risk assessment.

6.8.1.1 Fish

6.8.1.2 Short term toxicity to fish

No toxicity has been seen in the available acute studies with fish (EC, 2005 & 2007). The registration dossiers are consistent with these previous evaluations.

A few old (1970s) test results with *Leuciscus idus* mentioned in EC (2005) are not included in the registration dossiers, but these do not affect the assessment.

6.8.1.3 Long term toxicity to fish

No toxicity has been seen in the available long-term studies with fish exposed to aqueous solutions (EC, 2005 & 2007). The registration dossiers are consistent with these previous evaluations. The available data are deficient when compared to the current OECD TG 210, but comparison with SCCPs suggests that fish are unlikely to be more sensitive than *Daphnia* in chronic studies via aqueous exposure (for further explanation see EC, 2005).

EU (2005) summarised the results of a non-standard feeding study using juvenile Rainbow Trout *Oncorhynchus mykiss* (Cooley *et al.* 2001). Two specially synthesised C_{14} chlorinated n-alkanes (48 and 55% Cl wt.) were used, at three (different) dose levels each, with the test terminating after 21 days at the two higher doses, or 85 days for the low dose. Effects were observed at the two higher test concentrations for both substances (beginning at 0.78 or 29 mg/kg food, respectively), including abnormal behaviour (development of dark colouration, lack of response to tapping, spinal curvature, low activity levels and poor feeding), and/or mild to moderate hepatocyte necrosis and moderate to severe depletion of glycogen/lipids. No lesions or abnormalities were seen in the thyroid after 21 days, although only the mid-dose group was investigated. It is possible that these effects could be explained by the reduced feeding rate of the exposed fish, but it cannot be determined whether they were a direct toxic effect or an indirect consequence related to avoidance/unpalatability of the treated food. No effects were seen at the low doses (0.082 or 5.7 mg/kg food, respectively). The population relevance of these results is unknown. How representative the test substance is when compared to commercial MCCPs, which are produced by a different synthetic route, is unknown. These data are not included in the registration dossier.

6.8.1.4 Aquatic invertebrates

6.8.1.5 Short term toxicity to aquatic invertebrates

Several acute toxicity results are available for the cladoceran water flea *Daphnia magna* tested with $C_{14\text{-}17}$ chlorinated n-alkane 52% Cl wt. products (see Table 43).

Table 43

ACUTE AQUATIC TOXICITY OF MCCPS TO WATER FLEAS (*DAPHNIA MAGNA*)						
Chlorinated n-alkane test substance	**Method**	**Co-solvent**	**Analytical method**	**48-h EC_{50} (µg/L)**	**Reference**	**Registrant validity rating**
C_{14-17}, 52% Cl wt. (containing 0.3% epoxy soya bean oil stabiliser), mixed with n-pentadecane-8-^{14}C 51% Cl wt.	OECD TG 202 (static) GLP	Acetone	Non-specific liquid scintillation counting	7.7 (nominal) 5.9 (mean measured)	Thompson *et al*. (1996)	1
C_{14-17}, 52% Cl wt., mixed with n-pentadecane-8-^{14}C 51% Cl wt.	OECD TG 202 (static) GLP	Dilution of water soluble fraction	Non-specific liquid scintillation counting	ca. 2 200 (measured)	Unpublished *et al*. (1995)	2
C_{14-17} chlorinated paraffin (52% Cl wt.)	OECD TG 202 (static)[a] GLP status unknown	Acetone	None	<100 (nominal)	Thompson and Gore (1999)	2
C_{14-17}, 52% Cl wt.	OECD TG 202 (static) GLP	Acetone	None	< 6.5 (nominal)	Thompson (2004)[b]	-
		DMF		< 6.5 (nominal)		
		Water soluble fraction		≥350-360 (nominal)		
C_{14-17}, 52% Cl wt.	DIN 38 412, Teil 11 (static) GLP status unknown	Dilution of water soluble fraction	Adsorbable organic halogen analysis	> 379-423 (measured) 37 (measured)	Frank (1993)[b]; Frank and Steinhäuser (1994)[b]	-

Note: a – Fewer animals and test concentrations than usual.
b – Included in EC (2005) but not the REACH registrations (although some of the data are mentioned in the text/discussion within the endpoint summaries within the CSRs).

The key study reported in the registration dossiers provides a 48-h EC_{50} value of 5.9 µg/L, based on mean measured concentrations (Thompson *et al*., 1996). The original study report has been provided by the Registrants for review. It is considered to be well conducted and reliable by the eMSCA, and is also rated as 'reliable without restriction' by the Registrants. The eMSCA notes that geometric means could have been used to calculate measured concentrations rather than arithmetic means, but the difference is slight and does not impact the EC_{50} significantly.

The registration dossiers contain the results of one acute toxicity test with *D. magna* that was not previously considered in EC (2005 & 2007). Unpublished *et al.* (1995) is considered to be a supporting study by the Registrants, who consider it "reliable with restrictions". The full test report was provided to the eMSCA for evaluation. It was carried out to GLP using OECD TG 202. The test substance was a commercial C_{14-17}, 52% Cl wt. product. The starting material used to manufacture it contained 0.6% w/w chain lengths below C_{14} and 0.4% w/w chain lengths above C_{17}. The substance was mixed with an approximately equal weight of an n-pentadecane-8-^{14}C 51% Cl wt. prior to use in the test (reported to contain approximately 4% radiolabelled impurities, most of which were more polar than the chlorinated n-C_{15}). A saturated solution of the test substance was prepared by stirring a large excess of material (500 mg/L) in dilution water for 3 days followed by filtration (0.2 µm) prior to use. The following dilutions of the saturated solution were tested: 6.3, 12.5, 25, 50 and 100% (saturated solution). A control was also used. Analytical measurements of the 100% saturated solution using liquid scintillation counting (LSC) showed an initial measured concentration of 2.2 mg/L. Re-filtration of the solution

resulted in a similar measured concentration of 2.1 mg/L. The concentrations of the diluted test item were calculated from the measured concentration of the 100% saturated solution. A second saturated solution, prepared by stirring new dilution water with the original test substance[23] for 7 days gave a measured concentration after filtration of 0.8 mg/L. It should be noted that the concentrations measured are in excess of the water solubility of the test substance (see Section 6.4.2). Unpublished *et al.* (1995) noted that the concentrations may be influenced, in part, by the presence of more soluble radiolabelled impurities present in the test substance and so may not accurately reflect the actual MCCPs concentration.

At 48 hours, around 55% immobilization was observed at the highest concentration tested (the 100% saturated solution) but there was no immobilization or indication of toxicity in the 50% saturated solution. Thus the 48-h EC_{50} was approximately 2.2 mg/L. Only 24% of the radioactivity present in the saturated solution was extractable into hexane (recovery studies had previously shown 70 - 120% extraction of MCCPs into hexane). Therefore the toxicity seen in this study may have been the result of impurities present in the saturated solutions rather than MCCPs itself. The eMSCA considers that the results are inconclusive.

Other studies report 48-h EC_{50} values up to >100 µg/L. Such a wide range is surprising, and there are a number of potential explanations, most of which were considered in detail by EC (2005):

- *Variations in test substance composition and test solution preparation*: The key study used a composition that is representative of the current commercial substance (including a small amount (0.3% w/w) of stabiliser, which might not have been present in the other studies). Test solutions were prepared using acetone at 0.1 mL/L. Some of the older studies used dilutions of water soluble fractions, and the test substance in those cases might also have contained a higher proportion of $C_{10\text{-}13}$ chlorinated paraffin, which could have affected the results (reported 48-h EC_{50} values for SCCPs are in the range 75 - 140 µg/L (EU, 2000)).

- *Physical effects*: Studies performed with concentrations around the solubility limit in the test medium may have had a physical effect on the organisms (e.g. entrapment or smothering of gill surfaces). For example, in the Thompson *et al*. (1996) study, there was complete immobilisation at concentrations of 47 µg/L (measured) and above, which exceeds the solubility in pure water by a factor of around two (see Section 6.4.2). Nevertheless, the solubility in the test medium itself was not investigated, the study report does not note any cloudy solutions or entrapped *Daphnia* and 45% immobilisation was seen at a concentration of 4.1 µg/L (measured), which is below the reported water solubility limit. It therefore seems unlikely that physical effects were important in the key study.

- *Enhanced bioavailability caused by the use of co-solvent*: CPIA (2000) presented some preliminary results from a study of the effects of using a variety of different administration methods. This suggested that acetone co-solvent increased toxicity (48-h EC_{50} ca. 14 µg/L) compared to dimethylformamide or no co-solvent (48-h EC_{50} >100 µg/L). However, Thompson (2004) showed that the carrier solvent has little impact on acute toxicity to *Daphnia,* and obtained results that were reasonably

[23] This was prepared by adding dilution water to the test substance remaining in the original flask after preparation of the test solution.

consistent[24] with the earlier study of Thompson *et al.* (1996) (see EC, 2005 for further details[25]).

- *Uncertain reliability of measured concentrations*: Given the adsorptive properties of MCCPs it is important to measure test concentrations in aquatic tests, especially under static conditions (as used for many of the acute *Daphnia* studies). However, as described in Section 6.3.1, there can be a large degree of variation between different laboratories using the same analytical method, as well as between methods. The eMSCA considers that this makes it virtually impossible to compare measured results reported by different groups.

- There may potentially have been strain differences between laboratory populations.

The eMSCA finds no reason to doubt the reliability of the key study.

The registration dossiers include a RSS for the amphipod *Gammarus pulex*, which reported no acute effects over 96 hours up to 1 mg/L (nominal) (Thompson and Gore, 1999; cited in EC, 2005). One further acute study was summarised in EC (2005) but there is no RSS in the registration dossiers:

- A 96-h LC_{50} of 9 and >10 000 mg/L for a $C_{14\text{-}17}$, 45% Cl wt. and $C_{14\text{-}17}$, 52% Cl wt. substance, respectively, for the harpacticoid copepod *Nitocra spinipes* (Tarkpea *et al.*, 1981).

6.8.1.6 Long term toxicity to aquatic invertebrates

The key study reported in the registration dossiers provides a 21-d NOEC for *Daphnia magna* of 10 µg/L (based on mean measured concentrations) (Thompson *et al*., 1997). The original study report has been provided by the Registrants for review. It is considered to be well conducted and reliable by the eMSCA, and is also rated as 'reliable without restriction' by the Registrants. OECD TG 202 was the appropriate test guideline for reproductive studies at the time, but was superseded by OECD TG 211 in 2012. The study met the OECD TG 202 (1984) test validity criteria (i.e. <20% mortality in controls and satisfactory dissolved oxygen levels). The eMSCA notes that the study also meets the control validity criteria in the current OECD TG 211 for parental mortality, mean number of offspring per surviving parents and coefficient of variance around mean number of living offspring. Relevant data from the RSS are provided in Table 44. In line with the current OECD TG 211, the eMSCA has calculated an additional endpoint reflecting mean number of living offspring per parent animal which does not die accidentally of inadvertently during the test.

[24] 100% immobilisation was observed at nominal concentrations of 6.5 µg/L using either acetone or DMF as co-solvent, suggesting a 48-h EC_{50} < 6.5 µg/L (nominal).

[25] Another study performed in the same laboratory reported 72-h and 96-h LC_{50} values of >65 and 46 µg/L, respectively, for parent mortality based on measured concentrations (Thompson *et al*., 1997). This was a chronic study with feeding and so is not directly comparable with the acute studies performed in accordance with OECD TG 202.

Table 44

SUMMARY OF RESULTS OF A CHRONIC *DAPHNIA* TOXICITY TEST WITH MCCPs (THOMPSON ET AL., 1997)						
Treatment, µg/L		Parent mortality (no. of animals out of 10)	Study endpoint: Mean number of offspring per surviving parent **	eMSCA endpoint: Mean number of living offspring per parent***	Body length, mm	Total dead offspring
Nominal	Mean measured*					
Control	-	2	90.4	78.3	4.0	0
Solvent control	-	0	121.2	121.2	4.1	0
5.6	3.7	1	124.6	116.4	4.2	0
10	5	0	119.2	119.2	4.2	0
18	10	0	116.9	116.9	4.1	73
32	18	2	79.1	63.3	3.7	162
56	32	8	45	45	3.1	24
100	65	10	0	0	0	0

Note: Red text highlights the 21-day NOEC for reproduction based on comparison with the solvent control, since the blank control and solvent control were considered significantly different for the endpoint. The 21-day NOEC for parental mortality was 32 µg/L (nominal) based on comparison with the solvent control. The 21-day NOEC for length was 18 µg/L (nominal) based on comparison with the solvent control.
* Refer to notes below regarding applicability of study mean measured concentrations
** Offspring from parents that died are not included in this endpoint
*** No parent animals are considered to have died inadvertently so this endpoint considers mortality

Based on a detailed review of the original study, the eMSCA notes the following points:

- Exposure solutions were prepared with the aid of a solvent (acetone, at a concentration of 0.025 mL/L, which is lower than used in the acute study by the same group) and were observed to be 'clear and colourless'. No range-finding test was carried out. It is notable that concentrations for some treatment groups were nominally much higher than the reported upper solubility limit in pure water (27 µg/L), and also exceed the acute LC_{50}. Chronic studies are not usually conducted at concentrations where significant acute effects are expected, and this complicates the interpretation of the study.

- The reproduction NOEC endpoint is described as '*number of offspring produced per female (mean of 10 replicates)*'. This relates to the number of live offspring per surviving parent at the end of the study which was standard practice until the 2012 OECD 211 test guideline update. The eMSCA has calculated the number of offspring endpoint reflecting parent mortality in line with the current OECD TG 211, and does not consider that this affects the 21-day NOEC for reproduction. Given the observed effects, the eMSCA recommends that the Registrants calculate an EC_{10} by interpolation to reflect the reproduction endpoints described in OECD TG 211.

- The study recorded additional observations including dead offspring (see Table 48) which indicates a dose-response relationship. It is unclear why the offspring died although it is possible very young *Daphnia* may be more acutely sensitive than adults. The statistical significance of these data has not been considered by the eMSCA although it may be a population-relevant effect. The eMSCA recommends that the Registrants consider if a NOEC or EC_{10} can be calculated for offspring mortality, since it may be lower than the current reproduction and length NOECs.

- The study included analytical verification for 4 out of 8 renewal periods covering two periods of 2 days and two periods of 3 days. This means that analytical information for exposure solutions over the whole study is not available. Measured concentrations were 78-94% of nominal for fresh media, indicating the exposure solutions were prepared adequately. Losses were observed over the measured 2 and 3 day periods with measured concentrations ranging between 7.3-61% of nominal for expired solutions. The study report quotes an 'overall mean measured concentration' of 50-61% of nominal and the NOEC is expressed in terms of an arithmetic mean of the mean measured concentration for fresh media and mean measured concentration for expired media. While analytical verification was not performed for the whole study, the eMSCA considers the available renewal period data are representative enough to allow measured concentrations to be calculated. On this basis, the eMSCA notes that results should be expressed in terms of a time-weighted mean according to current best practice in the updated OECD TG 211. In line with this, the eMSCA has calculated a time-weighted mean of 0.0087 mg/L for the nominal 0.018 mg/L treatment, which is the 21-day NOEC for reproduction and length. The eMSCA recommends that this value is used in preference to the reported NOEC of 0.01 mg/L.

EU (2005) included other chronic *Daphnia* results for 52% Cl wt. MCCP products that are not included in the REACH registrations (see Table 45).

Table 45

CHRONIC AQUATIC TOXICITY OF MCCPs TO WATER FLEAS (*DAPHNIA MAGNA*)						
Chlorinated n-alkane test substance	**Method**	**Co-solvent**	**Analytical method**	**21-d NOEC (µg/L)**	**Reference**	**Registrant validity rating**
C_{14-17}, 52% Cl wt. (containing 0.3% epoxy soya bean oil stabiliser), mixed with n-pentadecane-8-^{14}C 51% Cl wt.	OECD TG 202 (semi-static) GLP	Acetone (0.025 mL/L)	Non-specific liquid scintillation counting	8.7 (see text)	Thompson *et al*. (1997)	1
C_{14-17}, 52% Cl wt.	OECD TG 202 (semi-static) GLP status unknown	Dilution of water soluble fraction	Adsorbable organic halogen analysis	12.6-15.6 (measured)	Frank (1993)[b]; Frank and Steinhäuser (1994)[b]	-
C_{14-17}, 52% Cl wt.			Total extractable organic halogen method	ca. 4-8 (measured) [0.18 vol.%]	TNO (1993)[b]	-

Note: a – Included in EC (2005) but not the REACH registrations.

Similar to the acute data set, there is a range of 21-d NOEC values, from (approximately) 4-8 to 15.6 µg/L (based on measured concentrations, although the reliability of the organic halogen analyses is unknown). Some of the issues highlighted for the acute studies may be applicable to the chronic studies too. This leads to some uncertainty as the acute and chronic values are of the same order of magnitude, and in some cases appear contradictory. For example, whilst Thompson *et al*. (1996) reported a 48-h EC_{50} of 5.9 µg/L, the chronic study performed in the same laboratory (Thompson *et al*., 1997) reported a 21-d NOEC of 10 µg/L (recalculated by the eMSCA as 8.7 µg/L) (see above). Both studies used the same test item and concentrations were measured using the same analytical method. One explanation for this discrepancy is that the addition of food might affect the bioavailability of the substance in the chronic studies. Frank and Steinhäuser (1994) found that the adsorption of chlorinated paraffin to the food (algae) in their test was small. However, a preliminary investigation performed by Thompson *et al*. (1997) concluded that the presence of food decreased the sensitivity of the *Daphnia* (<48 hours old), either directly by improving the nutritional status of the animals, or indirectly by

increasing the rate at which the dissolved test substance concentration declined (as a result of adsorption) between solution renewals. In this investigation all unfed animals died at 0.018 and 0.032 mg/L (nominal), while all fed animals at the 0.018 mg/L (nominal) treatment survived and 4 out 5 animals at the 0.032 mg/L (nominal) treatment survived. Castro *et al*. (2019) also suggest that elimination might increase when *Daphnia* are fed (see Section 6.7.5.1.1).

One additional long-term invertebrate toxicity study was summarised in EC (2005) but does not have a RSS in the registration dossier. This reported a 60-d NOEC of 0.22 mg/L [220 µg/L] for a C_{14-17}, 52% Cl wt. substance with Blue Mussel *Mytilus edulis* (Madeley and Thompson, 1983).

6.8.1.7 Algae and aquatic plants

No toxicity has been seen up to the limit of water solubility in the available studies with algae (EC, 2005 & 2007). Analyses were performed using non-specific LSC measurements. The registration dossiers include these data and the interpretation is consistent

6.8.1.8 Sediment organisms

Prolonged sediment toxicity tests are available for MCCPs with *Hyalella azteca, Lumbriculus variegatus* and *Chironomus riparius* and are summarised in EC (2005 & 2007). The tests were carried out sediment spiked with using a C_{14-17}, 52% Cl wt. substance. The lowest NOEC for the three species was 130 mg/kg dry weight sediment (~ 50 mg/kg wet weight), obtained both in the study with *Lumbriculus variegatus* and *Hyalella Azteca.* Analyses were performed using non-specific LSC measurements. The NOEC for *Chironomus riparius* was 3 800 mg/kg dry weight (~ 1 460 mg/kg wet weight). The registration dossiers include these data and the interpretation is consistent.

6.8.1.9 Other aquatic organisms

No other data are available.

6.8.1.10 Summary of aquatic toxicity

There is little information about how the aquatic toxicity of MCCPs varies with both chlorine content and carbon chain length, which is a limitation given the complex nature of the substance.

From the available database, aquatic effects have almost exclusively been observed with the water flea *Daphnia magna* (48-h EC_{50} 0.0059 mg/L; 21-d NOEC 0.0087 mg/L), for a C_{14-17} chlorinated n-alkane, 52% Cl wt. The similarity in end points is highly unusual, but is assumed to be related to differences in bioavailability (or elimination) caused by the presence of food in the chronic study.

No toxicity has been observed in the available aqueous exposure experiments with fish, other invertebrates or algae (other than at concentrations significantly in excess of the solubility limit in pure water). No effects were seen with MCCPs in a 20-day embryo-larval fish test; although the method was deficient when compared to the current OECD TG 210, comparison with SCCPs suggests that fish are unlikely to be more sensitive than *Daphnia* in chronic studies (see EC, 2005 for further explanation). Nevertheless, effects have been observed on behaviour and liver histology in juvenile Rainbow Trout (*Oncorhynchus mykiss*) in a non-standard dietary study. Long-term dietary fish toxicity could be considered a potential information gap, although the eMSCA notes that a standard test guideline does not exist, and there is no guidance about how such data should be used in hazard and risk assessment.

Commercial MCCPs contains ≤ 1% w/w of C_{10-13} chloroalkanes. These constituents are likely to behave in a similar way to SCCPs. The most relevant chronic *Daphnia* toxicity

value for SCCPs is a 21-day NOEC of 0.005 mg/L [5 µg/L] obtained using a C_{10-13} chlorinated n-alkane, 58% Cl wt. (ECHA, 2008). Although there are some differences in the chlorine contents between the substance tested in that study and C_{14-17} chlorinated n-alkane, 52% Cl wt., it seems reasonable to conclude that the $C_{<14}$ constituents of MCCPs with chlorine contents up to 52% by weight will have an aquatic toxicity profile that is similar to the main C_{14-17} constituents.

6.8.2 Terrestrial compartment

6.8.2.1 Toxicity test results

6.8.2.2 Toxicity to soil macro organisms

The registration dossiers include the results of an earthworm reproduction test using a radiolabelled C_{14-17}, 52% Cl wt. substance. The overall 56-d NOEC from the study was 280 mg/kg dry weight soil (~ 248 mg/kg wet weight). Analyses were performed using non-specific liquid scintillation counting. The Registrants consider the study to be "reliable without restriction", which is consistent with the interpretation given in EC (2005).

6.8.2.3 Toxicity to terrestrial plants

The registration dossiers contain the results from an OECD TG 208 (terrestrial plants test: seedling emergence and seedling growth test) study with wheat (*Triticum aestivum*), oilseed rape (*Brassica napus*) and mung bean (*Phaseolus aureus*) using a radiolabelled C_{14-17}, 52% Cl wt. substance. Analyses were performed using non-specific liquid scintillation counting. The overall 28-d NOEC was ≥5 000 mg/kg dry weight soil. The Registrants consider the study to be "reliable without restriction", which is consistent with the interpretation given in EC (2005).

6.8.2.4 Toxicity to soil micro-organisms

The registration dossiers contain the result of an OECD TG 216 (soil microorganisms: nitrogen transformation test) study using a radiolabelled C_{14-17}, 52% Cl wt. substance. The overall 28-d NOEC was ≥400 mg/kg dry weight soil. Analyses were performed using non-specific liquid scintillation counting. The Registrants consider the study to be "reliable without restriction", which is consistent with the interpretation given in EC (2005).

6.8.2.5 Toxicity to other terrestrial organisms

No other data are available.

6.8.3 Microbiological activity in sewage treatment systems

6.8.3.1 Toxicity to aquatic micro-organisms

The registration dossiers give the results of two tests with microorganisms. The lowest 24-h NOEC was 800 mg/L for a C_{14-17}, 41% Cl wt. substance using anaerobic bacteria from a domestic waste water treatment plant via the ETAD fermentation tube method. No details on the analytical method are available. The Registrants consider the study to be "reliable without restriction", which is consistent with the interpretation given in EC (2005).

6.8.4 PNEC derivation and other hazard conclusions

6.8.4.1 $PNEC_{water}$

The $PNEC_{water}$ derived in the registration dossiers is 1 µg/L for freshwater and 0.2 µg/L for marine water. These are derived using an assessment factor of 10 (freshwater) or 50 (marine water) with the 21-d NOEC for *Daphnia magna* of 0.01 mg/L. The same PNEC for marine water was also derived in a case study for the Stockholm Convention on Persistent Organic Pollutants (Brooke and Crookes, 2011).

The freshwater PNEC is the same as used in EC (2005 & 2007). However, as highlighted in Section 6.8.1.2.2, the eMSCA now believes that the 21-d NOEC should be 0.0087 mg/L. This means that the **$PNEC_{water}$ should be reduced to 0.87 µg/L for freshwater and 0.17 µg/L for marine water**.

The NOEC was derived from a chronic study performed in the presence of food, which is likely to be more environmentally realistic than studies performed without (such as the acute test). Nevertheless, the fact that significant acute effects may be observed around the same concentration should be considered further. For example, an additional assessment factor (e.g. 5) could be used to provide additional reassurance that the PNEC is sufficiently protective. Given the PBT conclusion (see Section 6.11), further risk management might be required for at least some uses of MCCPs. Remaining uses will need to be evaluated using the normal risk assessment approach, and the eMSCA recommends that the Registrants re-evaluate the chronic *Daphnia* study and produce an updated $PNEC_{water}$ for this purpose.

A marine water PNEC was not derived in EC (2005 & 2007). An assessment factor of 50 is in accordance with the REACH Guidance because long-term toxicity data are available for freshwater fish, invertebrates and algae, and a marine mollusc. However, given the uncertainty over protection against acute effects, the eMSCA recommends that the marine water PNEC should be re-evaluated once the Registrants produce an updated freshwater PNEC.

6.8.4.2 $PNEC_{sediment}$

The $PNEC_{sediment}$ (for a sediment with a 5% organic carbon content) derived in the registration dossiers is 13 mg/kg dry weight (~ 5 mg/kg wet weight) for freshwater sediment and 2.6 mg/kg dry weight (~ 1 mg/kg wet weight) for marine sediment. These are derived using an assessment factor of 10 (freshwater) or 50 (marine water) on the NOEC for *Lumbriculus variegatus* and *Hyalella azteca* of 130 mg/kg dry weight (~ 50 mg/kg wet weight).

This PNEC for freshwater sediment is the same as used in the EC (2005 & 2007) and is considered appropriate. A PNEC for marine sediment was not derived in EC (2005 & 2007). An assessment factor of 50 is in accordance with the REACH Guidance because long-term toxicity data are available for three sediment organisms representing different living and feeding conditions. The same PNEC for marine sediment was also derived in a case study for the Stockholm Convention on Persistent Organic Pollutants (Brooke and Crookes, 2011).

6.8.4.3 $PNEC_{soil}$

The $PNEC_{soil}$ derived in the registration dossier is 11.9 mg/kg dry weight using an assessment factor of 10. This is consistent with EC (2005), and is based on the following:

- As NOECs were available for three long-term tests covering earthworms, plants and microorganisms, the $PNEC_{soil}$ was derived using an assessment factor of 10 on the

lowest NOEC (280 mg/kg dry weight or 248 mg/kg wet weight for earthworms). Thus the $PNEC_{soil}$ is 28 mg/kg dry weight or 24.8 mg/kg wet weight.

- The earthworm test was carried out using a soil with a 4.7% organic carbon content. The "standard" organic carbon content assumed for the soil compartment is usually 2% and so the PNEC was then normalised to the standard organic carbon content. This leads to a $PNEC_{soil(standard)}$ of 11.9 mg/kg dry weight or 10.6 mg/kg wet weight.

6.8.4.4 PNEC for sewage treatment plant

The PNEC for sewage treatment plant derived in the registration dossier is 80 mg/L using an assessment factor of 10 on the lowest NOEC from the available studies. This is consistent with EC (2005).

6.8.4.5 Calculation of $PNEC_{oral}$ (secondary poisoning)

The $PNEC_{oral}$ for secondary poisoning derived in the registration dossiers is 10 mg/kg food. This is based on a mammalian NOEC of 300 mg/kg food (equivalent to a NOAEL of ~ 23 mg/kg body weight/day) from a 90-day study in rats, using an assessment factor of 30. In the absence of an avian reproduction NOEC for MCCPs, a $PNEC_{oral}$ cannot be derived for birds, but it is assumed that there is no significant difference in sensitivity, based on data for the analogue SCCPs[26]. The registration dossier notes that a higher assessment factor of 90 would normally be appropriate for the results of a 90-day study. However, several long-term reproduction studies are available that give NOAELs higher than the 90-day study and so a lower assessment factor of 30 can be justified (which takes account of both species variation and lab-to-field extrapolation).

The $PNEC_{oral}$ derivation is consistent with the approach taken in EC (2007).

The eMSCA's recommended PNECs are presented in Table 50.

[26] EC (2000) indicates that chronic effects on kidney, liver and thyroid were observed in laboratory rodents at SCCP concentrations of 100 mg/kg bw/day or above, which is equivalent to ~ 1 000 mg/kg food (using a conversion factor of 10). Reproductive effects were observed at higher concentrations. Birds therefore appear to be more sensitive than mammals when reproductive effects are considered (with effects at ~ 1 000 mg/kg food). Nevertheless, toxic effects in both birds and mammals begin to occur at similar dose levels. A $PNEC_{oral}$ based on the most sensitive mammalian data is therefore expected to be protective of birds (and *vice versa*).

Table 46

PNEC DERIVATION AND OTHER HAZARD CONCLUSIONS		
Hazard assessment conclusion for the environment compartment	**Hazard conclusion**	**Remarks/Justification**
Freshwater	$PNEC_{aqua}$ (freshwater): 0.87 µg/L	Assessment factor: 10 Extrapolation method: assessment factor
Marine water	$PNEC_{aqua}$ (marine water): 0.17 µg/L	Assessment factor: 50 Extrapolation method: assessment factor
Intermittent releases to water	No PNECs have been derived for intermittent releases to the environment	Intermittent releases of MCCPs to water have been reported, for example from their use in metal working fluids. However, TGD (R.16) states that "Intermittent releases are defined as occurring infrequently, i.e. less than once per month and for no more than 24 hours". It is not anticipated that such frequent releases will occur, therefore, a PNEC aqua for intermittent release has not been derived. If, however, such releases do occur in the future, the PNECs derived for continuous exposure are considered protective of intermittent releases, and can therefore be used.
Sediments (freshwater)	$PNEC_{sediment}$ (freshwater): 13.0 mg/kg sediment dry weight	Assessment factor: 10 Extrapolation method: assessment factor
Sediments (marine water)	$PNEC_{sediment}$ (marine water): 2.6 mg/kg sediment dry weight	Assessment factor: 50 Extrapolation method: assessment factor
Sewage treatment plant (STP)	PNECSTP: 80.0 mg/L	Assessment factor: 10 Extrapolation method: assessment factor
Soil	$PNEC_{soil}$: 11.9 mg/kg soil dry weight	Assessment factor: 10 Extrapolation method: assessment factor
Air	No hazard identified	Substance is not volatile and no exposure via the atmosphere is expected.
Secondary poisoning	$PNEC_{oral}$: 10 mg/kg food	Assessment factor: 30

6.8.5 Conclusions for classification and labelling

The existing harmonised environmental classification under the CLP Regulation is still appropriate for MCCPs. The decision letter issued in 2014 highlighted that no multiplication factor (M-factor) for mixtures was given in the harmonised classification. In response, the Registrants have included a proposed self-classification in their registration dossiers with M-factors of 100 and 10 for aquatic acute and chronic classifications, respectively. These are based on a 48-h EC_{50} 0.0059 mg/L and 21-d NOEC of 0.01 mg/L for *Daphnia magna* (see Section 6.8.1.4). As noted in Section 6.8.1.2.2, the eMSCA now believes that the 21-d NOEC should be 0.0087 mg/L, but this does not affect the chronic M-factor. The eMSCA therefore agrees with the proposal, and notes that the harmonised classification could be updated with this information.

6.9 Human Health hazard assessment

This substance evaluation is targeted for environmental end points, and so mammalian toxicity data have not been reviewed. A brief summary of relevant information is provided below. This is based on the human health risk assessment report produced under the Existing Substances Regulation EC (No.) 793/93 (HSE, 2008b), which can be consulted for further details. Since the reports have already been cited in public documents, they have not been anonymised for this report. One commercial product type (52% Cl wt.) has been used for the majority of regulatory studies.

- *Repeated dose toxicity*: The target organs for repeated oral dose toxicity are liver, thyroid and kidney. The lowest reliable NOAEL is 23 mg/kg/day from a 90-d study with F344 rats *Rattus norvegicus* (CXR Biosciences Ltd, 2005b), based on increased relative kidney weights. The European Food Safety Authority (in prep.) has derived a $BMDL_{10}$[27] of 36 mg/kg bw/day from this study.

- *Carcinogenicity*: No carcinogenicity studies have been conducted. MCCPs is generally unreactive and not mutagenic. The carcinogenic potential of MCCPs is expected to be similar – at least in qualitative terms – to that of SCCPs, although direct read across is not appropriate. SCCPs induce liver and thyroid adenomas and carcinomas and kidney tubular cell adenomas and carcinomas in animal studies. The liver and thyroid tumours are considered to be of little or no relevance to human health. It cannot be completely ruled out that the kidney toxicity observed for MCCPs might lead to kidney cancer in rats through a non-genotoxic mode of action. However, MCCPs is not classified for this end point under Regulation EC No. 1272/2008.

- *Toxicity to reproduction*: MCCPs has no apparent effect upon fertility in rats up to approximately 400 mg/kg/day in the diet. No adverse developmental effects occurred during gestation in rats or rabbits in two conventional developmental studies using maternal doses up to 5 000 and 100 mg/kg/day, respectively. In contrast, exposure of Wistar rats *R. norvegicus* to $C_{14\text{-}17}$ n-chloroalkane 52% Cl wt. at a maternal dietary dose of 74 mg/kg/day (1 000 ppm) up to approximately 400 mg/kg/day (6 250 ppm) produced internal haemorrhaging and deaths in the pups (IRDC, 1985). Follow-up studies with Sprague Dawley and CD rats (CXR Biosciences Ltd, 2003, 2004 & 2006) demonstrated that MCCPs can perturb blood clotting. In adult females that had been treated for 7-8 weeks including pregnancy and lactation, decreased levels of vitamin K and of the clotting factors VII and X were found, and 5 out of 32 dams showed signs of haemorrhaging during

[27] Benchmark Dose Level associated with a 10% response adjusted for background.

parturition. However, these decreases did not affect their prothrombin times, indicating that the functional reserve in the majority of these adult animals was sufficient. The foetus *in utero* apparently receives sufficient vitamin K via the placenta, but after birth becomes severely deficient in vitamin K and related clotting factors and relies on the mothers' milk to receive them. Exposure to MCCPs in the milk may also further reduce their vitamin K levels. This in turn leads to a severe vitamin K deficiency in the neonates and consequently to haemorrhaging. This is the basis for the harmonised classification for effects via lactation (H362 – May cause harm to breast-fed children) according to Regulation EC No. 1272/2008.

From the studies available, an overall NOAEL of 47 mg/kg/day (600 ppm) as a maternal dose can be identified for these effects mediated via lactation. However, it should be noted that the effects (11% reduction in pup survival and related haemorrhaging) observed at the LOAEL (74 mg/kg/day; 1 000 ppm) were not statistically significant. Haemorrhaging was also seen in one study at the time of parturition in 16% of dams given 538 mg/kg/day (6 250 ppm), but not up to 100 mg/kg/day (1 200 ppm) in other studies. The NOAEL of 100 mg/kg/day (1 200 ppm) was therefore selected for the risk characterisation of haemorrhaging effects potentially occurring in pregnant women at the time of parturition.

6.10 Assessment of endocrine disrupting (ED) properties

Endocrine disrupting (ED) properties are not considered in the registration dossiers, and have not been evaluated by the eMSCA.

6.11 PBT and vPvB assessment

Persistence

The estimated atmospheric half-life is estimated to be 1 - 2 days for MCCPs with chlorine contents between around 40 and 56% Cl wt. MCCPs with >65% chlorine have estimated half-lives which are longer than 2 days. There are no criteria in Annex XIII for half-lives in air. Although a half-life above 2 days in air is associated with long-range transport potential under the United Nations Stockholm Convention on Persistent Organic Pollutants, constituents of MCCPs have low vapour pressures and due to their intrinsic physico-chemical properties are likely to be primarily associated with particulates in air. No information is available on phototransformation potential in water or soil. It is noted that stabilizers are often added to commercial product types to improve light (and thermal) stability.

MCCPs is not expected to hydrolyse significantly. Several biodegradation (OECD TG 301) screening studies under conditions of enhanced bioavailability have been performed to investigate the influence of chain length and chlorination level on biodegradation potential:

- Constituents of MCCPs that contain up to around five chlorine atoms per molecule can be extensively degraded by micro-organisms under conditions of enhanced bioavailability. For example, C_{14} chlorinated n-alkanes with a chlorine content of 41.3 – 45.5% are readily biodegradable under these modified conditions. Although C_{14} chlorinated n-alkane, 50% Cl wt. failed to meet the criteria for ready biodegradation, it met the 60% pass threshold after 56 days when river water was used as the inoculum. These substances therefore do not screen as being persistent within the meaning of the Annex XIII criteria.

- Degradability reduces as the number of chlorine atoms per molecule increases. Both a 55% and 60% Cl wt. C_{14} chlorinated n-alkane failed to meet the pass threshold of 60% degradation even with a surfactant and after extended timescales using inocula derived from activated sludge. Similarly, C_{15} chlorinated n-alkane, 51% Cl wt. failed to meet the pass threshold after an extended timescale in river water (although it achieved up to 63% degradation after 60 days with a surfactant using inocula derived from activated sludge). These substances must therefore be considered to be potentially persistent.

- Longer chain lengths are expected to be less water soluble and more adsorptive than the C_{14} and C_{15} substances, but there are no degradation data for specific C_{16} or C_{17} substances, so the actual influence of chain length is unknown. C_{14-17} chlorinated n-alkane, 45.5% Cl wt. is not readily biodegradable; although more than 60% degradation occurred after extended timescales with a surfactant using activated sludge, no data are available using river water as the inoculum (the degradation rate would be expected to be slower). It must therefore be considered to be potentially persistent, even though it may contain a significant proportion of constituents (e.g. C_{14}) that are readily biodegradable.

- C_{14-17} chlorinated n-alkane, 51.7% Cl wt. was also extensively degraded over an extended period by activated sludge micro-organisms when bioavailability was enhanced, but it failed to meet the pass threshold (57% degradation was achieved after 60 days). In contrast, C_{14-17} chlorinated n-alkane, 63.2% Cl wt. only achieved 10% degradation under the same conditions. They must therefore both be considered to be potentially persistent.

It is not possible to extrapolate information from such tests to an environmental half-life.

No transformation of C_{14} chlorinated n-alkane, 50% Cl. wt. was observed over 120 days at 12 °C in an OECD TG 308 study, and so the sediment half-life exceeds 120 days (and is likely to exceed 180 days, although there is no empirical evidence to confirm this). The same test substance was found to degrade by 60% after 56 days in a ready test using surfactant and a river water inoculum. The negligible degradation rate in aerobic sediment may reflect a reduction in bioavailability caused by adsorption. Since the water-sediment simulation test is more environmentally relevant than the ready biodegradation test, it must be given more weight in the assessment of persistence.

All of the substances that were less degradable than C_{14} chlorinated n-alkane, 50% Cl. wt. in modified and enhanced ready tests are likely to have similar or longer sediment half-lives. It is possible that adsorption could cause substances that were found to be readily biodegradable in modified tests (C_{14} chlorinated n-alkanes, 41.3 – 45.5% Cl wt.) to have longer sediment half-lives than expected, but no data are available to allow a conclusion to be drawn.

Given the predicted and observed trends in physico-chemical properties, it is likely that C_{15-17} constituents with similar or higher chlorine contents to C_{14} chlorinated n-alkane, 50% Cl. wt. will be equally or more adsorptive to sediment. They are therefore likely to be equally or more persistent in sediment (i.e. sediment half-lives of ≥120 days).

Both C_{10} chlorinated n-alkane, 65% Cl wt. and C_{13} chlorinated n-alkane, 65% Cl wt. have degradation half-lives > 180 days in marine sediments. In contrast, C_{10-13} chlorinated n-alkane, 49.8% Cl wt. was found to be readily biodegradable when surfactant was used to enhance bioavailability.

The exact composition of the registered substance is claimed as confidential business information. However, commercial MCCPs contain a large proportion of C_{14} chlorinated n-alkanes (see Section 6.3). The eMSCA's conclusion is therefore that a significant proportion of the constituents of most current commercial MCCP products will have sediment half-lives that exceed exceed the Annex XIII 'persistent' criterion of 120 days (and some will exceed the 'very persistent' criterion of 180 days) in freshwater sediment at 12 °C. Some constituents with lower chlorine content (≤45% Cl wt.) are readily biodegradable. However, given the remaining uncertainties about the role of adsorption and the fact that $C_{14\text{-}17}$ chlorinated n-alkane, 45.5% Cl wt. is not readily biodegradable, the eMSCA believes that a firm conclusion cannot be drawn about whether all relevant constituents of such low chlorine content MCCPs would have sediment half-lives below 120 days.

Additional weight is given to this conclusion through monitoring data, including a study showing that MCCPs with chlorine contents of ~ 55% can persist in sediments for more than a decade.

The Registrants do not consider that MCCPs meets the Annex XIII P or vP criteria. In particular, they consider that evidence of aerobic mineralisation in modified screening level studies outweighs evidence from environmental simulation tests.

Bioaccumulation

The constituents of MCCPs have a range of log K_{OW} values, the majority of which are equal to or exceed 6.5. They therefore meet the Annex XIII screening criterion as being potentially 'very bioaccumulative' (vB) (i.e. log K_{OW} >5).

Two reliable aquatic fish BCF studies are available for MCCPs. The eMSCA has calculated growth-corrected and lipid-normalised kinetic BCFs of 10 500 – 14 600 L/kg for a C_{14} chlorinated n-alkane, 45% Cl wt. product using the data reported by Unpublished (2010h & 2010i) (without growth correction, the BCF is 3 230 – 4 460 L/kg). The growth-corrected kinetic BCF for a C_{15} chlorinated n-alkane, 51% Cl wt. substance is 2 164 L/kg based on data reported by Thompson *et al*. (2000) (lipid normalisation is not possible).

A new fish dietary bioaccumulation test with a C_{14} chlorinated n-alkane, 50% Cl wt. substance gave a growth-corrected depuration half-life of 108.9 days and growth-corrected and lipid-normalised BMF of 0.448 (Unpublished, 2019d). The eMSCA used the data from this study to calculate BCFs using the 15 models within the OECD TG 305 BCF estimation tool. All predict that the BCF significantly exceeds 5 000 L/kg.

Estimated BCF values from a series of fish dietary bioaccumulation studies by Fisk *et al*. (1996, 1998b & 2000) significantly exceed 5 000 L/kg for C_{14} (42 – 55% Cl wt.), C_{16} (32 – 68% Cl wt.) and C_{18} (49% Cl wt.) substances. Depuration from the fish is relatively slow (as it is in mammals) and dietary BMFs above one are estimated for C_{14} chlorinated paraffins with 4 to 6 chlorine atoms per molecule (corresponding to approximately 42 – 53% Cl wt.).

A high degree of accumulation has also been reported for aquatic invertebrates (*Daphnia magna* and *Mytilus edulis*) in three laboratory studies using $C_{14\text{-}17}$ chlorinated n-alkane, 52% Cl wt., C_{13}-C_{18} chlorinated n-alkane, 45% Cl wt. and C_{16} chlorinated n-alkane, 34% Cl wt. products, with BCFs and BAFs exceeding 2 000 L/kg (and 5 000 L/kg in two studies). There are significant uncertainties associated with these studies, and there may be some under-estimation in two studies due to the nominal exposure concentrations exceeding the water solubility limit. A BSAF of 4.4 on a lipid normalised basis was determined for a C_{16} chlorinated n-alkane, 35% Cl wt. in a study using *Lumbriculus variegatus*; the BSAF for a C_{16} chlorinated n-alkane, 69% Cl wt. substance was 0.6. An earthworm-soil accumulation factor of 2.4 for adults and 2.3 for juveniles was determined for a C_{15} chlorinated n-alkane, 51% Cl wt. in a 56-day study using *Eisenia fetida*.

The Annex XIII criteria state that a substance can be considered 'bioaccumulative' (B) if it has a BCF in aquatic organisms greater than 2 000 L/kg and 'very bioaccumulative' (vB) if it has a BCF greater than 5 000 L/kg. The eMSCA concludes that the whole UVCB substance that C_{14} and C_{15} chlorinated n-alkanes (45 – 50% Cl wt.) represent has a significant number of constituents that are B and some that are vB. The Registrants indicate that C_{14} chlorinated n-alkanes with higher chlorine content include the same congener groups and so the eMSCA concludes that C_{14} chlorinated n-alkane, 55 – 60% Cl wt. also has constituents with BCFs above 5 000 L/kg. C_{14} constituents are a major congener group in commercial MCCP products.

Conclusions for constituents with higher carbon chain length and chlorine contents cannot be made with certainty, but they are also likely to be bioaccumulative based on the evidence of the estimates from the Fisk *et al*. series of studies and Castro *et al*. (2019).

Additional weight is given to this conclusion by monitoring studies which demonstrate widespread contamination of wildlife by MCCPs at all trophic levels (including predatory species and people). The available (limited) field bioaccumulation studies are equivocal: trophic magnification factors below and above 1 have been derived for MCCPs, and although most BMFs are below 1, some individual BMF values above 1 have been derived.

The registration dossiers contain a report which focuses on the biomagnification of MCCPs (Unpublished, 2014c). A weight of evidence approach involving bioaccumulation factors (BAF), biomagnification factors (BMF) and trophic magnification factors (TMF) is presented to argue that MCCPs is not bioaccumulative. The suggestion is that BCF data cannot be used to assess the biomagnification of MCCPs as dietary exposure is not involved. However, as ECHA stated in the decision letter issued in February 2014, the absence of biomagnification cannot be used to dismiss BCF data when considering the Annex XIII criteria (ECHA, 2014). This view was upheld by the Board of Appeal decision dated 9 September 2015. Field biomagnification studies generally have significant experimental limitations and lack of biomagnification in one food chain does not automatically mean that it can be excluded for all others. The PBT guidance (ECHA, 2017) states "*If a substance has a valid and plausible aquatic BCF > 2 000 (or 5 000) L/kg (indicating a significant accumulation in the test organism), the substance is defined as B (or vB) regardless of whether biomagnification or trophic magnification occurs*".

C_{13} chlorinated n-alkanes, 49 – 58% Cl wt. also meet the B criterion on the basis of steady state BCFs (normalised to a 5% lipid content) in the range 1 962 – 3 630 L/kg. A C_{11} chlorinated n-alkane, ~58% Cl wt. had a steady state fish BCF of 5 300 - 7 816 (not lipid normalised or growth corrected) so meets the vB criterion. It is inferred that $C_{<14}$ constituents of MCCPs with a similar degree of chlorination will also meet the B/vB criteria.

Toxicity

Since MCCPs contains thousands of constituents, the reported toxicity end points effectively reflect an average of the contributions that individual constituents make. The influence of varying degrees of chlorination and chain length on toxicity is not known. It is therefore assumed that if toxicity is demonstrated for one type of product, it will be applicable for all.

Aquatic toxicity: A $C_{14\text{-}17}$ chlorinated n-alkane 52% Cl wt. has a 48-h EC_{50} of 0.0059 mg/L for *Daphnia magna.* The 21-day NOEC for the same species and substance is 0.0087 mg/L. It is therefore concluded that this substance meets the Annex XIII criteria for being "toxic" (T).

A $C_{10\text{-}13}$ chlorinated n-alkane 58% Cl wt. also meets the T criterion on the basis of toxicity to *Daphnia* (21-day NOEC of 0.005 mg/L; ECHA, 2008). It is inferred that $C_{<14}$ constituents of MCCPs with a similar degree of chlorination will also meet the T criterion.

Mammalian toxicity: MCCPs does not meet the criteria for classification as carcinogenic (category 1A or 1B), germ cell mutagenic (category 1A or 1B), toxic for reproduction (category 1A, 1B, or 2) or specific target organ toxicity after repeated exposure (STOT RE category 1 or 2) according to Regulation EC No. 1272/2008.

Internal haemorrhaging and death observed in rodent offspring may be a relevant factor but no conclusion has been drawn for the purposes of this Substance Evaluation.

Conclusion

MCCPs meets the PBT and vPvB criteria. This conclusion is assumed to apply to all MCCP product types because they will contain shared constituents with PBT/vPvB properties above 0.1% w/w. Longer chain length constituents appear to be significantly bioaccumulative in invertebrates even if bioaccumulation in fish is reduced. It is possible that lower chlorine content MCCP products (≤45% Cl wt.) might not be persistent within the meaning of the Annex XIII criteria, but definitive data to confirm this are not available.

In addition, the registered substance contains unintentional $C_{10\text{-}13}$ constituents that are structural analogues of SCCPs in the range 0.1-1% w/w. SCCPs is on the ECHA Candidate List of Substances of Very High Concern due to its PBT properties, and is also listed as a persistent organic pollutant under the United Nations Stockholm Convention on Persistent Organic Pollutants. The $C_{10\text{-}13}$ constituents of MCCPs are likely to have the same PBT properties as SCCPs. As they are present above 0.1% w/w, MCCPs is therefore also a "PBT-containing substance".

6.12 Exposure assessment

6.12.1 Human health

Since this substance evaluation is targeted for environmental end points, human exposure has not been evaluated.

6.12.2 Environment

6.12.2.1 Overview of uses and exposure scenarios

The environmental exposure assessment in the registration dossiers is based on seventeen exposure scenarios. These are summarised in Table 47 and broadly correspond to those developed in EC (2005). For the purposes of this substance evaluation, a detailed comparison between the approaches used in the registrations and those used in EC (2005) has been made, along with an assessment of whether the Registrants' exposure scenarios adequately cover the registered tonnage and the identified uses. Up-to-date tonnage information has not been provided by all Registrants. Information on the chlorine contents of all MCCP product types supplied by the Registrants, as well as a description of chlorine content for each registered use was requested by ECHA. This information is confidential. In addition, a number of exposure scenarios in Section 9 of the Chemical Safety Report were asked to be updated to identify the appropriate operational conditions and risk management measures. These have been checked by the eMSCA and are now appropriate.

Table 47

ENVIRONMENTAL EXPOSURE SCENARIOS AND THEIR CORRESPONDING TONNAGES		
Use	**Exposure Scenario**	**Percentage of total tonnage**
Manufacturing	ES1: Manufacturing	100%
PVC, Polymer and Rubber	ES2: Formulation ES3: Conversion ES4: Service life	63.8%
Sealants and Adhesives	ES5: Formulation and use ES6: Outdoor service life ES7: Indoor service life	27.0%
Metalworking Fluids	ES8: Formulation ES9: Use (emulsion) ES10: Use (neat oil)	7.0%
Paints	ES14: Formulation and use ES15: Outdoor service life ES16: Indoor service life	1.3%
Textiles	ES11: Formulation and use ES12: Outdoor service life ES13: Indoor service life	0.9%
Paper Products	ES17: Manufacture of paper and recycled paper	0.3%

The PECs in the registration dossiers are calculated using EUSES version 2.1.1. The key properties of MCCPs used in the EUSES calculations are summarised in Table 48. The

equivalent values used in the previous assessments under the Existing Substances Regulation are shown alongside for comparison.

Table 48

SUBSTANCE SPECIFIC INPUT PARAMETERS FOR ECETOC/EUSES MODEL		
Parameter	**Values used in CSR**	**Values used in EC, 2005 & 2007**
Physical State	Liquid	Not specified
Chlorine Content	52%	The main modelling was based on 52% chlorine content but the effect of a lower chlorine content (45%) on volatility was also explored.
Molecular Weight	488 g/mol	488 g/mol
Vapour Pressure at 20 °C	0.00027 Pa	0.00027 Pa
Melting Point (pour point)	0 °C	Not specified
Boiling Point	200 °C	Not specified
Water Solubility at 20 °C	0.027 mg/L	0.027 mg/L
Partition coefficient – log K_{ow}	7	7
Half-life for degradation in air	HL = 48 hours k_{OH} = 8×10^{-12} cm^3 $molecule^{-1}$ s^{-1}	k_{OH} = 8×10^{-12} cm^3 $molecule^{-1}$ s^{-1}
Bioconcentration factor for fish (BCF_{fish})	1 087 L/kg ww 1.087 m^3/kg ww	1 087 L/kg
Bioconcentration factor for earthworms ($BCF_{earthworm}$)	5.6 unit less [$K_{earthworm,porewater}$ = 58.194 m^3/kg ww = 58 194 L/kg ww]	5.6
Bioconcentration factor for plants (BCF_{plant})	0.034	0.034
Bioaccumulation/ biomagnification factor for fish/predators (BMF)	3	Range of 1-3 (food accumulation factors)

SUBSTANCE SPECIFIC INPUT PARAMETERS FOR ECETOC/EUSES MODEL		
Parameter	**Values used in CSR**	**Values used in EC, 2005 & 2007**
Partition coefficient between plant and water, $K_{plant-water}$	330 m^3/m^3	330 m^3/m^3
Chemical class for Koc-QSAR	Predominantly hydrophobics	Predominantly hydrophobics
Biodegradability	Although biodegradation does occur, considered not biodegradable	Considered to be not biodegradable
Sewage treatment plant removal rate (sludge)	97.1%	93%

As can be seen from Table 48, the basic property information used in the registration dossiers is in broad agreement with that used in the previous risk assessment under the Existing Substances Regulation (EC, 2005 & 2007). However the eMSCA notes the following points:

- **Sewage treatment plant removal rate:** The eMSCA considers that MCCPs is likely to be more adsorptive than SCCPs, and so the removal rate of 93% used in previous assessments was a "worst case" in terms of release to water. The higher percentage used by the Registrants is probably more realistic.

  A single value has been chosen for the K_{oc} as derived from the K_{ow} using QSAR in EUSES; the K_{oc} estimated from a log K_{ow} of 7 is 588 844 L/kg. The possible variation of K_{oc} with chain length and chlorine content is not considered, but it is likely to affect the predicted environmental concentrations. The eMSCA suggests that a sensitivity analysis could be performed by the Registrants, to investigate how variation in log K_{ow} affects behaviour in a sewage treatment plant. As an exploratory exercise, the eMSCA has briefly considered how this might affect the exposure assessment and risk characterisation (discussed below). The eMSCA recognises that this could add to the complexity in the recommended risk management measures, but believes it is worthwhile if in future certain types of commercial MCCP products are no longer permitted to be used.

- **Bioconcentration factor for fish:** The fish BCF used in EC (2005) was 1 087 L/kg and the same value has been used in the registration dossiers. As noted in Section 6.7.5.1.2, this value has been growth-corrected to give a BCF of around 2 000 L/kg. In addition, higher BCF values (up to 20 000 L/kg) have been derived from other studies.

  The choice of the most appropriate BCF value to use in the PEC calculations is problematic because, as discussed in Section 6.7.5, the BCF value varies with carbon chain length and chlorine content, and MCCPs is a UVCB substance containing thousands of different constituents with different BCF values. In terms of the objectives of the exposure assessment in REACH, which is to determine the operational conditions and risk management measures for safe use, it may not be so important to define a precise BCF for MCCPs provided that the assumptions in the

assessment are such that safe use can be demonstrated for a reasonable range of BCF values.

The secondary poisoning assessment is superseded by the PBT assessment. However, similar to the situation with sewage treatment plant removal, the eMSCA believes that a sensitivity analysis would be worthwhile if in future certain types of commercial MCCP products are no longer permitted to be used.

Sensitivity analysis performed by the eMSCA

To take account of a range of possible scenarios for sewage sludge removal and fish bioconcentration, the eMSCA has performed modelling with EUSES 2.03 using the range of parameter values summarised in Table 49. The environmental releases from current exposure scenarios in the registration dossiers are confidential, but were the basis for the modelling.

Table 49

SUBSTANCE SPECIFIC INPUT PARAMETERS FOR SENSITIVITY ANALYSIS				
Parameter	**Range of values**			
Log K_{ow}	5.5	6.58	7	8.2
K_{oc} (estimated from 'predominantly hydrophobics' QSAR and K_{ow})	3.59×10^4	2.69×10^5	5.89×10^5	5.53×10^6
Fish BCF (L/kg)	1 087	2 490	11 214	21 469

The use of a log K_{ow} of 5.5 generates a lower log K_{oc} with reduced partitioning to solids and higher predicted concentrations in surface water. It is only relevant for some $C_{<14}$ constituents, which are present significantly below 1% w/w in commercial products.

6.12.2.2 Aquatic compartment (incl. sediment)

Overview of uses and exposure scenarios

See Section 6.12.2.1.

Monitoring data

Monitoring data compiled from a literature review were included in the registration dossiers, and have also been summarised in Appendix D by the eMSCA. Concerns over the reliability of analytical methods complicates interpretation but they generally show widespread occurrence of MCCPs in water (at concentrations typically up to a few µg/L), sediment (at concentrations typically up to around 2 mg/kg, although higher concentrations up to 65 mg/kg dry weight have been measured in some studies) and biota (typically <1 mg/kg ww but higher concentrations up to around 80 mg/kg ww have been reported in some studies).

Modelled data

The PECs in the CSRs have been calculated using the EUSES program. These calculations have been checked by the eMSCA as part of this substance evaluation (re-calculations carried out using EUSES 2.0.3) and the agreement between the re-calculations and the PECs presented in the CSRs was generally good. Therefore the eMSCA considers that the PECs are calculated appropriately in the CSRs with the caveat that the variability in the log K_{ow} and BCF values could be subject to a sensitivity analysis (see Section 6.13).

Comparison of monitoring and modelled data

The highest levels are found in industrial/urban areas and so probably reflect point source releases (for example, monitoring points close to chlorinated paraffin manufacturing plants). However, there is generally insufficient information available on the actual industries present in the sampling localities and, in particular, on the operational conditions and risk management measures in place at the time of sampling. Therefore it is not possible to directly compare the available monitoring data with the PECs calculated in the exposure scenarios.

The registration dossiers include a comparison of the PECs calculated with the monitoring data contained in the literature and EC (2005) and the eMSCA agrees that there is generally a good comparison between the predicted PECs with measured concentrations where a comparison was possible.

6.12.2.3 Terrestrial compartment

Overview of uses and exposure scenarios

See Section 6.12.2.1

Monitoring data

See Section 6.12.2.1. In addition to the information reported in Appendix D, Smith (2009) carried out a review of the levels of various contaminants in sewage sludge published in the literature and reported that the concentration of MCCPs in sewage sludge ranged between 30 and 9 700 mg/kg dw, with an overall mean value of around 1 800 mg/kg dw.

Modelled data

See Section 6.12.2.2

Comparison of monitoring and modelled data

See Section 6.12.2.2

6.12.2.4 Atmospheric compartment

Overview of uses and exposure scenarios

See Section 6.12.2.1

Monitoring data

No monitoring data were included in the registration dossiers. This EC (2005) indicated that little or no information was available on levels in air at that time. Since then the following studies have become available (studies from outside the EU are recorded in Appendix D):

- Barber *et al.* (2005) determined MCCPs to be present at concentrations of <0.81 to 14.5 ng/m^3 (mean 3.0 ng/m^3) in air samples from the Hazelrigg field station near Lancaster, UK.
- Fridén *et al.* (2011) determined that low levels of chlorinated paraffins (determined as the sum of SCCPs and MCCPs) were present in indoor air samples from apartments in Stockholm, Sweden. The levels measured ranged between <5 and 210 ng/m^3 but the levels were dominated by the more volatile SCCPs. Levels in dust were reported to be in the low mg/kg range. These data are not directly relevant to atmospheric concentrations.

Modelled data

See Section 6.12.2.2

Comparison of monitoring and modelled data

See Section 6.12.2.2

6.12.3 Combined exposure assessment

The regional concentrations were estimated in the registration dossiers using EUSES. These calculations have been checked by the eMSCA for the purposes of this evaluation using EUSES 2.0.3, and similar PECs are obtained.

6.13 Risk characterisation

6.13.1 Environment

6.13.1.1 Aquatic compartment (incl. sediment)

The eMSCA concludes that the comparison of local exposure scenarios and PNECs lead to the derivation of risk characterisation ratios (RCRs) below one using both the PNECs derived by the Registrants and the revised $PNEC_{water}$ recommended by the eMSCA, i.e. the deterministic risk is low.

However, two of the exposure scenarios (textiles formulation (ES 11) and manufacture of paper (ES 17) may result in RCRs above one for secondary poisoning via fish where the log K_{ow} is set at 5.5 and the BCF fish is set at 21 469 L/kg in EUSES. This combination of properties is unlikely, but the eMSCA believes that the Registrants should perform their own sensitivity analysis to provide reassurance that the risk management measures are appropriate for all relevant constituents of MCCPs.

6.13.1.2 Terrestrial compartment

The eMSCA concludes that the comparison of local exposure scenarios and PNECs lead to RCRs below one. Any further sensitivity analysis performed by the Registrants could consider secondary poisoning via earthworms.

6.13.1.3 Atmospheric compartment

No quantitative risk characterisation is possible for the atmospheric compartment in the absence of any effects data.

6.13.1.4 Microbiological activity in sewage treatment systems

The local exposure scenarios in the registration dossiers all lead to RCRs below one, indicating that the risk to sewage treatment plant is adequately controlled for these scenarios.

6.13.2 Overall risk characterisation

6.13.2.1 Human health (combined for all exposure routes)

Since this substance evaluation is targeted for environmental end points, risks to human health have not been evaluated. A scientific opinion on human health risks related to the presence of chlorinated paraffins in food is currently in preparation by the European Food Safety Authority (EFSA, 2019). The draft conclusion is that the margin of exposure for MCCPs does not indicate a health concern for consumption of 'fish meat'. No other conclusions can be drawn due to lack of data.

6.13.2.2 Environment (combined for all exposure routes)

The eMSCA concludes that MCCPs meets the Annex XIII PBT/vPvB criteria, and so a risk exists for any level of environmental exposure. The Registrants should review their exposure scenarios to ensure the minimisation of emissions.

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Additional studies

The eMSCA performed a literature search in Google, Google Scholar, Science Direct, Scopus, Wiley Publications and the Royal Society of Chemistry Virtual Library on 1 November 2019 using the following search terms: Medium-chain chlorinated paraffins * environmental persistence * environmental accumulation * environmental bioaccumulation * aquatic bioaccumulation * environmental and aquatic toxicity. In addition, a review by Glüge *et al*. (2018) highlighted some additional studies that are not included in this substance evaluation. The eMSCA has not reviewed the following articles for relevance or reliability, but notes that some may need to be taken into account in future evaluations:

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Note: Norway has been active in monitoring a range of substances in recent years. The reference list includes recent reports that are cited in the text or appendices, but additional information on MCCPs is available in the following (the eMSCA has not checked these reports specifically, and this list might not be exhaustive):

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Abbreviations

APCI-QToF-HRMS	Atmospheric-Pressure Chemical Ionization Quantitative Time of Flight High Resolution Mass Spectrometry
BAF	Bioaccumulation Factor
BCF	Bioconcentration Factor
BMF	Biomagnification Factor
BOD	Biological Oxygen Demand
BSAF	Biota-sediment accumulation factor
Cl wt.	Chlorine content by weight
CLP	Classification, Labelling and Packaging
CoRAP	Community rolling action plan
CSR	Chemical Safety Report
DOC	Dissolved Organic Carbon
dw	Dry weight
EC_{50}	Half maximal effective concentration
ECHA	European Chemicals Agency
ED	Endocrine disrupters
eMSCA	Evaluating Member State Competent Authority
ESR	Existing Substances Regulation
GC-ECNI-LRMS	Gas Chromatography Electron Capture Negative Ionisation Low Resolution Mass Spectrometry
GCxGC-ECD	Two Dimensional Gas Chromatography with Electron Capture Detector
GLP	Good Laboratory Practise
k_1	Uptake rate constant
k_2	Overall depuration rate constant
kM	Rate constant for metabolism
K_{OC}	Organic carbon-water partition coefficient
K_{OW}	Octanol/water partition coefficient
LCCP(s)	Long Chain Chlorinated Paraffin(s)
LOD	Limit of detection
lw	Lipid weight
MCCP(s)	Medium-Chain Chlorinated Paraffin(s)
M-factors	Multiplication Factors
NOEC	No Observed Effect Concentration
NER	Non-extractable residues
NPOC	Non-Purgeable Organic Carbon
OECD	Organisation for Economic Co-operation and Development
PAAP	Polyalkoxylated alkylphenol (alkylphenol polyalkoxylate), Agnique BP NP1530

PBT	Persistent, Bioaccumulative and Toxic
PEC	Predicted Effect Concentration
PNEC	Predicted No Effect Concentration
POC	Particulate Organic Carbon
QSAR	Quantitative Structure Activity Relationships
RCR	Risk Characterisation Ratio
REACH	Registration, Evaluation and Authorisation of Chemicals
RMOA	Risk Management Option Analysis
SCCP(s)	Short Chain Chlorinated Paraffin(s)
SMILES	Simplified Molecular Input Line Entry System
SVHC	Substances of very high concern
TG	Test Guideline
ThOD	Theoretical Oxygen Demand
TMF	Trophic Magnification Factor
UVCB	Unknown Variable Concentration or Biological
vPvB	very Persistent very Bioaccumulative
ww	Wet weight

Appendix A: Modelling of physico-chemical properties and degradation potential

As part of the initial evaluation of MCCPs in 2012, the eMSCA produced predictions of vapour pressure, water solubility, log K_{OW} and degradation potential for a series of hypothetical chlorinated paraffin structures with a range of carbon chain lengths and chlorine contents.

- Vapour pressure was estimated using the MPBPVP v1.43 model contained within the EPI Suite™ v4.11 platform (US EPA, 2012).

- Water solubility was estimated using the WSKOWWIN v1.41 and WATERNT v1.01 models contained within the EPI Suite™ v4.11 platform (US EPA, 2012).

- The predictions for log K_{OW} were carried out using KOWWIN v1.68 from EPI Suite™ v 4.11 (US EPA, 2012), Sijm and Sinnige (1995) and Hilger *et al*. (2011a).

- The biodegradation predictions were carried out using the Biowin v4.10 model in the EPI Suite™ v 4.11 (US EPA, 2012). The summary of persistence is based on the Biowin 3 prediction. A prediction of >1.5 is considered to be not persistent, a prediction <1.4 is considered to be potentially persistent and a prediction between 1.4 and 1.5 is considered to be not clear.

The results are summarised in the following tables. The shaded boxes in Table A3 represent cases where the substance is predicted to be persistent (or is not clear on persistence). It should be noted that there have been updates to the models since these predictions were made, which could affect some values. The main text of the report should be consulted for further discussion.

Table A1

STRUCTURES AND ESTIMATED VAPOUR PRESSURE AND WATER SOLUBILITY FOR A SERIES OF HYPOTHETICAL CHLORINATED PARAFFIN STRUCTURES							
Formula	**Molecular weight (g/mol)**	**Chlorine content (% by weight)**		**SMILES notation used for estimations**	**Water solubility (mg/L)**		**Vapour pressure (mm Hg at 25 °C)**
		Actual	**Group**		**WSKOWWIN v1.41**	**WATERNT v1.01**	**MPBPVP v1.43**
$C_{10}H_{19}Cl_3$	245.5	43.4	45.0	CC(Cl)CC(Cl)CCC(Cl)CCC	0.2819	0.73229	0.0225
$C_{11}H_{20}Cl_4$	294.0	48.3		CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC	0.03999	0.13402	0.0024
$C_{12}H_{22}Cl_4$	308.0	46.1		CC(Cl)CC(Cl)CC(Cl)CCCC(Cl)CC	0.01261	0.040775	0.00121
$C_{13}H_{24}Cl_4$	322.0	44.1		CC(Cl)CC(Cl)CC(Cl)CCCCC(Cl)CC	0.003967	0.01238	0.000508
$C_{14}H_{26}Cl_4$	336.0	42.3		C(Cl)CCCCC(Cl)CCCC(Cl)CC(Cl)CC	0.001078	0.0022385	6.64E-5
$C_{15}H_{27}Cl_5$	384.5	46.2		CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CCCC(Cl)CC	0.0001689	0.00065611	2.16E-5
$C_{16}H_{29}Cl_5$	398.5	44.5		CC(Cl)CC(Cl)CCC(Cl)CCC(Cl)CCC(Cl)CCC	5.267E-5	0.00019748	9.02E-6
$C_{17}H_{31}Cl_5$	412.5	43.0		C(Cl)CC(Cl)CC(Cl)CCCC(Cl)CCCC(Cl)CCCC	1.42E-5	3.5421E-5	1.12E-6
$C_{18}H_{32}Cl_6$	461.0	46.2		CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CCC(Cl)CCC(Cl)CCC	2.172E-6	1.014E-5	3.54E-7
$C_{10}H_{18}Cl_4$	280.0	50.7	52.0	CC(Cl)CC(Cl)C(Cl)CC(Cl)CCC	0.1265	0.43952	0.00563
$C_{11}H_{19}Cl_5$	328.5	54.0		C(Cl)CC(Cl)CCC(Cl)CC(Cl)CC(Cl)C	0.01522	0.047025	0.00025
$C_{12}H_{21}Cl_5$	342.5	51.8		CC(Cl)C(Cl)CC(Cl)CCC(Cl)CCC(Cl)C	0.005518	0.023863	0.000325
$C_{13}H_{22}Cl_6$	391.0	54.5		C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CCC(Cl)C	0.0006457	0.0024844	1.2E-5
$C_{14}H_{24}Cl_6$	405.0	52.6		C(Cl)CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC(Cl)CC	0.0002013	0.00074733	4.99E-6
$C_{15}H_{26}Cl_6$	419.0	50.8		C(Cl)CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC(Cl)CCC	6.268E-5	0.00022453	1.74E-6
$C_{16}H_{27}Cl_7$	467.5	53.2		CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC(Cl)CCC(Cl)C(Cl)C	9.572E-6	6.417E-5	5.51E-7
$C_{17}H_{29}Cl_7$	481.5	51.6		CC(Cl)CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC(Cl)CC(Cl)CC	2.967E-6	1.9193E-5	2.29E-7
$C_{18}H_{31}Cl_7$	495.5	50.2		C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CCCC(Cl)CCC	7.952E-7	3.4226E-6	3.31E-8

Formula	Molecular weight (g/mol)	Chlorine content (% by weight)		SMILES notation used for estimations	Water solubility (mg/L)		Vapour pressure (mm Hg at 25 °C)
		Actual	Group		WSKOWWIN v1.41	WATERNT v1.01	MPBPVP v1.43
$C_{10}H_{16}Cl_6$	349.0	61.0	60.0	CC(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)	0.02114	0.090539	0.000162
$C_{11}H_{17}Cl_7$	397.5	62.5		C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)	0.002469	0.0094049	6.65E-6
$C_{12}H_{19}Cl_7$	411.5	60.4		C(Cl)CC(Cl)C(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)CC	0.0008887	0.0047385	7.86E-6
$C_{13}H_{20}Cl_8$	460.0	61.7		C(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)CC(Cl)CC(Cl)CC(Cl)	0.0001018	0.00048311	2.61E-7
$C_{14}H_{22}Cl_8$	474.0	59.9		C(Cl)CC(Cl)C(Cl)C(Cl)CC(Cl)CCC(Cl)CC(Cl)C(Cl)C	3.65E-5	0.00024228	3.05E-7
$C_{15}H_{23}Cl_9$	522.5	61.1		C(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)C(Cl)CC(Cl)CC(Cl)C	4.766E-6	4.0821E-5	3.33E-8
$C_{16}H_{25}Cl_9$	536.5	59.6		C(Cl)CC(Cl)C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)C	1.473E-6	1.2172E-5	1.36E-8
$C_{17}H_{26}Cl_{10}$	585.0	60.7		C(Cl)CC(Cl)C(Cl)C(Cl)C(Cl)C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC	1.902E-7	2.0287E-6	1.42E-9
$C_{18}H_{27}Cl_{11}$	633.5	61.6		C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)CC(Cl)C(Cl)C(Cl)CC(Cl)C(Cl)C	2.44E-8	6.334E-7	1.44E-10

Table A2

STRUCTURES AND ESTIMATED LOG K_{OW} FOR A SERIES OF HYPOTHETICAL CHLORINATED PARAFFIN STRUCTURES							
Formula	**Molecular weight (g/mol)**	**Chlorine content (% by weight)**		**SMILES notation used for estimating log K_{OW}**	**Log K_{OW} estimate**		
		Actual	**Group**		**KOWWIN v1.68**	**Sijm and Sinnige (1995)**	**Hilger *et al.* (2011a)**
$C_{10}H_{19}Cl_3$	245.5	43.4	45.0	CC(Cl)CC(Cl)CCC(Cl)CCC	5.79	5.50	5.09
$C_{11}H_{20}Cl_4$	294.0	48.3		CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC	6.47	6.07	5.37
$C_{12}H_{22}Cl_4$	308.0	46.1		CC(Cl)CC(Cl)CC(Cl)CCCC(Cl)CC	6.96	6.32	5.65
$C_{13}H_{24}Cl_4$	322.0	44.1		CC(Cl)CC(Cl)CC(Cl)CCCCC(Cl)CC	7.45	6.55	5.93
$C_{14}H_{26}Cl_4$	336.0	42.3		C(Cl)CCCCC(Cl)CCCC(Cl)CC(Cl)CC	8.01	6.75	6.21
$C_{15}H_{27}Cl_5$	384.5	46.2		CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CCCC(Cl)CC	8.61	7.09	6.50
$C_{16}H_{29}Cl_5$	398.5	44.5		CC(Cl)CC(Cl)CCC(Cl)CCC(Cl)CCC(Cl)CCC	9.1	7.23	6.78
$C_{17}H_{31}Cl_5$	412.5	43.0		C(Cl)CC(Cl)CC(Cl)CCCC(Cl)CCCC(Cl)CCCC	9.67	7.34	7.06
$C_{18}H_{32}Cl_6$	461.0	46.2		CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CCC(Cl)CCC(Cl)CCC	10.26	7.51	7.34
$C_{10}H_{18}Cl_4$	280.0	50.7	52.0	CC(Cl)CC(Cl)C(Cl)CC(Cl)CCC	5.97	5.80	5.09
$C_{11}H_{19}Cl_5$	328.5	54.0		C(Cl)CC(Cl)CCC(Cl)CC(Cl)CC(Cl)C	6.72	6.32	5.37
$C_{12}H_{21}Cl_5$	342.5	51.8		CC(Cl)C(Cl)CC(Cl)CCC(Cl)CCC(Cl)C	7.14	6.55	5.65
$C_{13}H_{22}Cl_6$	391.0	54.5		C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CCC(Cl)C	7.88	6.93	5.93
$C_{14}H_{24}Cl_6$	405.0	52.6		C(Cl)CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC(Cl)CC	8.37	7.09	6.21
$C_{15}H_{26}Cl_6$	419.0	50.8		C(Cl)CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC(Cl)CCC	8.79	7.23	6.50
$C_{16}H_{27}Cl_7$	467.5	53.2		CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC(Cl)CCC(Cl)C(Cl)C	9.46	7.44	6.78
$C_{17}H_{29}Cl_7$	481.5	51.6		CC(Cl)CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC(Cl)CC(Cl)CC	9.95	7.51	7.06
$C_{18}H_{31}Cl_7$	495.5	50.2		C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CCCC(Cl)CCC	10.52	7.55	7.34

Formula	Molecular weight (g/mol)	Chlorine content (% by weight)		SMILES notation used for estimating log K_{OW}	Log K_{OW} estimate		
		Actual	Group		KOWWIN v1.68	Sijm and Sinnige (1995)	Hilger *et al.* (2011a)
$C_{10}H_{16}Cl_6$	349.0	61.0	60.0	CC(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)	6.41	6.32	5.28
$C_{11}H_{17}Cl_7$	397.5	62.5		C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)	7.15	6.75	5.55
$C_{12}H_{19}Cl_7$	411.5	60.4		C(Cl)CC(Cl)C(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)CC	7.57	6.93	5.83
$C_{13}H_{20}Cl_8$	460.0	61.7		C(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)CC(Cl)CC(Cl)CC(Cl)	8.32	7.23	6.10
$C_{14}H_{22}Cl_8$	474.0	59.9		C(Cl)CC(Cl)C(Cl)C(Cl)CC(Cl)CCC(Cl)CC(Cl)C(Cl)C	8.73	7.34	6.38
$C_{15}H_{23}Cl_9$	522.5	61.1		C(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)C(Cl)CC(Cl)CC(Cl)C	9.41	7.51	6.66
$C_{16}H_{25}Cl_9$	536.5	59.6		C(Cl)CC(Cl)C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)C	9.9	7.55	6.93
$C_{17}H_{26}Cl_{10}$	585.0	60.7		C(Cl)CC(Cl)C(Cl)C(Cl)C(Cl)C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC	10.57	7.58	7.21
$C_{18}H_{27}Cl_{11}$	633.5	61.6		C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)CC(Cl)C(Cl)C(Cl)CC(Cl)C(Cl)C	11.24	7.51	7.48

Table A3

Formula			Smiles used	Cl content (% wt.)	EPI Suite™ Predictions					Summary of persistence
					Biowin					
C	H	Cl			1	2	3	5	6	
13	28	0	CCCCCCCCCCCCC	0.0	0.8766	0.9833	3.3884	0.708	0.8772	Not P
13	27	1	CCCC(CL)CCCCCCCCC	16.2	0.6404	0.4731	2.8408	0.5066	0.4511	Not P
13	26	2	CCCC(CL)CCC(CL)CCCCCC	28.1	0.5126	0.0795	2.5915	0.3051	0.0863	Not P
13	25	3	CCCC(CL)CCC(CL)CCC(CL)CCC	37.0	0.2764	0.0013	2.0438	0.1036	0.0108	Not P
13	24	4	CC(CL)CC(CL)CCC(CL)CCC(CL)CCC	44.1	0.1486	0.0001	1.7945	-0.0979	0.0012	Not P
13	23	5	CC(CL)CC(CL)CC(CL)C(CL)CCC(CL)CCC	49.8	0.0208	0	1.5452	-0.2993	0.0001	Not P
13	22	6	CC(CL)CC(CL)CC(CL)C(CL)CC(CL)C(CL)CCC	54.5	-0.107	0	1.2959	-0.5008	0	Potentially P
13	21	7	CC(CL)CC(CL)CC(CL)C(CL)CC(CL)C(CL)CC(CL)C	58.4	-0.2347	0	1.0466	-0.7023	0	Potentially P
13	20	8	CC(CL)C(CL)C(CL)CC(CL)C(CL)CC(CL)C(CL)CC(CL)C	61.7	-0.3625	0	0.7973	-0.9037	0	Potentially P
13	19	9	CC(CL)C(CL)C(CL)CC(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C	64.6	-0.4903	0	0.5481	-1.1052	0	Potentially P
13	18	10	C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C	67.1	-0.6181	0	0.2988	-1.1576	0	Potentially P
13	17	11	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C	69.3	-0.7459	0	0.0495	-1.3591	0	Potentially P
13	16	12	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C	71.2	-0.8737	0	-0.1998	-1.5606	0	Potentially P
13	15	13	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)	73.0	-1.0015	0	-0.4491	-1.6129	0	Potentially P
14	30	0	CCCCCCCCCCCCCC	0.0	0.87	0.9797	3.3574	0.7157	0.8799	Not P
14	29	1	CCCC(CL)CCCCCCCCCC	15.3	0.6337	0.4239	2.8098	0.5143	0.4572	Not P
14	28	2	CCCC(CL)CCCCC(CL)CCCCC	26.6	0.5059	0.0661	2.5605	0.3128	0.0883	Not P
14	27	3	CCCC(CL)CCC(CL)CC(CL)CCCCC	35.3	0.3782	0.0068	2.3112	0.1113	0.011	Not P
14	26	4	CCCC(CL)CCC(CL)CC(CL)CCC(CL)CC	42.3	0.1419	0.0001	1.7635	-0.0902	0.0013	Not P
14	25	5	CCCC(CL)C(CL)CC(CL)CC(CL)CCC(CL)CC	47.9	0.0142	0	1.5142	-0.2916	0.0001	Not P

Formula			Smiles used	Cl content (% wt.)	EPI Suite™ Predictions					Summary of persistence
					Biowin					
C	H	Cl			1	2	3	5	6	
14	24	6	CC(CL)CC(CL)C(CL)CC(CL)CC(CL)CCC(CL)CC	52.6	-0.1136	0	1.2649	-0.4931	0	Potentially P
14	23	7	CC(CL)CC(CL)C(CL)CC(CL)CC(CL)CC(CL)C(CL)CC	56.5	-0.2414	0	1.0157	-0.6946	0	Potentially P
14	22	8	C(CL)C(CL)CC(CL)C(CL)CC(CL)CC(CL)CC(CL)C(CL)CC	59.9	-0.3692	0	0.7664	-0.747	0	Potentially P
14	21	9	C(CL)C(CL)CC(CL)C(CL)CC(CL)C(CL)C(CL)CC(CL)C(CL)CC	62.8	-0.497	0	0.5171	-0.9484	0	Potentially P
14	20	10	C(CL)C(CL)CC(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC	65.4	-0.6248	0	0.2678	-1.1499	0	Potentially P
14	19	11	C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC	67.6	-0.7526	0	0.0185	-1.3514	0	Potentially P
14	18	12	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC	69.6	-0.8804	0	-0.2308	-1.5529	0	Potentially P
14	17	13	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C	71.4	-1.0082	0	-0.4801	-1.7543	0	Potentially P
14	16	14	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)	73.0	-1.1359	0	-0.7294	-1.8067	0	Potentially P
15	32	0	CCCCCCCCCCCCCCC	0.0	0.8633	0.9754	3.3264	0.7234	0.8824	Not P
15	31	1	CCCCCC(CL)CCCCCCCCC	14.4	0.7355	0.7921	3.0771	0.5219	0.4633	Not P
15	30	2	CCCCCC(CL)CCCCC(CL)CCCC	25.3	0.6077	0.2681	2.8278	0.3205	0.0903	Not P
15	29	3	CC(CL)CCCC(CL)CCCCC(CL)CCCC	33.8	0.3715	0.0055	2.2802	0.119	0.0113	Not P
15	28	4	CC(CL)CCCC(CL)CC(CL)CCC(CL)CCCC	40.6	0.2437	0.0005	2.0309	-0.0825	0.0013	Not P
15	27	5	CC(CL)CCCC(CL)CC(CL)CCC(CL)CC(CL)CC	46.2	0.0075	0	1.4832	-0.284	0.0002	Not clear
15	26	6	CC(CL)CC(CL)CC(CL)CC(CL)CCC(CL)CC(CL)CC	50.8	-0.1203	0	1.234	-0.4854	0	Potentially P
15	25	7	CC(CL)C(CL)C(CL)CC(CL)CC(CL)CCC(CL)CC(CL)CC	54.8	-0.2481	0	0.9847	-0.6869	0	Potentially P
15	24	8	CC(CL)C(CL)C(CL)CC(CL)CC(CL)CC(CL)C(CL)CC(CL)CC	58.2	-0.3759	0	0.7354	-0.8884	0	Potentially P

Formula			Smiles used	Cl content (% wt.)	EPI Suite™ Predictions					Summary of persistence
					Biowin					
C	H	Cl			1	2	3	5	6	
15	23	9	CC(CL)C(CL)C(CL)CC(CL)CC(CL)CC(CL)C(CL)CC(CL)C(CL)C	61.1	- 0.5037	0	0.4861	-1.0899	0	Potentially P
15	22	10	CC(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CC(CL)C(CL)C	63.7	-0.6315	0	0.2368	-1.2913	0	Potentially P
15	21	11	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CC(CL)C(CL)C	66.0	-0.7593	0	-0.0125	-1.3437	0	Potentially P
15	20	12	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)CC(CL)C(CL)C	68.1	-0.887	0	-0.2618	-1.5452	0	Potentially P
15	19	13	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C(CL)C	69.9	-1.0148	0	-0.5111	-1.7467	0	Potentially P
15	18	14	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C	71.5	-1.1426	0	-0.7604	-1.9481	0	Potentially P
15	17	15	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)	73.0	-1.2704	0	-1.0097	-2.0005	0	Potentially P
16	34	0	CCCCCCCCCCCCCCCC	0.0	0.8566	0.9701	3.2954	0.7311	0.8849	Not P
16	33	1	CCCC(CL)CCCCCCCCCCC	13.6	0.6204	0.3307	2.7478	0.5296	0.4694	Not P
16	32	2	CCCC(CL)CCCCCCCCC(CL)CCC	24.1	0.3842	0.0075	2.2001	0.3282	0.0923	Not P
16	31	3	CCCC(CL)CCCCC(CL)CCCC(CL)CCC	32.3	0.2564	0.0007	1.9508	0.1267	0.0116	Not P
16	30	4	CC(CL)CC(CL)CCCCC(CL)CCCC(CL)CCC	39.0	0.1286	0.0001	1.7016	-0.0748	0.0013	Not P
16	29	5	CC(CL)CC(CL)CC(CL)CCC(CL)CCCC(CL)CCC	44.5	0.0008	0	1.4523	-0.2763	0.0002	Not clear
16	28	6	CC(CL)CC(CL)CC(CL)CCC(CL)CC(CL)CC(CL)CCC	49.2	-0.127	0	1.203	-0.4777	0	Potentially P
16	27	7	CC(CL)CC(CL)CC(CL)CCC(CL)CC(CL)CC(CL)CC(CL)C	53.2	-0.2548	0	0.9537	-0.6792	0	Potentially P
16	26	8	CC(CL)CC(CL)CC(CL)CC(CL)C(CL)CC(CL)CC(CL)CC(CL)C	56.6	-0.3826	0	0.7044	-0.8807	0	Potentially P
16	25	9	CC(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CC(CL)CC(CL)CC(CL)C	59.6	-0.5104	0	0.4551	-1.0822	0	Potentially P
16	24	10	C(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CC(CL)CC(CL)CC(CL)C	62.2	-0.6381	0	0.2058	-1.1345	0	Potentially P

Formula			Smiles used	Cl content (% wt.)	EPI Suite™ Predictions					Summary of persistence
					Biowin					
C	H	Cl			1	2	3	5	6	
16	23	11	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)CC(CL)CC(CL)CC(CL)C	64.5	-0.7659	0	-0.0435	-1.336	0	Potentially P
16	22	12	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)CC(CL)C	66.6	-0.8937	0	-0.2928	-1.5375	0	Potentially P
16	21	13	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C	68.4	-1.0215	0	-0.5421	-1.739	0	Potentially P
16	20	14	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C	70.1	-1.1493	0	-0.7914	-1.9404	0	Potentially P
16	19	15	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C	71.6	-1.2771	0	-1.0407	-2.1419	0	Potentially P
16	18	16	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)	73.0	-1.4049	0	-1.29	-2.1943	0	Potentially P
17	36	0	CCCCCCCCCCCCCCCCC	0.0	0.8499	0.9638	3.2644	0.7388	0.8874	Not P
17	35	1	CCCCCCCCCCC(CL)CCCCCC	12.9	0.7221	0.719	3.0151	0.5373	0.4755	Not P
17	34	2	CCCC(CL)CCCCCCC(CL)CCCCCC	23.0	0.4859	0.0375	2.4675	0.3358	0.0944	Not P
17	33	3	CCCC(CL)CCCCCCC(CL)CCC(CL)CCC	31.0	0.2497	0.0006	1.9199	0.1344	0.0118	Not P
17	32	4	CCCC(CL)CCC(CL)CCCC(CL)CCC(CL)CCC	37.6	0.1219	0.0001	1.6706	-0.0671	0.0014	Not P
17	31	5	CC(CL)CC(CL)CCC(CL)CCCC(CL)CCC(CL)CCC	43.0	-0.0059	0	1.4213	-0.2686	0.0002	Not clear
17	30	6	CC(CL)CC(CL)CCC(CL)CC(CL)CC(CL)CCC(CL)CCC	47.7	-0.1337	0	1.172	-0.4701	0	Potentially P
17	29	7	CC(CL)CC(CL)CCC(CL)CC(CL)CC(CL)CC(CL)C(CL)CCC	51.6	-0.2615	0	0.9227	-0.6715	0	Potentially P
17	28	8	CC(CL)CC(CL)CCC(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CCC	55.0	-0.3892	0	0.6734	-0.873	0	Potentially P
17	27	9	CC(CL)CC(CL)CC(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CCC	58.0	-0.517	0	0.4241	-1.0745	0	Potentially P
17	26	10	CC(CL)C(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CCC	60.7	-0.6448	0	0.1748	-1.276	0	Potentially P

Formula			Smiles used	Cl content (% wt.)	EPI Suite™ Predictions					Summary of persistence
					Biowin					
C	H	Cl			1	2	3	5	6	
17	25	11	CC(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CCC	63.0	-0.7726	0	-0.0745	-1.4774	0	Potentially P
17	24	12	CC(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)CCC	65.1	-0.9004	0	-0.3238	-1.6789	0	Potentially P
17	23	13	CC(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)CC(CL)C	67.0	-1.0282	0	-0.5731	-1.8804	0	Potentially P
17	22	14	CC(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C	68.7	-1.156	0	-0.8224	-2.0818	0	Potentially P
17	21	15	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C	70.3	-1.2838	0	-1.0717	-2.1342	0	Potentially P
17	20	16	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C	71.7	-1.4116	0	-1.321	-2.3357	0	Potentially P
17	19	17	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)	73.0	-1.5393	0	-1.5703	-2.3881	0	Potentially P

Appendix B: Growth correction of the BCF for a C_{15}, 51% Cl wt. substance

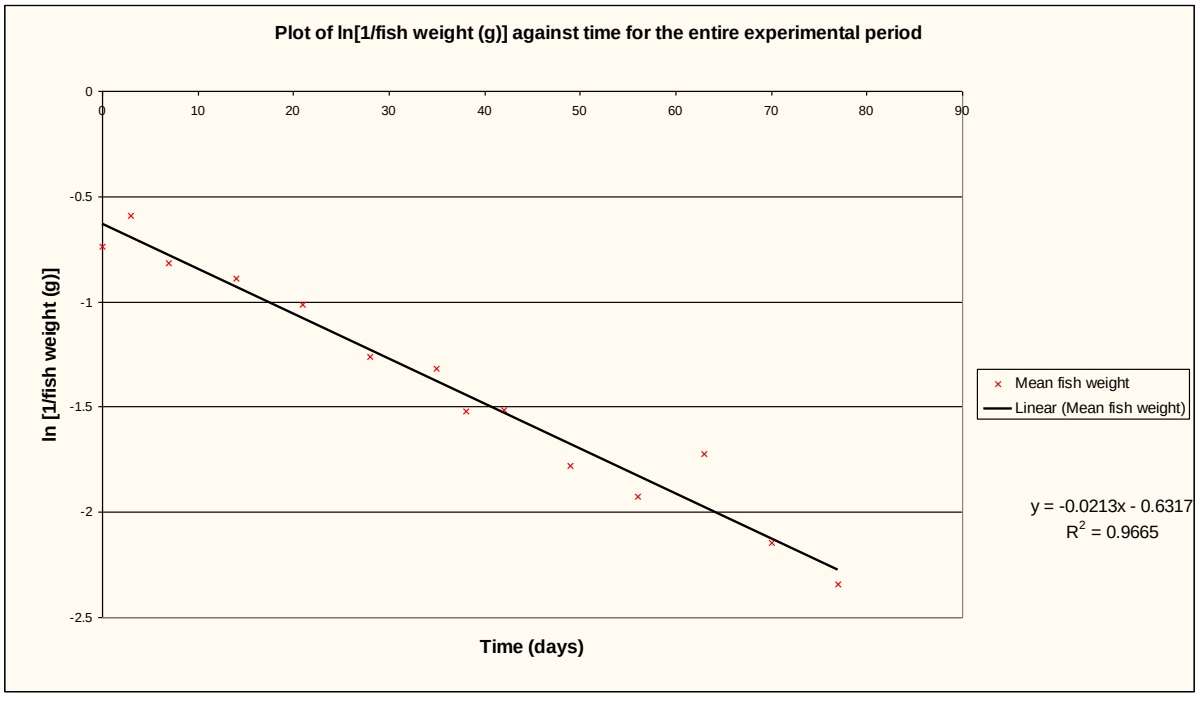
The background to the corrections made in this appendix is discussed in detail in EA (2011). The study performed by AstraZeneca (2000) was originally summarised in EC (2005). The relevant kinetic parameters are summarised in Table B1.

Table B1:

SUMMARY OF KINETIC PARAMETERS FROM THE UNPUBLISHED (2000) STUDY			
Exposure concentration (mg/L)	**Uptake rate constant k_{uptake} (L/kg/day)**	**Overall depuration rate constant $k_{depuration\_overall}$ (day^{-1})**	**Kinetic BCF (L/kg)**
0.00093	48.7	0.0448	1 087
0.0049	14.2	0.0407	349

The fish weights were determined at various time points during the uptake phase (days 0 to 35) and the depuration phase (days 38 to 77). The rate constant for growth dilution (k_{growth}) can be obtained from a plot of ln [1/fish weight] against time. The slope of such a plot is the negative of the growth dilution constant ($-k_{growth}$). Such a plot is shown in Figure B1 for the entire duration of the experiment (uptake and depuration phase). Similar plots were also constructed for the depuration period (day 35 to day 77 and day 38 to 77).

Figure B1: Determination of growth rate constant over the uptake and depuration phase



Based on these plots the following growth rate constants are determined:

For the entire experiment duration (day 0 to 77) k_{growth} = 0.0213 day^{-1} (R^2=0.97)

For depuration period days 35 to 77 k_{growth} = 0.0209 day^{-1} (R^2=0.88)

For depuration period days 38 to 77 k_{growth} = 0.0197 day^{-1} (R^2=0.84)

As can be seen, the rate constant for growth dilution appears to have been relatively constant over the entire period of the experiment. As the growth correction is applied to the depuration rate constant, the rate constant for growth dilution determined over the depuration period is most relevant to the analysis. However, the correlation (as measured by the R2 value) is slightly better for the growth rate constant determined over the entire experimental period than those determined during the depuration phase. Therefore the effect of the growth rate constants obtained using all three datasets are considered here.

The growth corrected depuration rate constant can be obtained from the following equation assuming additivity of first order rate constants.

$$k_{depuration\_overall} = k_{depuration\_growth\ corrected} + k_{growth}$$

thus $k_{depuration\_growth\ corrected} = k_{depuration\_overall} - k_{growth}$.

The growth corrected rate constants and growth corrected BCF values are summarised in Table B2.

Table B2

SUMMARY OF GROWTH CORRECTED KINETIC PARAMETERS FROM THE UNPUBLISHED (2000) STUDY				
Exposure concentration (mg/L)	**Uptake rate constant k_{uptake} (L/kg/day)**	**Rate constant for growth dilution k_{growth} (day^{-1})**	**Growth corrected depuration rate constant $k_{depuration\ growth\ corrected}$ (day-1)**	**Kinetic BCF (L/kg)**
0.00093	48.7[a]	0.0197 0.0209 0.0213	0.0251 0.0239 0.0235	1 940 2 038 2 072
0.00093	46.0[b]	0.0197 0.0209 0.0213	0.0251 0.0239 0.0235	1 833 1 925 1 957
0.0049	14.2	0.0197 0.0209 0.0213	0.0210 0.0198 0.0194	676 717 732

Notes: a) Value taken from the Unpublished (2000) test report. The value has been estimated by forcing the curve fitting routine to pass through the measured concentration in fish at day 35.

b) Value recalculated by Euro Chlor without constraint of the day 35 value.

The uptake rate constant of 48.7 L/kg/day given in the Unpublished (2000) study was estimated from the uptake curve by forcing the curve fitting routine through the point for the concentration measured at day 35 of the uptake period (the concentration measured at this time point was 0.80 mg/kg). There is some rationale for this approach as a larger number of fish samples were analysed on day 35 (and also day 28) of the study compared with the earlier time points[28]. Thus it could be argued that the actual concentration in fish is known more reliably at day 35 (and day 28) than the earlier time points and so fitting the curve through this point is appropriate. However, it has been pointed out by Euro Chlor (2009) that a better overall fit to the data is obtained if the curve fitting is carried out without the constraint of the day 35 point. When this is carried out the uptake rate constant for the 0.00093 mg/L treatment group was 46.0 L/kg/day (and the estimated concentration in fish at day 35 from the regression was 0.76 mg/kg). The effect of using this uptake rate

[28] Eight fish were sampled on each of day 35 and day 28 of the study compared with four fish on each of days 21, 14, 7 and 3 of the study.

constant on the predicted growth corrected BCF is shown in Table B2 – the estimated BCF is slightly lower.

Appendix C: Consideration of bioavailability in laboratory bioconcentration tests

MCCPs have a low water solubility and a high log K_{OW}. These factors mean that the substance is considered "difficult to test" in laboratory BCF test systems. In particular, these properties mean that the substance can adsorb onto surfaces and particles present in the test media, and also potentially associate with dissolved organic carbon (DOC) present in the test system. This can then lead to a reduction of the actual dissolved concentration in the test below that indicated by the analytical measurements (most analytical methods will not distinguish between the adsorbed and dissolved fractions). If the adsorbed fraction is not bioavailable, this may therefore lead to an underestimate of the true BCF based on the freely dissolved concentration (for those studies that do not estimate BCF using the kinetic method).

Although current test guidelines for bioconcentration studies (e.g. OECD TG 305) are designed to minimize the amount (concentration) of both particulate and dissolved organic matter present in the test system, it is practically impossible to carry out such tests without such confounding factors being present.

The potential impact of the presence of particulate matter and DOC on the BCF of MCCPs has been considered in Unpublished (2013). Unpublished (2013) indicates that the dissolved fraction can be estimated from the following equation:

$$Fraction\ dissolved = \frac{1}{1 + [POC] \times 0.35 \times K_{OW} + 0.08 \times K_{OW}}$$

Where [POC] = concentration of Particulate Organic Carbon in the test system (kg/kg or kg/L)

[DOC] = concentration of Dissolved Organic Carbon in the test system (kg/kg or kg/L)

K_{OW} = octanol/water partition coefficient

0.35 and 0.08 are proportionality constants relating K_{OW} to the types of organic carbon.

For the BCF study for a C_{15} chlorinated n-alkane, 51% Cl wt. substance with Rainbow Trout (Thompson *et al*., 2000, as summarised in EC, 2005), the concentration of non-purgeable organic carbon (NPOC) was measured during the test and the values generally ranged between 0.69 and 2.4 mg/L. The exact nature of the organic carbon measured was uncertain but Unpublished (2013) concluded that the BCFs based on the dissolved (bioavailable) water concentration were likely to be higher than reported in the study. Although it was not possible to apply a correction directly to the data, Unpublished (2013) indicated that the above equation, assuming a DOC concentration of around 1 mg/L and a log K_{OW} of around 8 for the substance tested, would suggest a dissolved concentration of around 10% of the total measured concentration.

A further BCF study (Unpublished, 2010h) reported the total organic carbon concentration in the test medium as < 3.0 mg/L (mean of 15 samples in each of the solvent control and exposed groups). In his review of this study, Unpublished (2013) indicated that a DOC concentration of 0.45 mg/L was reported at one sampling point. Assuming a DOC concentration of around 0.5 mg/L and a log K_{OW} of 7.5 for the substance tested, Unpublished (2013) estimated that the dissolved fraction may be around 40% of the total measured concentration (ignoring any influence of POC).

The DOC value in the Unpublished (2010h) study appears to be taken from a single analysis of a representative sample of laboratory dechlorinated water that was sampled between 6 August and 22 October 2009, rather than the test solutions themselves.

The equation used in the Unpublished (2013) review is of a similar form to that used in the REACH Guidance for calculation of predicted environmental concentrations (PECs) on a freely dissolved basis, although in this case only adsorption onto particulate matter is taken into account (DOC is not considered in the PEC calculations). The equivalent equation from the REACH Guidance, modified to the current situation, would be as follows:

$$Fraction\ dissolved = \frac{1}{1 + [POC] \times K_{OC}}$$

Where [POC] = concentration of Particulate Organic Carbon in the test system (kg/kg or kg/L).

K_{oc} = organic carbon-water partition coefficient (kg/L)

For MCCPs, a representative K_{oc} value of 588 844 L/kg was used in EC (2005). This was an estimated value but was supported by two measured values of 103 846 L/kg for a C_{16}, 35% Cl wt. substance and 175 333 L/kg for a C_{16}, 69% Cl wt. substance (for further details see EC, 2005).

Assuming that the maximum POC concentration in the test was 3 mg/L, then the K_{oc} value of 588 844 L/kg would lead to an estimate for the minimum fraction dissolved of around 36% (this would increase as the assumed [POC] decreases below 3 mg/L; at a [POC] of 1 mg/L the fraction dissolved would be around 63%). The equivalent for the minimum fraction dissolved using the lower of the two measured K_{oc} values would be around 76% at a [POC] of 3 mg/L and 90% at a [POC] of 1 mg/L.

Overall, although the presence of POC and DOC can clearly influence the bioavailability of the test substance in these systems, there is currently insufficient information on their concentrations in the available tests to allow a reliable correction to be applied. Should the concentrations of POC and DOC have been significant in these tests then it is likely that the reported BCF will be underestimated when considered on a freely dissolved concentration basis. It should also be noted that any correction for adsorption onto POC or association with DOC is dependent on knowledge of the partitioning properties of the substance tested. In the correction applied in the Unpublished (2013) review, these partitioning properties are estimated directly from estimates of the log K_{OW}. This introduces further uncertainty into the interpretation of the data and the exact magnitude of the fraction dissolved.

Validity criteria for the quality of water used in any fish study (detailed in OECD TG 305) is routinely measured outside of studies as part of laboratory compliance. This is documented in the robust study summary supplied by the Registrant. POC and TOC concentrations in the blank flow-through water will be tightly controlled. This in-study single time point measurement cannot be taken as indicative of POC or TOC throughout the study. There will be short periods of time when an elevated DOC/POC concentration may be measured in test waters i.e. after feeding or prior to cleaning of waste. However, as a flow-through system was utilised, it is likely that this could be considered an aberrant result in the scale of the study. Therefore though the eMSCA do not disagree that there is a possibility that POC or TOC could influence the freely dissolved concentration MCCPs, there are also other factors that the above equation does not include (e.g. surface adsorption to the glass of the tanks may also cause reduction in the observed freely dissolved concentration). Daily determinations of the concentration of MCCP in the waters are documented in the robust study summary. The average concentration was calculated to be ~ 0.34 µg/L.

Appendix D: Summary of environmental monitoring data

The following tables outline the available environmental monitoring data for MCCPs in surface water, sediment and biota.

Table D1

SUMMARY OF LEVELS OF MCCPs IN SURFACE WATER AND SLUDGE				
Location	**Year/Comment**	**Units**	**Concentration**	**Reference**
Derwent Reservoir	1986	µg/L	1.46	ICI (1992)
River Trent, Newark	1986	µg/L	0.86	ICI (1992)
Trent Mersey Canal	1986	µg/L	0.62	ICI (1992)
River Derwent, Derby	1986	µg/L	0.64	ICI (1992)
Walton on Trent	1986	µg/L	1.07	ICI (1992)
River Ouse, Goole	1986	µg/L	0.94	ICI (1992)
River Don, Rotherham	1986	µg/L	1.13	ICI (1992)
River Aire/Ouse	1986	µg/L	1.13	ICI (1992)
River Ouse, York	1986	µg/L	1.36	ICI (1992)
River Cover, Wilton	1986	µg/L	0.84	ICI (1992)
River Ure, Mickley	1986	µg/L	1.46	ICI (1992)
River Trent, Gainsborough	1986	µg/L	2.49	ICI (1992)
River Trent, Burton	1986	µg/L	2.46	ICI (1992)
River Rother	1986	µg/L	2.11	ICI (1992)
River Trent, Humber	1986	µg/L	3.75	ICI (1992)
Hull Docks	1986	µg/L	2.69	ICI (1992)
River Lech at Augsburg	1987	µg/L		Ballschmiter (1984)
	1994	µg/L	<0.05	
River Lech at Gersthofen (upstream from a chlorinated paraffin production plant)	1987	µg/L	4.5	Ballschmiter (1984)
	1994	µg/L	0.094	
River Lech at langweid (downstream from a chlorinated paraffin production plant)	1987	µg/L	4	Ballschmiter (1984)
	1994	µg/L	0.185	
River Lech at Rain	1987	µg/L		Ballschmiter (1984)
	1994	µg/L	0.170	
River Danube at Marxheim (downstream from the mouth of the River Lech)	1987	µg/L	20	Ballschmiter (1984)
	1994	µg/L	0.072	
River Danube at Marxheim (upstream from the mouth of the River Lech)	1987	µg/L	4	Ballschmiter (1984)
	1994	µg/L	≤0.055	
Irish Sea: Site a	Relates to C_{10-20}	µg/L	1	Campbell and McConnell (1980)

SUMMARY OF LEVELS OF MCCPs IN SURFACE WATER AND SLUDGE				
Location	**Year/Comment**	**Units**	**Concentration**	**Reference**
Irish Sea: Site b	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
Irish Sea: Site c	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
Irish Sea: Site d	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
Irish Sea: Site e	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
Irish Sea: Site f	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
Barmouth Harbour	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
Menai Straights (Caernarvon)	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
Tremadoc Bay (Llandanwg)	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
North Minch: Ardmair	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
North Minch: Port Bùn á Ghlinne	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
North Minch: Port of Ness	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
Goile Chròic (Lewis)	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
Sound of Taransay (Harris)	Relates to C_{10-20}	µg/L	4.0	Campbell and McConnell (1980)
Sound of Arisaig	Relates to C_{10-20}	µg/L	1.0	Campbell and McConnell (1980)
North Sea: N55° 5.7' W1° 9.3'	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
North Sea: N57° 26.2' W1° 17.0'	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
North Sea: N57° 56.5' W1° 22.0'	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
River Banwy, Llangadfan	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
River Lea, Welwyn	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)

SUMMARY OF LEVELS OF MCCPs IN SURFACE WATER AND SLUDGE				
Location	**Year/Comment**	**Units**	**Concentration**	**Reference**
River Lea, Batford	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
River Clwyd, Ruthin	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
Bala Lake	Relates to C_{10-20}	µg/L	1.0	Campbell and McConnell (1980)
River Dee, Corwen	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
River Wnion, Merioneth	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
Firth of Lorne, Ganevan	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
Loch Linnhe, Corran Narrows	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
Firth of Clyde, Ashcraig	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
Firth of Clyde, Girvan	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
An Garbh Allt	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
Five drinking water reservoirs, Manchester area	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
River Aire, Leeds	Relates to C_{10-20}	µg/L	2.0	Campbell and McConnell (1980)
River Aire, Woodlesford	Relates to C_{10-20}	µg/L	2.0	Campbell and McConnell (1980)
River Ouse, Boothberry edge	Relates to C_{10-20}	µg/L	1 - 2	Campbell and McConnell (1980)
River Trent, West Bromwich	Relates to C_{10-20}	µg/L	1 - 2	Campbell and McConnell (1980)
River Trent, Walton-upon-Trent	Relates to C_{10-20}	µg/L	2 - 3	Campbell and McConnell (1980)
River Trent, Swarkestone	Relates to C_{10-20}	µg/L	1 - 2	Campbell and McConnell (1980)
River Trent, Newark	Relates to C_{10-20}	µg/L	4.0	Campbell and McConnell (1980)
River Trent, Gainsborough	Relates to C_{10-20}	µg/L	2.0	Campbell and McConnell (1980)
River Trent, confluence with Humber	Relates to C_{10-20}	µg/L	6.0	Campbell and McConnell (1980)

SUMMARY OF LEVELS OF MCCPs IN SURFACE WATER AND SLUDGE				
Location	**Year/Comment**	**Units**	**Concentration**	**Reference**
Humber Estuary, Hull	Relates to C_{10-20}	µg/L	1 - 2	Campbell and McConnell (1980)
Humber Estuary, Grimsby	Relates to C_{10-20}	µg/L	3.0	Campbell and McConnell (1980)
Mersey Estuary, New Brighton	Relates to C_{10-20}	µg/L	3.0	Campbell and McConnell (1980)
Mersey Estuary, Liverpool Pier Head	Relates to C_{10-20}	µg/L	4.0	Campbell and McConnell (1980)
River Thames, Oxford	Relates to C_{10-20}	µg/L	2.0	Campbell and McConnell (1980)
River Thames, Sanford	Relates to C_{10-20}	µg/L	1 - 2	Campbell and McConnell (1980)
Wyre Estuary	Relates to C_{10-20}	µg/L	not detected - 1.5	Campbell and McConnell (1980)
River Tees, Low Dinsdale	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
River Tees, North Gare breakwater	Relates to C_{10-20}	µg/L	0.5	Campbell and McConnell (1980)
River Tees, Middlesbrough	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
Sugar Creek, upstream of discharge		µg/L (particulate)	not detected	Murray *et al.* (1987a and 1987b)
Sugar Creek, just upstream of discharge		µg/L (particulate)	0.05 - 0.17	Murray *et al.* (1987a and 1987b)
Sugar Creek, just downstream of discharge		µg/L (particulate)	0.16 - 0.2	Murray *et al.* (1987a and 1987b)
Sugar Creek, downstream of discharge		µg/L (particulate)	0.20 - 0.24	Murray *et al.* (1987a and 1987b)
Upstream of sewage treatment plant, Germany		µg/L	not detected	Rieger and Ballschmiter (1985)
Downstream of sewage treatment plant, Germany		µg/L	not detected	Rieger and Ballschmiter (1985)
Tibutary, upstream of sewage treatment plant, Germany		µg/L	not detected	Rieger and Ballschmiter (1985)
Downstream of a chlorinated paraffin manufacturing plant, Canada		µg/L	<1	Tomy *et al.* (1998)

SUMMARY OF LEVELS OF MCCPs IN SURFACE WATER AND SLUDGE				
Location	**Year/Comment**	**Units**	**Concentration**	**Reference**
Surface water near to industrial sites, UK	1998	µg/L	<0.1	Cefas (1999)
Water samples from Norway	Two samples. Concentration refers to total (dissolved + particulate) in one sample. The concentrations present in the other sample was much lower (shown graphically only but was probably <0.1 µg/L.	µg/L	1.49	Petersen *et al.* (2006)
Filtered river water samples, Europe	8 Samples filtered using a membrane glass fibre filter before analysis	µg/L	<0.10	Coelhan (2009 & 2010)
Influent to waste water treatment plants, Europe	15 Samples. MCCPs detectable in 12 samples.	µg/L (particulate)	not detected – 4.6	Coelhan (2009 & 2010)
Effluent from waste water treatment plants, Norway	Samples from 8 waste water treatment plants (4 samples from each location). MCCPs detectable in 13% of samples analysed.	µg/L	not detected – 0.942	Thomas *et al.* (2011)
Dewatered sludge from waste water treatment plants, Norway	Samples from 8 waste water treatment plants (4 samples from each location). MCCPs detectable in all samples.	µg/kg	14 - 7 000 (median 385)	Thomas *et al.* (2011)
Snow (melted) from urban areas of Gothenburg, Sweden	8 Samples. MCCPs detectable in 2 samples (the concentrations may relate to SCCPs + MCCPs in the samples)	µg/L	0.33 - 32	Björklund *et al.* (2011)
Great Lakes Basin	Mean concentration based on an analysis of published studies	µg/L	9×10^{-7}	Klečka *et al.* (2010)
Storm water	Norway	µg/L	0.0685	Ruus *et al.* (2018)
Sludge	Norway average (minimum-maximum)	µg/kg	4 031 (120-17 000)	Norsk Vann (2018)
Sludge	Norway average (minimum-maximum)	µg/kg	3 964 (77-11 800)	Fjeld (2008)

Table D2

SUMMARY OF LEVELS OF MCCPs IN SEDIMENT Location	Year/ Comment	Units	Concentration	Reference
River Lech, upstream from chlorinated paraffin production plant	1987	µg/kg dry wt.	2200	Unpublished (1987)
	1994	µg/kg dry wt.	<10	Ballschmiter (1994)
River Lech, downstream from chlorinated paraffin production plant	1987	µg/kg dry wt.	1 700	Unpublished (1987) [reference no long attributable]
	1994	µg/kg dry wt.	325	Ballschmiter (1994)
Bodensee (middle) - 0 to 5 cm depth	1994	µg/kg dry wt.	70	Ballschmiter (1994)
River Rhein (141 km) at Rheinfelden	1994	µg/kg dry wt.	60	Ballschmiter (1994)
River Rhein (152 km) at Rheinfelden, upper layer	1994	µg/kg dry wt.	140	Ballschmiter (1994)
River Rhein (152 km) at Rheinfelden, lower layer	1994	µg/kg dry wt.	85	Ballschmiter (1994)
River Rhein (853.8 km), near German-Dutch border	1994	µg/kg dry wt.	205	Ballschmiter (1994)
River Rhein (863.8 km), near German-Dutch border	1994	µg/kg dry wt.	145	Ballschmiter (1994)
River Main (16.2 km)	1994	µg/kg dry wt.	260	Ballschmiter (1994)
River Main (at Griesheim)	1994	µg/kg dry wt.	190	Ballschmiter (1994)
River Main (55 km)	1994	µg/kg dry wt.	160	Ballschmiter (1994)
Outer Alster, Hamburg	1994	µg/kg dry wt.	370	Ballschmiter (1994)
River Elbe, Hamburg (610 km)	1994	µg/kg dry wt.	130	Ballschmiter (1994)
River Elbe, Hamburg (629.9 km)	1994	µg/kg dry wt.	230	Ballschmiter (1994)
River Danube, downstream of the confluence with the River Lech		µg/kg dry wt.	1800	BUA (1992)
Irish Sea: Site a	Relates to C_{10-20}	µg/kg	100	Campbell and McConnell (1980)

SUMMARY OF LEVELS OF MCCPs IN SEDIMENT				
Location	**Year/ Comment**	**Units**	**Concentration**	**Reference**
Irish Sea: Site b	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
Irish Sea: Site c	Relates to C_{10-20}	µg/kg	not measured	Campbell and McConnell (1980)
Irish Sea: Site d	Relates to C_{10-20}	µg/kg	100	Campbell and McConnell (1980)
Irish Sea: Site e	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
Irish Sea: Site f	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
Barmouth Harbour	Relates to C_{10-20}	µg/kg	500	Campbell and McConnell (1980)
Menai Straights (Caernarvon)	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
Tremadoc Bay (Llandanwg)	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
North Minch: Ardmair	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
North Minch: Port Bùn á Ghlinne	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
North Minch: Port of Ness	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
Goile Chròic (Lewis)	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
Sound of Taransay (Harris)	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
Sound of Arisaig	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
North Sea: N55° 5.7' W1° 9.3'	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
North Sea: N57° 26.2' W1° 17.0'	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
North Sea: N57° 56.5' W1° 22.0'	Relates to C_{10-20}	µg/kg	50	Campbell and McConnell (1980)
River Banwy, Llangadfan	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
River Lea, Batford	Relates to C_{10-20}	µg/kg	1 000	Campbell and McConnell (1980)

SUMMARY OF LEVELS OF MCCPs IN SEDIMENT				
Location	**Year/ Comment**	**Units**	**Concentration**	**Reference**
River Clwyd, Ruthin	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
River Dee, Corwen	Relates to C_{10-20}	µg/kg	300	Campbell and McConnell (1980)
River Wnion, Merioneth	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
Five drinking water reservoirs, Manchester area	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
River Aire, Leeds	Relates to C_{10-20}	µg/kg	10 000	Campbell and McConnell (1980)
River Ouse, Goole	Relates to C_{10-20}	µg/kg	2 000	Campbell and McConnell (1980)
River Trent, West Bromwich	Relates to C_{10-20}	µg/kg	6 000	Campbell and McConnell (1980)
River Trent, Walton-upon-Trent	Relates to C_{10-20}	µg/kg	1 000	Campbell and McConnell (1980)
River Trent, Swarkestone	Relates to C_{10-20}	µg/kg	14 000	Campbell and McConnell (1980)
River Trent, Newark	Relates to C_{10-20}	µg/kg	8 000	Campbell and McConnell (1980)
River Trent, Gainsborough	Relates to C_{10-20}	µg/kg	3 000	Campbell and McConnell (1980)
Humber Estuary, Hull	Relates to C_{10-20}	µg/kg	2 000	Campbell and McConnell (1980)
Humber Estuary, Stone Creek	Relates to C_{10-20}	µg/kg	2 000	Campbell and McConnell (1980)
Mersey Estuary, New Brighton	Relates to C_{10-20}	µg/kg	3 000	Campbell and McConnell (1980)
Mersey Estuary, Liverpool Pier Head	Relates to C_{10-20}	µg/kg	8 000	Campbell and McConnell (1980)
River Thames, Sanford	Relates to C_{10-20}	µg/kg	1 000	Campbell and McConnell (1980)
Wyre Estuary	Relates to C_{10-20}	µg/kg	not detected - 1 600	Campbell and McConnell (1980)
Mersey Estuary, 14 sediment samples	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
River Tees, Low Dinsdale	Relates to C_{10-20}	µg/kg	300	Campbell and McConnell (1980)

SUMMARY OF LEVELS OF MCCPs IN SEDIMENT				
Location	**Year/ Comment**	**Units**	**Concentration**	**Reference**
River Tees, North Gare breakwater	Relates to C_{10-20}	µg/kg	50	Campbell and McConnell (1980)
River Tees, Middlesbrough	Relates to C_{10-20}	µg/kg	15 000	Campbell and McConnell (1980)
Japan	1979 – no information on type	µg/kg	600 - 10 000	Environment Agency Japan (1991)
Japan	1980 – no information on type	µg/kg	500 - 8 500	Environment Agency Japan (1991)
Downstream of production site, US		µg/kg dry wt.	6.8 - 8.2	Murray *et al.* (1987a and 1987b)
Rotterdam harbour mud		µg/kg	7 - 10	Greenpeace (1995)
Hamburg harbour mud		µg/kg	8	Greenpeace (1995)
Mud flats, Kaiser Wilhelm Koog		µg/kg	98	Greenpeace (1995)
Mud flats, Den Helder		µg/kg	3	Greenpeace (1995)
St. Lawrence River, Canada, downstream of a chlorinated paraffin manufacturing plant		µg/kg dry wt.	<3 500	Tomy *et al.* (1998)
Industrial areas of the UK	A total of 77 samples from 1998. Highest concentration, downstream of a lubricant blending/metal working site.	µg/kg dry wt.	65 000	Cefas (1999)
Mersey and Seine estuaries	Mean levels of total chlorinated paraffins - predominantly LCCPs (only traces of MCCPs present)	µg/kg dry wt.	10.5	van Zeijl (1997)
Schelde estuary	Mean levels of total chlorinated paraffins - predominantly LCCPs (only traces of MCCPs present)	µg/kg dry wt.	5.5	van Zeijl (1997)
Liffey River estuary	Mean levels of total chlorinated paraffins - predominantly LCCPs (only traces of MCCPs present)	µg/kg dry wt.	4.8	van Zeijl (1997)

SUMMARY OF LEVELS OF MCCPs IN SEDIMENT				
Location	**Year/ Comment**	**Units**	**Concentration**	**Reference**
Forth estuary	Mean levels of total chlorinated paraffins - predominantly LCCPs (only traces of MCCPs present)	µg/kg dry wt.	3.3	van Zeijl (1997)
Humber estuary	Mean levels of total chlorinated paraffins - predominantly LCCPs (only traces of MCCPs present)	µg/kg dry wt.	1.2	van Zeijl (1997)
Sediment core, Lake St. Francois, St. Lawrence River	1972	µg/kg dry wt.	1 200	Muir *et al.* (2002)
Sediment core, Lake St. Francois, St. Lawrence River	1976	µg/kg dry wt.	1 000	Muir *et al.* (2002)
Sediment core, Lake St. Francois, St. Lawrence River	1981	µg/kg dry wt.	700	Muir *et al.* (2002)
Sediment core, Lake St. Francois, St. Lawrence River	1986	µg/kg dry wt.	750	Muir *et al.* (2002)
Sediment core, Lake St. Francois, St. Lawrence River	1990	µg/kg dry wt.	400	Muir *et al.* (2002)
Sediment core, Lake St. Francois, St. Lawrence River	1995	µg/kg dry wt.	700	Muir *et al.* (2002)
Lake Zürich		µg/kg	5	Schmid and Müller (1985)
Close to chlorinated paraffin manufacturing site, Australia	Sample I	µg/kg dry weight	1 108	Kemmlein *et al.* (2002)
Close to chlorinated paraffin manufacturing site, Australia	Sample II	µg/kg dry weight	1 168	Kemmlein *et al.* (2002)
Close to chlorinated paraffin manufacturing site, Australia	Sample II	µg/kg dry weight	3 108	Kemmlein *et al.* (2002)

SUMMARY OF LEVELS OF MCCPs IN SEDIMENT				
Location	**Year/ Comment**	**Units**	**Concentration**	**Reference**
Close to chlorinated paraffin manufacturing site, Australia	Sample IV	µg/kg dry weight	16 403	Kemmlein *et al.* (2002)
Lake Thun, Switzerland	Sediment core, surface layer corresponding to around 2004	µg/kg dry weight	26	Iozza *et al.* (2008)
Czech Republic	Highest concentration	µg/kg	5 575	Pribylová *et al.* (2006)
North and Baltic Sea	Sample 1 (relates to C_{14-15} chlorinated paraffins)	µg/kg dry weight	87	Hüttig and Oehme, (2006)
North and Baltic Sea	Sample 2 (MCCP relates to C_{14-15} chlorinated paraffins)	µg/kg dry weight	48	Hüttig and Oehme, (2006)
North and Baltic Sea	Sample 3 (MCCP relates to C_{14-15} chlorinated paraffins)	µg/kg dry weight	34	Hüttig and Oehme, (2006)
North and Baltic Sea	Sample 4 (MCCP relates to C_{14-15}chlorinated paraffins)	µg/kg dry weight	149	Hüttig and Oehme, (2006)
North and Baltic Sea	Sample 5 (MCCP relates to C_{14-15}chlorinated paraffins)	µg/kg dry weight	23	Hüttig and Oehme, (2006)
North and Baltic Sea	Sample 6 (MCCP relates to C_{14-15}chlorinated paraffins)	µg/kg dry weight	43	Hüttig and Oehme, (2006)
North and Baltic Sea	Sample 7 (MCCP relates to C_{14-15}chlorinated paraffins)	µg/kg dry weight	85	Hüttig and Oehme, (2006)
North and Baltic Sea	Sample 8 (MCCP relates to C_{14-15}chlorinated paraffins)	µg/kg dry weight	72	Hüttig and Oehme, (2006)
North and Baltic Sea	Sample 9 (MCCP relates to C_{14-15}chlorinated paraffins)	µg/kg dry weight	39	Hüttig and Oehme, (2006)
North and Baltic Sea	Sample 10 (MCCP relates to C_{14-15}chlorinated paraffins)	µg/kg dry weight	22	Hüttig and Oehme, (2006)
North and Baltic Sea	Sample 11 (MCCP relates to C_{14-15}chlorinated paraffins)	µg/kg dry weight	33	Hüttig and Oehme, (2006)

SUMMARY OF LEVELS OF MCCPs IN SEDIMENT				
Location	**Year/ Comment**	**Units**	**Concentration**	**Reference**
North and Baltic Sea	Highest concentration - relates to SCCP+MCCP (MCCP/SCCP ratio 1.7 - 2.4)	µg/kg dry weight	499	Hüttig and Oehme, (2005)
Firth of Clyde, Scotland	MCCPs detected but not quantified		detected	Hussy *et al.* (2012)
Sediments from Norway	Twenty sediments analysed	µg/kg dry weight	50 - 3 240	Petersen *et al.* (2006)
Pearl River Delta, South China	Range	µg/kg dry weight	880 to 38 000	Chen *et al.* (2011)
Pearl River Delta, South China. Pond sediments in the vicinity of an electronic waste recycling area	Mean	µg/kg dry weight	21 000	Chen *et al.* (2011)
Pearl River Delta, South China. River sediments from industrialised areas.	Mean	µg/kg dry weight	3 900	Chen *et al.* (2011)
Yellow River, China	2018 (mean, normal season)	ng/g	35	Li *et al.* (2018)
Yellow River, China	2018 (mean, wet season)	ng/g	89	Li *et al.* (2018)
Yellow River, China	2018 (mean, dry season)	ng/g	167	Li *et al.* (2018)
Yellow River, China	2016	ng/g dw	44.81538462	Qiao *et al.* (2016)
Pearl River Delta, China	2017	ng/g dw	102 - 6650	Zeng *et al.* (2017)
Shenzhen, China	2017	ng/g dw	10.9 - 2500	Zeng *et al.* (2017)
Hong Kong, China	2017	ng/g dw	<LOD - 286	Zeng *et al.* (2017)
Tokyo Bay. Japan	2017	ng/g dw	3.2 - 56.8	Zeng *et al.* (2017)
Laizhou Bay, China	2009	ng/g dw	6 - 63	Pan *et al.* (2018)
Rivers around Laizhou Bay, China	2009	ng/g dw	1.8 - 3200	Pan *et al.* (2018)
Inner Oslofjord, Norway	2017	mg/kg dw	0.14	Ruus *et al.* (2018)
Oslo, Norway	Soil	ng/g dw	Mean = 183 Median = 193 Minimum = 57 Maximum = 282	Heimstad *et al.* (2017)

SUMMARY OF LEVELS OF MCCPs IN SEDIMENT				
Location	**Year/ Comment**	**Units**	**Concentration**	**Reference**
Chongming Island, China	Soil	ng/g	Minimum = 2.56 Maximum = 96.3 Median = 7.32	Sun *et al.* (2013).
Jiaojiang River, China	Soil samples within 5 km of the e-waste dismantling centres	ng/g dw	507 to 4.40×10^6	Xu *et al.* (2019)
Jiaojiang River, China	Sediment samples from the surrounding area	ng/g dw	$271 - 2.72 \times 10^4$	Xu *et al.* (2019)
Yangtze River, China	Sediments from the middle reaches of the Yangtze River	ng/g dw	Not detected to 14.6 ng/g dw	Qiao *et al.* (2017)
Yellow River, China	Sediment samples from the middle reaches of the Yellow River	ng/g dw	20.5 – 93.7	Xia *et al.* (2016)
Pearl River Delta, South China	Soil	ng/g	Minimum = 1.95 Maximum = 188 Median = 7.98	Wang *et al.* (2014)
Switzerland	Soil	ng/g	5.1 – 160	Bogdal *et al.* (2015)
China	Core soils from Chinese nation-wide agricultural lands	ng/g dw	127 – 1969	Aamir *et al.* (2019)
Dongjiang River, China	Top soils (0−5 cm) at 60 sites	ng/g	59.3	Wang *et al.* (2013)
China	In-plant coniferous leaves and soil, 2016 (average)	ng/g dry weight	3481.8	Xu *et al.* (2016)
Shanghai, China	Suburb soils, 2017	ng/g dry weight	ND – 666	Wang *et al.* (2017)
Australia (Sewage sludge)	2017	ng/g dry weight	542 - 3645	Brandsma *et al.* (2017)
Effluent water	Bekkelaget STP, Norway	µg/L	0.08	Ruus *et al.* (2018)
Sludge	Bekkelaget STP, Norway	ng/g dry weight	2470-2500	Ruus *et al*. (2018)

Table D3

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
Mussel	United Kingdom	Mean concentration – relates to C_{10-20}	µg/kg	3 250	Campbell and McConnell (1980)
Plaice *Pleuronectes platessa*	United Kingdom	Mean concentration – relates to C_{10-20}	µg/kg	30	Campbell and McConnell (1980)
Pouting *Trisopterus luscus*	United Kingdom	Mean concentration – relates to C_{10-20}	µg/kg	100	Campbell and McConnell (1980)
Pike *Esox lucius*	United Kingdom	Mean concentration – relates to C_{10-20}	µg/kg	25	Campbell and McConnell (1980)
Grey Seal *Halichoerus grypus*	United Kingdom	Mean concentration – relates to C_{10-20}	µg/kg	75 (liver and blubber)	Campbell and McConnell (1980)
Grey Heron *Ardea cinerea*	United Kingdom	Relates to C_{10-20}	µg/kg	100 - 1 200 (liver)	Campbell and McConnell (1980)
Common Guillemot *Uria aalge*	United Kingdom	Relates to C_{10-20}	µg/kg	100 - 1 100 (liver)	Campbell and McConnell (1980)
Herring Gull *Larus argentatus*	United Kingdom	Relates to C_{10-20}	µg/kg	200 – 900 (liver)	Campbell and McConnell (1980)
Seabirds' eggs	United Kingdom	Relates to C_{10-20}	µg/kg	up to 2 000	Campbell and McConnell (1980
Dairy products	United Kingdom	Mean concentration – relates to C_{10-20}	µg/kg	300	Campbell and McConnell (1980)
Vegetable oils and derivatives	United Kingdom	Mean concentration – relates to C_{10-20}	µg/kg	150	Campbell and McConnell (1980)
Fruit and vegetables	United Kingdom	Mean concentration – relates to C_{10-20}	µg/kg	5	Campbell and McConnell (1980)
Beverages	United Kingdom	Mean concentration – relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
Domestic Sheep *Ovis aries*	United Kingdom, remote from industry	Relates to C_{10-20}	µg/kg	not detected in liver, brain kidney, mesenteric fat	Campbell and McConnell (1980)
	United Kingdom, close to chlorinated paraffin production site			200 (liver); 50 (mesenteric fat); 50 (kidney); not detected in heart, lung or perinephritic fat	
Mussel	Upstream of chlorinated paraffin manufacturing plant		µg/kg	<7	Murray *et al*. (1987a)
	Downstream of chlorinated paraffin manufacturing plant			170	
Mackerel			µg/kg lipid	46	Greenpeace (1995)
Herring oil			µg/kg lipid	12	Greenpeace (1995)
Margarine containing fish oil			µg/kg lipid	28	Greenpeace (1995)
Common Porpoise *Phocoena phocoena*			µg/kg lipid	3 - 7	Greenpeace (1995)
Fin Whale *Balaenoptera physalus*			µg/kg lipid	144	Greenpeace (1995)
Pork			µg/kg lipid	11	Greenpeace (1995)
Cow's milk			µg/kg lipid	16	Greenpeace (1995)
Rabbit *Oryctolagus cuniculus*	Revingehed, Skåne, Sweden 1986	Unspecified chain length, with 6-16 chlorine atoms/molecule	µg/kg lipid	2 900 (muscle)	Jansson *et al.* (1993)

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
Moose *Alces alces*	Grimsö, Västtmanland, Sweden 1985 - 86	Unspecified chain length, with 6-16 chlorine atoms/molecule	µg/kg lipid	4 400 (muscle)	Jansson *et al.* (1993)
Reindeer *Rangifer tarandus*	Ottsjö, Jämtland, Sweden 1986	Unspecified chain length, with 6-16 chlorine atoms/molecule	µg/kg lipid	140 (suet)	Jansson *et al.* (1993)
Osprey *Pandion haliaetus*	Sweden, 1982 - 1986	Unspecified chain length, with 6-16 chlorine atoms/molecule	µg/kg lipid	530 (muscle)	Jansson *et al.* (1993)
Arctic Char *Salvelinus alpinus*	Lake Vättern, Central Sweden, 1987	Unspecified chain length, with 6-16 chlorine atoms/molecule	µg/kg lipid	570 (muscle)	Jansson *et al*. (1993)
Whitefish *Coregonus sp.*	Lake Storvindeln, Lapland, 1986	Unspecified chain length, with 6-16 chlorine atoms/molecule	µg/kg lipid	1 000 (muscle)	Jansson *et al*. (1993)
	Bothnian Sea, Sweden 1986			1 400 (muscle)	
Herring *Clupea harengus*	Baltic proper, Sweden 1987	Unspecified chain length, with 6-16 chlorine atoms/molecule	µg/kg lipid	1 500 (muscle)	Jansson *et al*. (1993)
	Skagerrak, Sweden 1987			1 600 (muscle)	
Ringed Seal *Pusa hispida*	Kongsfjorden, Svalbard 1981	Unspecified chain length, with 6-16 chlorine atoms/molecule	µg/kg lipid	130 (blubber)	Jansson *et al*. (1993)
Grey Seal *Halichoerus grypus*	Baltic Sea, Sweden 1979 - 85	Unspecified chain length, with 6-16 chlorine atoms/molecule	µg/kg lipid	280 (blubber)	Jansson *et al*. (1993)

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
Benthos	Industrial areas of the United Kingdom 1998	Highest concentration - tentatively identified as MCCPs	µg/kg	800	Cefas (1999)
Fish	Industrial areas of the United Kingdom 1998	Highest concentration - tentatively identified as MCCPs	µg/kg	2 800 (pike liver)	Cefas (1999)
Human milk			µg/kg lipid	7	Greenpeace (1995)
Human milk	Lancaster and London, UK	Highest concentration	µg/kg lipid	61	Thomas and Jones (2002)
Human milk	Lancaster and London, UK	95th percentile	µg/kg lipid	127.5	Thomas *et a*l. (2003)
Human milk	Bavaria	60 Samples. MCCPs detected in 58% of the samples. Range reflects the quantified levels.	µg/kg lipid	9.6 - 903 [median 115.4]	Hilger *et al*. (2011b)
Human milk	China	2007 (median value)	µg/kg lipid weight	60.4	Xia *et al*. (2017)
Human milk	China	2011 (median value)	µg/kg lipid weight	64.3	Xia *et al*. (2017)
Human blood	China	2017	µg/kg lipid weight	130 - 3200	Li *et al*. (2017)
Human placenta	China	2018	µg/kg lipid weight	80.8 - 954	Wang *et al*. (2018)
Cows' milk	Lancaster, UK		µg/kg lipid	63	Thomas and Jones (2002)
Butter	Denmark Wales Ireland		µg/kg lipid	11 8.8 52	Thomas and Jones (2002)
Beluga Whale *Delphinapterus leucas*	St. Lawrence River, Canada	Blubber samples from 15 females	µg/kg ww	79 000 (max.)	Bennie *et al.* (2000)
		Blubber samples from 10 males		80 000 (max.)	
		Liver samples from 3 females		20 900 (max.)	

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
		Liver samples from 3 males		5 820 (max.)	
Carp	Lake Ontario, Canada	Whole body homogenates from 3 individuals	µg/kg ww	563 (max.)	Bennie *et al.* (2000)
Trout	Lake Ontario, Canada	Whole body homogenates from 10 individuals	µg/kg ww	4 390 (max.)	Bennie *et al.* (2000)
Mussel	Close to a chlorinated paraffin manufacturing plant in Australia		µg/kg lipid	23 200	Kemmlein *et al.* (2002)
Crabs	Close to a chlorinated paraffin manufacturing plant in Australia		µg/kg lipid	30 500	Kemmlein *et al.* (2002)
Lake Trout *Salvelinus namaycush*	Lake Ontario	Archived samples from 1998	µg/kg	25	Ismail *et al.* (2009)
		Archived samples from 2004		8	
Diporeia	Lake Ontario	Mean concentration, 2001	µg/kg	12	Muir *et al.* (2002)
Rainbow Smelt *Osmerus mordax*	Lake Ontario	Mean concentration, 2001	µg/kg	109	Muir *et al.* (2002)
Slimy Sculpin *Cottus cognatus*	Lake Ontario	Mean concentration, 2001	µg/kg	108	Muir *et al.* (2002)
Alewife *Alosa pseudoharengus*	Lake Ontario	Mean concentration, 2001	µg/kg	35	Muir *et al.* (2002)
Lake Trout *Salvelinus namaycush*	Lake Ontario	Mean concentration, 2001	µg/kg	15	Muir *et al.* (2002)
Plankton	Lake Ontario	Mean concentration, 1999 - 2004	µg/kg	not detected	Houde *et al.* (2008)
	Lake Michigan			not detected	

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
Diporeia	Lake Ontario Lake Michigan	Mean concentration, 1999 - 2004	µg/kg	4.2 not detected	Houde *et al.* (2008)
Mysis	Lake Ontario Lake Michigan	Mean concentration, 1999 - 2004	µg/kg	not detected not detected	Houde *et al.* (2008)
Rainbow Smelt *Osmerus mordax*	Lake Ontario Lake Michigan	Mean concentration, 1999 - 2004	µg/kg	109 not detected	Houde *et al.* (2008)
Slimy Sculpin *Cottus cognatus*	Lake Ontario Lake Michigan	Mean concentration, 1999 - 2004	µg/kg	108 2.9	Houde *et al.* (2008)
Alewife *Alosa pseudoharengus*	Lake Ontario Lake Michigan	Mean concentration, 1999 - 2004	µg/kg	35 5.6	Houde *et al.* (2008)
Lake Trout *Salvelinus namaycush*	Lake Ontario Lake Michigan	Mean concentration, 1999 - 2004	µg/kg	24 5.6	Houde *et al.* (2008)
Dab, cod and flounder	North and Baltic Sea	Highest	µg/kg	260 (liver)	Reth *et al*. (2005)
Atlantic Cod *Gadus morhua*	Iceland and Norway	Highest concentration	µg/kg	47 (liver)	Reth *et al.* (2006)
Arctic Char *Salvelinus alpinus*	Bear Island	Highest concentration	µg/kg	43 (liver) 47 (muscle)	Reth *et al.* (2006)
Little Auk *Alle alle*	Bear Island	Highest concentration	µg/kg	370 (liver) 55 (muscle)	Reth *et al.* (2006)
Black-legged Kittiwake *Rissa tridactyla*	Bear Island	Highest concentration	µg/kg	39 (liver) 38 (muscle)	Reth *et al.* (2006)
Spruce needles	The Alps	Eight samples collected in October 2004. Concentrations refer to MCCPs.	µg/kg	5.2 - 95	Iozza *et al.* (2009a)

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
Spruce needles	The Alps	Samples from various altitudes from 7 locations collected in Autumn 2004. Concentrations refer to total chlorinated paraffins	µg/kg	26 - 450	Iozza *et al.* (2009b)
Masson pine needles	Shanghai, China	2016	µg/kg	12.4 – 33 500	Wang *et al.* (2016)
"Biota"	Great Lakes Basin	Mean concentration based on an analysis of published studies	µg/kg	21	Klečka *et al.* (2010)
Porpoises	South China Sea	2004 - 2014	µg/kg dry weight	320 – 8 600	Zeng *et al.* (2015)
Dolphins	South China Sea	2004 - 2014	µg/kg dry weight	530 – 23 000	Zeng *et al.* (2015)
Bastard halibut	Liaodong Bay, North China	2017	µg/kg lipid weight	706.5 ± 240.2	Huang *et al.* (2017)
Turbot	Liaodong Bay, North China	2017	µg/kg lipid weight	5 097 ± 2 242	Huang *et al.* (2017)
Ray	Liaodong Bay, North China	2017	µg/kg lipid weight	109.0 ± 44.6	Huang *et al.* (2017)
Navodon septentrionalis	Liaodong Bay, North China	2017	µg/kg lipid weight	375.9 ± 120.2	Huang *et al.* (2017)
Yellow croaker	Liaodong Bay, North China	2017	µg/kg lipid weight	55.19 ± 23.73	Huang *et al.* (2017)
Bass	Liaodong Bay, North China	2017	µg/kg lipid weight	24.57 ± 10.31	Huang *et al.* (2017)
Capelin	Liaodong Bay, North China	2017	µg/kg lipid weight	30.26 ± 11.49	Huang *et al.* (2017)
Spanish Mackerel	Liaodong Bay, North China	2017	µg/kg lipid weight	53.92 ± 22.64	Huang *et al.* (2017)
Abalone	Liaodong Bay, North China	2017	µg/kg lipid weight	63.48 ± 24.75	Huang *et al.* (2017)

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
Cod	Liaodong Bay, North China	2017	µg/kg lipid weight	22.37 ± 9.17	Huang *et al.* (2017)
	Chéran River (mean)	2019	µg/kg lipid weight	7 123	
	Usses River (mean)	2019	µg/kg lipid weight	4 615	
Common Barbel *Barbus barbus*	Combeauté River (mean)	2019	µg/kg lipid weight	5 423	Labadie *et al.* (2019)
	Rhône River (mean)	2019	µg/kg lipid weight	904	
	Morge Canal (mean)	2019	µg/kg lipid weight	3 292	
Earthworms	Oslo, Norway	2017	µg/kg ww	Mean: 37 Median: 39 Minimum: 25 Maximum: 46	Heimstad *et al.* (2017)
Fieldfare *Turdus pilaris*	Oslo, Norway	2017, eggs	µg/kg ww	Mean: 21 Median: 7.35 Minimum: 4.70 Maximum: 135	Heimstad *et al.* (2017)
Eurasian Sparrowhawk *Accipter nisus*	Oslo, Norway	2017, eggs	µg/kg ww	Mean: 12.2 Median: <LOD Minimum: <LOD Maximum: 74.0	Heimstad *et al.* (2017)
Tawny Owl *Strix aluco*	Oslo, Norway	2017, eggs	µg/kg ww	Mean: <LOD Median: <LOD Minimum: <LOD Maximum: <LOD	Heimstad *et al.* (2017)
Rat *Rattus norvegicus*	Oslo, Norway	2017, liver	µg/kg ww	Mean: 183 Median: 177 Minimum: 81.0 Maximum: 327	Heimstad *et al.* (2017)

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
Red Fox *Vulpes vulpes*	Oslo, Norway	2017, liver	µg/kg ww	Mean: 68.1 Median: 61 Minimum: 23 Maximum: 130	Heimstad *et al.* (2017)
Badger *Meles meles*	Oslo, Norway	2017, liver	µg/kg ww	Mean: 43 Median: 41 Minimum: 37 Maximum: 51	Heimstad *et al.* (2017)
Blue Mussel *Mytilus edulis*	Gressholmen, Inner Oslofjord, Norway	2017	µg/kg ww	Median: 11.9	Green *et al.* (2018)
	Færder, Outer Oslofjord, Norway	2017	µg/kg ww	Median: 9.89	
	Singlekalven, Hvaler, Norway	2017	µg/kg ww	Median: 5.82	
	Bjørkøya, Langesundfjord, Norway	2017	µg/kg ww	Median: 22.7	
	Sylterøya, Langesundfjord, Norway	2017	µg/kg ww	Median: 10.5	
	Nordnes, Bergen harbour, Norway	2017	µg/kg ww	Median: 44.9	
	Vågsvåg, Outer Nordfjord, Norway	2017	µg/kg ww	Median: 27.3	
	Ålesund harbour, Norway	2017	µg/kg ww	Median: 41.6	
	Ørland area, Outer Trondheimsfjord, Norway	2017	µg/kg ww	Median: 4.46	
	Bodø harbour, Norway	2017	µg/kg ww	Median: 52.4	
	Mjelle, Bodø area, Norway	2017	µg/kg ww	Median: 17.3	
	Svolvær airport area, Norway	2017	µg/kg ww	Median: 22.2	
Atlantic Cod	Inner Oslofjord, Norway	2017, liver	µg/kg ww	Median: 498.0	

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
Gadus morhua	Tjøme, Outer Oslofjord, Norway	2017, liver	µg/kg ww	Median: 35.15	Green *et al.* (2018)
	Kirkøy, Hvaler, Norway	2017, liver	µg/kg ww	Median: 77.2	
	Stathelle area, Langesundfjord, Norway	2017, liver	µg/kg ww	Median: 143.0	
	Kristiansand harbour area, Norway	2017, liver	µg/kg ww	Median: 226.5	
	Inner Sørfjord, Norway	2017, liver	µg/kg ww	Median: 100.0	
	Bømlo, Outer Selbjørnfjord, Norway	2017, liver	µg/kg ww	Median: 74.6	
	Bergen harbour area, Norway	2017, liver	µg/kg ww	Median: 310.0	
	Ålesund harbour area, Norway	2017, liver	µg/kg ww	Median: 842.0	
	Trondheim harbour, Norway	2017, liver	µg/kg ww	Median: 102.0	
	Austnesfjord, Lofoten, Norway	2017, liver	µg/kg ww	Median: 71.6	
	Tromsø harbour area, Norway	2017, liver	µg/kg ww	Median: 123.0	
	Isfjorden, Svalbard, Norway	2017, liver	µg/kg ww	Median: 35.4	
Common Eider *Somateria mollissima*	Breøyane, Kongsfjorden, Svalbard, Norway	2017	µg/kg ww	Median: 2.5 (blood) Median: 8.6 (egg)	Green *et al.* (2018)
Cereal	19 Chinese provinces	1710 cereal samples giving 19 pooled samples	µg/kg ww	Mean: 213	Wang *et al.* (2019)
Legume	19 Chinese provinces	1710 legume samples giving 19 pooled samples	µg/kg ww	Mean: 184	Wang *et al.* (2019)
Herring *Clupea harengus*	Scandinavia	2011, female 4–6 years, muscle	µg/kg lipid	44	Yuan *et al.* (2019)
		2014, female 4–5 years, muscle	µg/kg lipid	30	
		2017, female 3–5 years, muscle	µg/kg lipid	51	

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
		2014, female and male 7 – 13 years, liver	µg/kg lipid	140	
		2014 female and male, 7–13 years, muscle	µg/kg lipid	120	
		2016 female and male, 6 – 12 years, liver	µg/kg lipid	170	
		2016, female and male 6 – 12 years, muscle	µg/kg lipid	140	
		2015, female adults, liver	µg/kg lipid	440	
Common Eider *Somateria mollissima*	Scandinavia	2015, egg	µg/kg lipid	140-200	Yuan *et al.* (2019)
		2015, female adults, liver	µg/kg lipid	290	
Common Guillemot *Uria aalge*	Scandinavia	2016, egg	µg/kg lipid	58-67	Yuan *et al.* (2019)
White-tailed Sea-eagle *Haliaeetus albicilla*	Scandinavia	2015, egg	µg/kg lipid	140-250	Yuan *et al.* (2019)
Grey Seal *Halichoerus grypus*	Scandinavia	2006 – 2008, males juveniles (0 – 1 year)	µg/kg lipid	210 (liver) 83 (blubber)	Yuan *et al.* (2019)
		2009 – 2010, males adults (8 – 11 year)	µg/kg lipid	230 (liver) 32 (blubber)	
		2014 – 2015, juveniles	µg/kg lipid	540 (liver)	
		2014 – 2015, juveniles, blubber	µg/kg lipid	100	
Harbour Seal *Phoca vitulina*	Scandinavia	2012 – 2016, adults	µg/kg lipid	230 (liver) 64 (blubber)	Yuan *et al.* (2019)
Harbour Porpoise	Scandinavia	2006 – 2012, 3 females and 1 male adults, liver	µg/kg lipid	140 (liver)	Yuan *et al.* (2019)
		2006 – 2012, 3 females and 1 male adults	µg/kg lipid	36 (blubber)	

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
Phocoena phocoena		2008, 1 female and 1 male adults	µg/kg lipid	440 (liver)	
			µg/kg lipid	59 (blubber)	
Moose *Alces alces*	Scandinavia	2012 – 2015, female and male adults, muscle	µg/kg lipid	1 600	Yuan *et al.* (2019)
Bank Vole *Myodes glareolus*	Scandinavia	2014, female and male adults, muscle	µg/kg lipid	370	Yuan *et al.* (2019)
Eurasian Lynx *Lynx lynx*	Scandinavia	2012 – 2016 female and male adults, muscle	µg/kg lipid	750	Yuan *et al.* (2019)
Grey Wolf *Canis lupus*	Scandinavia	2012 – 2016 female and male adults, muscle	µg/kg lipid	830	Yuan *et al.* (2019)
Starling *Sturnus vulgaris*	Scandinavia	2012 – 2015, female and male fledglings, muscle	µg/kg lipid	310	Yuan *et al.* (2019)
Common Kestrel *Falco tinnunculus*	Scandinavia	2014, egg	µg/kg lipid	85	Yuan *et al.* (2019)
Tawny Owl *Strix aluco*	Scandinavia	2014, egg	µg/kg lipid	87	Yuan *et al.* (2019)
Eagle Owl *Bubo bubo*	Scandinavia	2013 – 2017, female and male adults, muscle	µg/kg lipid	720	Yuan *et al.* (2019)
Marsh Harrier *Circus aeruginosus*	Scandinavia	2012 – 2015 female and male adults, muscle	µg/kg lipid	180	Yuan *et al.* (2019)
Golden Eagle *Aquila chrysaetos*	Scandinavia	2012 – 2016 female and male adults, muscle	µg/kg lipid	360	Yuan *et al.* (2019)
Peregrine Falcon *Falco peregrinus*	Scandinavia	2012 – 2016 female and male adults, muscle	µg/kg lipid	410	Yuan *et al.* (2019)
Salmon	Southern Germany	2014 - 2017, 122 farmed and 11 wild salmon samples	µg/kg ww	1.1 - 79	Krätschmer *et al.* (2019)
Pond Loach *Misgurnus anguillicaudatus*	Paddy fields in the Yangtze River Delta, China	Median (min-max)	µg/kg lw	2 500 (1 400 – 2 600)	Du *et al.* (2018)
			µg/kg dw	270 (170 – 430)	
Rice Field Eel *Monopterus albus*	Paddy fields in the Yangtze River Delta, China	Median (min-max)	µg/kg lw	2 600 (820 – 3 700)	Du *et al.* (2018)
			µg/kg dw	140 (50 – 270)	

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
Red-backed Rat Snake *Elaphe rufodorsata*	Paddy fields in the Yangtze River Delta, China	Median (min-max)	µg/kg lw µg/kg dw	3 800 (2 100 – 7 900) 170 (100 – 330)	Du *et al.* (2018)
Red-banded Snake *Dinodon rufozonatum*	Paddy fields in the Yangtze River Delta, China	Median (min-max)	µg/kg lw µg/kg dw	13 000 570	Du *et al.* (2018)
Short-tailed Mamushi *Gloydius brevicaudus*	Paddy fields in the Yangtze River Delta, China	Median (min-max)	µg/kg lw µg/kg dw	17 000 (7 400 – 19 000) 990 (450 – 1 300)	Du *et al.* (2018)
Yellow Weasel *Mustela sibirica*	Paddy fields in the Yangtze River Delta, China	Median (min-max)	µg/kg lw µg/kg dw	12 000 (6 700 – 33 000) 990 (640 – 2 900)	Du *et al.* (2018)
Peregrine Falcon *Falco peregrinus*	Paddy fields in the Yangtze River Delta, China	Median (min-max)	µg/kg lw µg/kg dw	2 100 (1 300 – 29 000) 260 (190 – 4 700)	Du *et al.* (2018)
Collared Scops-owl *Otus lettia*	Paddy fields in the Yangtze River Delta, China	Median (min-max)	µg/kg lw µg/kg dw	270 (96 – 440) 74 (39 – 110)	Du *et al.* (2018)
Common Cuckoo *Cuculus canorus*	Paddy fields in the Yangtze River Delta, China	Median (min-max)	µg/kg lw µg/kg dw	200 (<170 – 1 400) 25 (<12 – 92)	Du *et al.* (2018)
Fish (no further information provided)	Bohai Bay, China	Range	µg/kg dw	42.1 – 5 307	Xia *et al.* (2016)
Polychaetes	Inner Oslofjord	3 pooled samples (whole individuals)	µg/kg ww	Average: 12	Ruus *et al.* (2018)
Blue Mussel *Mytilus edulis*	Inner Oslofjord	3 pooled samples (soft tissue)	µg/kg ww	Average: 10	Ruus *et al.* (2018)
Krill *Euphausiacea*	Inner Oslofjord	3 pooled samples (whole individuals)	µg/kg ww	60	Ruus *et al.* (2018)
Prawn *Pandalus borealis*	Inner Oslofjord	3 pooled samples (tail soft tissue)	µg/kg ww	2	Ruus *et al.* (2018)
Herring *Clupea harengus*	Inner Oslofjord	3 pooled samples (muscle)	µg/kg ww	Average: 17	Ruus *et al.* (2018)

SUMMARY OF LEVELS OF MCCPs IN BIOTA (and some foodstuffs)					
Sample	**Location**	**Comment**	**Units**	**Level**	**Reference**
Atlantic Cod *Gadus morhua*	Inner Oslofjord	Liver (detected in all 15 samples)	µg/kg ww	Arithmetic mean 216 (range: 51-1050)	Ruus *et al*. (2018)
	Inner Oslofjord	Blood (detected in all 15 samples)	µg/kg ww	Arithmetic mean 28.23 (range: 8.2-76)	Ruus *et al*. (2018)
	Outer Oslofjord	Blood (detected in all 15 samples)	µg/kg ww	Arithmetic mean 38.87 (range: 5.8-200)	Ruus *et al*. (2018)
Herring Gull *Larus argentatus*	Inner Oslofjord	Egg (detected in all 15 samples)	µg/kg ww	Arithmetic mean 29.14 (range: 6.1-68)	Ruus *et al*. (2018)
	Outer Oslofjord	Egg (detected in all 15 samples)	µg/kg ww	Arithmetic mean 69.58 (range: 3.1-630)	Ruus *et al*. (2018)

Table D4

SUMMARY OF LEVELS OF MCCP$_S$ IN AIR				
Location	**Comment**	**Units**	**Concentration**	**Reference**
Dongjiang River, China	Air samples	µg/sampler	4.1	Wang *et al.* (2013)
	Atmospheric depositions (wet and dry) at 11 sites	µg/(m^{2}d)	5.3	
Shergyla Mountain and Lhasa (Tibetan Plateau)	Air samples	pg/m^3	50 – 690 800 – 6 700	Wu *et al.* (2019)
Georgia King Island, Fildes Peninsula of Antarctica (Great Wall Station)	Air samples	pg/m^3	3.7 – 5.2 (average: 4.5)	Ma *et al.* (2014)
India	Air samples (average)	ng/m^3	3.62	Chaemfa *et al.* (2014)
Pakistan	Air samples (average)	ng/m^3	4.21	Chaemfa *et al.* (2014)
Shenzhen, Guangzhou Province, China	Air samples (28 samples collected over 4 seasons, September 2013 to August 2014)	ng/m^3	0.70–12.2	Li *et al.* (2018)

Appendix E: Biodegradability of Chlorinated n-alkanes C_{10-13} (50%; SCCP); Closed Bottle Test Method

The Registrants provided a finalised non-GLP certified study report for inclusion into this Substance Evaluation, although it is not part of the registration dossier. The study examined the biodegradability of a C_{10-13} chlorinated n-alkanes, 50% Cl wt. using a Closed Bottle Test (Unpublished, 2018g).

The purity of the test substance was stated to be ~100%. The total chlorine content was measured to be 49.75% w/w, as per the certificate of analyses presented in the test report.

Two inocula were assessed: 1) secondary activated sludge from a plant treating predominantly domestic waste water, and 2) river water. In order to reduce the endogenous respiration rates both activated sludge (0.4 g dw/L activated sludge solids) and river water were aerated for one week prior to addition to test vessels. Nutrient medium was prepared as per OECD TG 301D, with ammonium chloride omitted to prevent nitrification. For both inocula the following test systems were prepared:

1) Inocula and nutrient medium only.
2) The test substance was solubilised in dichloromethane (DCM) to give a stock solution concentration of 1 g/L. Aliquots of 0.6 mL were transferred to test vessels that were then placed on a roller system, where the solvent was removed overnight to leave a coating of the substance on the test vessel walls.
3) The test substance was solubilised in silicone oil (AR 20; Fluka Chemika) at a concentration of 1 g/L. Aliquots of 0.6 mL were transferred directly to the test vessels.
4) The test substance was solubilised in the surfactant polyalkoylate alkylphenol (PAAP) to form a suspension at a concentration of 1 g/L. Aliquots of 0.6 mL were transferred directly to the test vessels.

All test vessels were 300 mL in volume. For the activated sludge vessels, aerated sludge and mineral medium were added to give a final concentration of 2 mg dw/L (sludge solids). River water test vessels were filled entirely with the aerated river water. All test vessels were agitated using a magnetic stirring and incubated in the dark. The incubation temperature range was 22 – 24 °C. Dissolved oxygen concentrations were measured in duplicate bottles for each exposure scenario. Sampling intervals for all exposure scenarios were 28 d, 42 d and 56 d. In addition to dissolved oxygen concentrations, temperature and pH measurements were made during the study. No, positive control, or toxic/inhibitory assessment of the test substance on the test systems were incorporated into the study design.

The ThOD for was calculated to be 1.36 mg O_2/mg. The results are summarised in Table E1.

Table E1

RESULTS OF THE CBT WITH ACTIVATED SLUDGE AND RIVER WATER C_{10-13} CHLORINATED N-ALKANE, 50% CL WT. SUBSTANCE						
Time (days)	**Percentage degradation (based on O_2 consumption; %)**					
	Sludge			**River water**		
	DCM	**Silicone oil**	**PAAP**	**DCM**	**Silicone oil**	**PAAP**
28	36	7	72	18	10	42
42	-	-	75	-	-	63
56	47	25	-	37	38	64

The substance achieved the pass threshold of 60% after 28 days in the activated sludge inoculum when dosed within PAAP, and so can be considered to be readily biodegradable. This pass level was also achieved by 42 days in the river water inoculum, again using PAAP.

Due to limited information presented in the study report, the eMSCA has not been able to assess the results against the validity criteria of OECD TG 301D. This includes, but is not necessarily limited to, a lack of data or graphical representations of biodegradation of the test chemical that would allow verification of lag- and biodegradation- phases; the omission of a positive control (preventing an assessment of the health/viability of the test systems); and lack of toxicity controls (to assess the potential detrimental influence of application in DCM or silicone oil). No investigation of adsorption to glassware was reported.

Appendix F Analysis of bioaccumulation using fish dietary studies

The following tables As well as BMF data, fish feeding studies provide information on the growth-corrected depuration half-life. This can be used to estimate an equivalent BCF value using the models within the OECD TG 305 BCF estimation tool (Excel® spread sheet). Further information can be found in Brooke *et al*. (2012). The eMSCA has calculated fish BCFs using this tool based on relevant data from the Fisk *et al.* (1996), Fisk *et al.* (1998b), Fisk *et al.* (2000) and Unpublished (2019d) studies. The data are provided in the following tables.

ESTIMATION OF UPTAKE RATE CONSTANT VALUES FROM DIETARY ACCUMULATION STUDIES WITH FISH

Substance[a]			Cl content (% wt.)	Fish weights (g)		Ref.	Estimated uptake rate constant (L/kg/day)[C]												
C	H	Cl		Range at start of study	Est. at day 40[b]		1	2	3	4	5	6	7	8	9	10	11	12	13
10	18	4	50.7	2 - 7	8.3	Fisk *et al.* 1998	264	235	471	493	463	482	351	332	292	293	282	680	793
10	17	5	56.4	2 - 7	8.3	Fisk *et al.* 1998	264	237	471	493	463	482	351	332	292	293	282	746	856
10	17	5	56.4	2 - 7	8.3	Fisk *et al.* 1998	264	237	471	493	463	482	351	332	292	293	282	746	856
10	16	6	61.0	2 - 7	8.7	Fisk *et al.* 1998	261	235	466	489	459	479	348	330	290	291	278	811	919
10	16	6	61.0	2 - 7	8.7	Fisk *et al.* 1998	261	235	466	489	459	479	348	330	290	291	278	811	919
10	16	6	61.0	2 - 7	8.7	Fisk *et al.* 1998	261	235	466	489	459	479	348	330	290	291	278	811	919
10	15.3	6.7	63.7	1 - 5	5.5	Fisk *et al.* 2000	302	264	523	527	500	515	387	361	312	318	335	857	961
10	15.3	6.7	63.7	1 - 5	5.5	Fisk *et al.* 2000	302	264	523	527	500	515	387	361	312	318	335	857	961
10	15	7	64.8	2 - 7	8.7	Fisk *et al.* 1998	261	236	466	489	459	479	348	330	290	291	278	876	979

10	15	7	64.8	2 - 7	8.7	Fisk *et al.* 1998	261	236	466	489	459	479	348	330	290	291	278	876	979
10	14	8	67.9	2 - 7	8.7	Fisk *et al.* 1998	261	236	466	489	459	479	348	330	290	291	278	939	1 037
10	14	8	67.9	2 - 7	8.7	Fisk *et al.* 1998	261	236	466	489	459	479	348	330	290	291	278	939	1 037
11	20	4	48.3	2 - 7	8.7	Fisk *et al.* 1998	261	235	466	489	459	479	348	330	290	291	277	746	856
11	19	5	54.0	2 - 7	8.7	Fisk *et al.* 1998	261	235	466	489	459	479	348	330	290	291	278	811	919
11	18	6	58.7	2 - 7	8.7	Fisk *et al.* 1998	261	236	466	489	459	479	348	330	290	291	278	876	979
11	16	8	65.7	2 - 7	8.7	Fisk *et al.* 1998	261	236	466	489	459	479	348	330	290	291	278	999	1 092
12	20	6	56.5	2 - 7	10.6	Fisk *et al.* 1996	244	224	443	474	443	464	332	317	281	279	255	939	1 037
12	20	6	56.5	2 - 7	7.9	Fisk *et al.* 1996	269	242	478	497	467	486	356	336	294	296	289	939	1 037
12	16	10	68.9	2 - 7	8.6	Fisk *et al.* 1996	261	237	467	490	460	480	349	330	290	291	278	1 147	1 225
12	16	10	68.9	2 - 7	8.3	Fisk *et al.* 1996	264	239	471	493	463	482	352	333	292	293	283	1 147	1 225
14	26	4	42.3	2 - 7	8.3	Fisk *et al.* 1998	264	238	471	493	463	482	351	332	292	293	282	939	1 037
14	25	5	47.9	2 - 7	8.3	Fisk *et al.* 1998	264	238	471	493	463	482	351	332	292	293	282	999	1 092
14	25	5	47.9	2 - 7	8.3	Fisk *et al.* 1998	264	238	471	493	463	482	351	332	292	293	282	999	1 092
14	24	6	52.6	2 - 7	8.3	Fisk *et al.* 1998	264	238	471	493	463	482	351	332	292	293	282	1 054	1 141
14	24	6	52.6	2 - 7	8.3	Fisk *et al.* 1998	264	238	471	493	463	482	351	332	292	293	282	1 054	1 141

14	23.3	6.7	55.4	1 - 5	5.3	Fisk *et al.* 2000	306	268	528	531	503	518	390	364	314	321	341	1 090	1 173
14	23.3	6.7	55.4	1 - 5	5.7	Fisk *et al.* 2000	298	262	518	524	496	512	383	358	310	316	330	1 090	1 173
16	31	3	32.3	2 - 7	8.5	Fisk *et al.* 1996	263	237	469	491	461	481	350	331	291	292	280	999	1 092
16	31	3	32.3	2 - 7	6.7	Fisk *et al.* 1996	282	251	497	510	481	498	369	347	302	306	308	999	1 092
16	21	13	68.4	2 - 7	7.2	Fisk *et al.* 1996	277	248	489	505	476	494	364	342	299	302	300	1 214	1 283
16	21	13	68.4	2 - 7	7.1	Fisk *et al.* 1996	278	248	490	505	476	494	364	343	299	302	301	1 214	1 283
16	21	13	68.4	2 - 7	7.2	Fisk *et al.* 1996	277	248	489	505	476	494	364	342	299	302	300	1 214	1 283
18	31.4	6.6	48.6	1 - 5	5.5	Fisk *et al.* 2000	302	265	523	527	500	515	387	361	312	318	335	1 224	1 292
18	31.4	6.6	48.6	1 - 5	5.3	Fisk *et al.* 2000	306	268	528	531	503	518	390	364	314	321	341	1 224	1 292
14	24.6	5.4	50	1.4-2.9	2.58	Un-published (2019c)	409	106	81	614	593	597	480	435	116	384	494	886	988

Note: a) Data for medium-chain length chlorinated paraffins are highlighted in green.

b) Estimated from the mid-point of the starting weight range and the growth rate constant derived from the paper. The uptake period was 40 days in all studies.

c) Uptake rate constant estimated for day 40 using the following methods:

1 - Sijm *et al.* 1995 (method given in the REACH Guidance)
2 - Omega/Hendriks, 2001
3 - QEAFDCHN/Thomann, 1989
4 - BASS/Barber, 2001
5 - FGETS/Barber *et al.* 1991
6 - Erickson and McKim, 1990a
7 - Erickson and McKim, 1990b
8 - Hayton and Barron, 1990
9 - Streit and Sire, 1993
10 - Barber, 2003 observed

11 - Barber, 2003 calibrated
12 - Spacie and Hamelink, 1982
13 - Tolls and Sijm, 1995

Where needed, the log K_{OW} values were estimated using the equations derived by Sijm and Sinnige (1995).

ESTIMATION OF GROWTH CORRECTED BCF VALUES FROM DIETARY ACCUMULATION STUDIES WITH FISH																	
Substance[a]			Cl content (% wt.)	Growth corrected depuration rate constant (d^{-1})[b]	Estimated uptake rate constant (L/kg/day)[C]												
C	H	Cl			1	2	3	4	5	6	7	8	9	10	11	12	13
10	18	4	50.7	0.083	3 179	2 836	5 673	5 935	5 575	5 808	4 232	4 005	3 516	3 531	3 398	8 192	9 559
10	17	5	56.4	0.089	2 965	2 662	5 291	5 535	5 199	5 417	3 947	3 735	3 279	3 293	3 170	8 378	9 623
10	17	5	56.4	0.097	2 720	2 442	4 854	5 078	4 770	4 970	3 622	3 427	3 008	3 021	2 908	7 687	8 830
10	16	6	61.0	0.068	3 831	3 460	6 856	7 197	6 756	7 045	5 119	4 851	4 264	4 276	4 081	11 932	13 511
10	16	6	61.0	0.069	3 775	3 410	6 756	7 093	6 658	6 943	5 045	4 780	4 202	4 214	4 022	11 759	13 315
10	16	6	61.0	0.034	7 662	6 920	13 711	14 395	13 511	14 091	10 238	9 701	8 528	8 551	8 162	23 864	27 021
10	15.3	6.7	63.7	0.016	18 872	16 524	32 700	32 948	31 226	32 192	24 170	22 567	19 493	19 901	20 957	53 557	60 083
10	15.3	6.7	63.7	0.027	11 183	9 792	19 378	19 525	18 505	19 077	14 323	13 373	11 551	11 793	12 419	31 737	35 605
10	15	7	64.8	0.047	5 543	5 014	9 919	10 413	9 774	10 193	7 406	7 018	6 169	6 186	5 905	18 642	20 835
10	15	7	64.8	0.081	3 216	2 910	5 755	6 042	5 671	5 915	4 298	4 072	3 580	3 590	3 426	10 817	12 089
10	14	8	67.9	0.023	11 326	10 256	20 269	21 279	19 973	20 830	15 135	14 341	12 607	12 641	12 066	40 826	45 093
10	14	8	67.9	0.050	5 210	4 718	9 324	9 788	9 187	9 582	6 962	6 597	5 799	5 815	5 550	18 780	20 743
11	20	4	48.3	0.064	4 070	3 664	7 284	7 647	7 178	7 486	5 439	5 154	4 530	4 543	4 336	11 650	13 383
11	19	5	54.0	0.077	3 383	3 056	6 054	6 356	5 966	6 222	4 521	4 284	3 766	3 776	3 604	10 537	11 932
11	18	6	58.7	0.041	6 354	5 748	11 370	11 937	11 204	11 685	8 490	8 045	7 072	7 091	6 769	21 371	23 884
11	16	8	65.7	0.019	13 711	12 422	24 536	25 759	24 178	25 215	18 321	17 360	15 261	15 303	14 606	52 559	57 449
12	20	6	56.5	0.018	13 558	12 453	24 612	26 312	24 591	25 777	18 460	17 607	15 597	15 517	14 181	52 166	57 619
12	20	6	56.5	0.009	29 847	26 847	53 057	55 227	51 941	54 040	39 534	37 346	32 709	32 922	32 073	104 332	115 239

12	16	10	68.9	0.008	32 646	29 579	58 390	61 257	57 505	59 960	43 592	41 295	36 290	36 401	34 804	143 415	153 100
12	16	10	68.9	0.009	29 355	26 530	52 372	54 767	51 452	53 600	39 068	36 967	32 441	32 587	31 397	127 480	136 089
14	26	4	42.3	0.018	14 659	13 237	26 160	27 366	25 707	26 783	19 516	18 469	16 210	16 281	15 673	52 166	57 619
14	25	5	47.9	0.013	20 297	18 337	36 221	37 891	35 595	37 084	27 023	25 572	22 445	22 542	21 701	76 817	83 963
14	25	5	47.9	0.015	17 590	15 892	31 392	32 839	30 849	32 140	23 420	22 163	19 453	19 537	18 807	66 575	72 768
14	24	6	52.6	0.024	10 994	9 936	19 620	20 524	19 280	20 087	14 637	13 852	12 158	12 210	11 755	43 914	47 562
14	24	6	52.6	0.016	16 491	14 904	29 430	30 787	28 921	30 131	21 956	20 778	18 237	18 316	17 632	65 872	71 342
14	23.3	6.7	55.4	0.012	25 487	22 305	44 038	44 215	41 939	43 194	32 522	30 326	26 155	26 745	28 406	90 793	97 780
14	23.3	6.7	55.4	0.017	17 536	15 433	30 470	30 811	29 176	30 109	22 542	21 074	18 230	18 584	19 404	64 089	69 021
16	31	3	32.3	0.014	18 751	16 960	33 500	35 094	32 956	34 349	25 001	23 671	20 789	20 866	20 019	71 330	77 966
16	31	3	32.3	0.019	14 862	13 230	26 132	26 826	25 312	26 232	19 405	18 239	15 880	16 082	16 196	52 559	57 449
16	21	13	68.4	0.012	23 084	20 650	40 759	42 066	39 643	41 145	30 307	28 541	24 907	25 163	25 021	101 133	106 936
16	21	13	68.4	0.011	25 247	22 573	44 554	45 949	43 309	44 942	33 122	31 185	27 205	27 494	27 385	110 327	116 658
16	21	13	68.4	0.009	30 779	27 534	54 346	56 088	52 857	54 860	40 409	38 055	33 209	33 551	33 361	134 844	142 581
18	31.4	6.6	48.6	0.009	34 313	30 122	59 454	59 906	56 775	58 532	43 946	41 031	35 441	36 184	38 105	139 080	146 849
18	31.4	6.6	48.6	0.008	40 243	35 229	69 534	69 813	66 220	68 200	51 351	47 883	41 297	42 229	44 852	161 040	170 036
14	24.6	5.4	50	0.006	52 282	13 546	10 387	78 396	75 807	76 305	61 318	55 523	14 847	49 015	63 280	112 902	125 951

Note: a) Data for medium-chain length chlorinated paraffins are highlighted in green.
b) Taken from the corresponding paper by Fisk *et al.* (1996, 1998b or 2000).
c) Uptake rate constant estimated for day 40 using the following methods:

1 - Sijm *et al.* 1995 (method given in the REACH Guidance)
2 - Omega/Hendriks, 2001
3 - QEAFDCHN/Thomann, 1989
4 - BASS/Barber, 2001
5 - FGETS/Barber *et al.* 1991
6 - Erickson and McKim, 1990a
7 - Erickson and McKim, 1990b
8 - Hayton and Barron, 1990

9 - Streit and Sire, 1993
10 - Barber, 2003 observed
11 - Barber, 2003 calibrated
12 - Spacie and Hamelink, 1982
13 - Tolls and Sijm, 1995

ESTIMATION OF NON-GROWTH CORRECTED BCF VALUES FROM DIETARY ACCUMULATION STUDIES WITH FISH

Substance[a]				Overall depuration rate constant (d^{-1})[b]	Estimated non-growth corrected BCF (L/kg)[c]												
C	H	Cl	Cl content (% wt.)		1	2	3	4	5	6	7	8	9	10	11	12	13
10	18	4	50.7	0.098	2 681	2 392	4 785	5 006	4 703	4 899	3 570	3 378	2 965	2 978	2 867	6 910	8 063
10	17	5	56.4	0.104	2 527	2 269	4 510	4 718	4 432	4 618	3 365	3 184	2 795	2 807	2 702	7 142	8 204
10	17	5	56.4	0.112	2 347	2 107	4 189	4 382	4 117	4 289	3 125	2 958	2 596	2 607	2 510	6 634	7 620
10	16	6	61	0.084	3 086	2 788	5 524	5 799	5 443	5 676	4 124	3 908	3 435	3 445	3 288	9 613	10 885
10	16	6	61	0.085	3 050	2 755	5 459	5 731	5 379	5 610	4 076	3 862	3 395	3 405	3 250	9 501	10 758
10	16	6	61	0.05	5 169	4 668	9 250	9 711	9 115	9 506	6 907	6 545	5 753	5 769	5 506	16 099	18 229
10	15.3	6.7	63.7	0.031	9 740	8 529	16 877	17 005	16 117	16 615	12 475	11 647	10 061	10 272	10 817	27 642	31 010
10	15.3	6.7	63.7	0.042	7 189	6 295	12 457	12 552	11 896	12 264	9 208	8 597	7 426	7 581	7 984	20 403	22 889
10	15	7	64.8	0.063	4 109	3 717	7 353	7 720	7 246	7 556	5 491	5 203	4 573	4 586	4 377	13 820	15 446
10	15	7	64.8	0.097	2 675	2 420	4 786	5 025	4 716	4 919	3 574	3 387	2 977	2 985	2 849	8 996	10 054
10	14	8	67.9	0.039	6 612	5 987	11 832	12 422	11 659	12 159	8 835	8 372	7 359	7 379	7 044	23 832	26 324
10	14	8	67.9	0.066	3 923	3 553	7 021	7 371	6 918	7 215	5 243	4 968	4 367	4 379	4 180	14 141	15 620
11	20	4	48.3	0.08	3 240	2 917	5 798	6 087	5 714	5 959	4 330	4 103	3 606	3 616	3 451	9 274	10 653
11	19	5	54	0.093	2 789	2 519	4 991	5 240	4 918	5 129	3 727	3 532	3 104	3 113	2 971	8 687	9 836
11	18	6	58.7	0.057	4 538	4 106	8 122	8 527	8 003	8 346	6 065	5 746	5 051	5 065	4 835	15 265	17 060
11	16	8	65.7	0.035	7 359	6 667	13 169	13 826	12 977	13 533	9 833	9 318	8 191	8 213	7 840	28 210	30 834
12	20	6	56.5	0.04	6 178	5 675	11 215	11 990	11 206	11 746	8 412	8 023	7 108	7 071	6 462	23 772	26 257
12	20	6	56.5	0.023	11 679	10 505	20 761	21 611	20 325	21 146	15 470	14 614	12 799	12 883	12 550	40 826	45 093
12	16	10	68.9	0.024	10 792	9 778	19 303	20 250	19 010	19 822	14 411	13 651	11 997	12 033	11 506	47 410	50 612
12	16	10	68.9	0.024	10 872	9 826	19 397	20 284	19 056	19 852	14 470	13 691	12 015	12 069	11 629	47 215	50 403
14	26	4	42.3	0.033	7 900	7 134	14 098	14 748	13 854	14 434	10 518	9 953	8 736	8 774	8 446	28 114	31 052
14	25	5	47.9	0.028	9 291	8 394	16 580	17 345	16 293	16 975	12 369	11 706	10 274	10 319	9 933	35 163	38 434

14	25	5	47.9	0.03	8 679	7 842	15 489	16 203	15 221	15 858	11 556	10 936	9 598	9 640	9 280	32 849	35 905
14	24	6	52.6	0.039	6 697	6 052	11 951	12 502	11 744	12 236	8 916	8 438	7 406	7 438	7 160	26 750	28 972
14	24	6	52.6	0.031	8 403	7 594	14 996	15 687	14 737	15 353	11 188	10 587	9 293	9 333	8 984	33 565	36 353
14	23.3	6.7	55.4	0.026	11 763	10 295	20 325	20 407	19 357	19 935	15 010	13 997	12 071	12 344	13 110	41 904	45 129
14	23.3	6.7	55.4	0.033	9 034	7 950	15 697	15 872	15 030	15 511	11 613	10 856	9 391	9 573	9 996	33 016	35 556
16	31	3	32.3	0.03	8 809	7 968	15 738	16 487	15 483	16 137	11 745	11 121	9 767	9 803	9 405	33 511	36 628
16	31	3	32.3	0.029	9 704	8 638	17 062	17 515	16 527	17 128	12 670	11 909	10 369	10 500	10 575	34 317	37 509
16	21	13	68.4	0.024	11 738	10 500	20 725	21 389	20 157	20 921	15 410	14 512	12 664	12 795	12 723	51 423	54 374
16	21	13	68.4	0.022	12 398	11 085	21 879	22 564	21 268	22 070	16 265	15 314	13 360	13 502	13 448	54 178	57 287
16	21	13	68.4	0.021	13 447	12 029	23 743	24 504	23 093	23 968	17 654	16 626	14 509	14 658	14 575	58 912	62 293
18	31.4	6.6	48.6	0.024	12 687	11 138	21 983	22 150	20 993	21 642	16 249	15 171	13 104	13 379	14 089	51 424	54 297
18	31.4	6.6	48.6	0.022	14 159	12 395	24 466	24 564	23 300	23 996	18 068	16 848	14 530	14 858	15 781	56 662	59 827
14	26.4	5.4	50.1	0.006	52 934	13 678	10 387	78 886	76 344	76 771	61 862	55 947	14 942	49 391	64 293	112 902	125 952

Note: a) Data for medium-chain length chlorinated paraffins are highlighted in green.
b) Estimated from the data reported in the corresponding paper by Fisk *et al.* (1996, 1998b or 2000).
c) Uptake rate constant estimated for day 40 using the following methods:

1 - Sijm *et al.* 1995 (method given in the REACH Guidance)
2 - Omega/Hendriks, 2001
3 - QEAFDCHN/Thomann, 1989
4 - BASS/Barber, 2001
5 - FGETS/Barber *et al.* 1991
6 - Erickson and McKim, 1990a
7 - Erickson and McKim, 1990b
8 - Hayton and Barron, 1990
9 - Streit and Sire, 1993
10 - Barber, 2003 observed
11 - Barber, 2003 calibrated
12 - Spacie and Hamelink, 1982
13 - Tolls and Sijm, 1995